

Numerical Methods Course Notes  
Version 0.11  
(UCSD Math 174, Fall 2004)

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# Preface

These notes were originally prepared during Fall quarter 2003 for UCSD Math 174, Numerical Methods. In writing these notes, it was not my intention to add to the glut of Numerical Analysis texts; they were designed to complement the course text, *Numerical Mathematics and Computing*, Fourth edition, by Cheney and Kincaid [7]. As such, these notes follow the conventions of that text fairly closely. If you are at all serious about pursuing study of Numerical Analysis, you should consider acquiring that text, or any one of a number of other fine texts by *e.g.*, Epperson, Hamming, etc. [3, 4, 5].

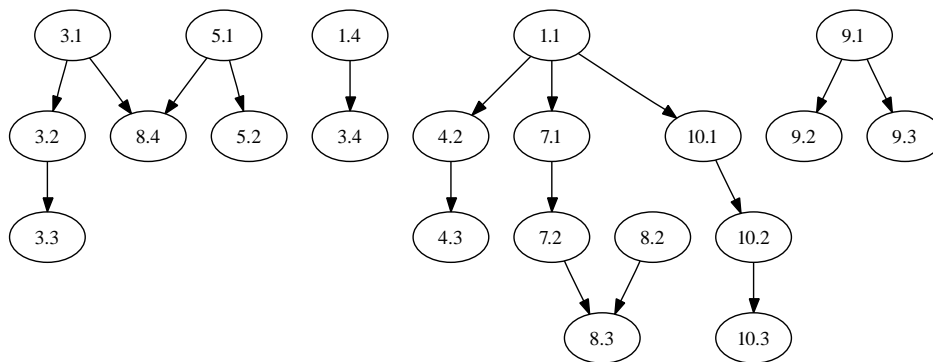


Figure 1: The chapter dependency of this text, though some dependencies are weak.

Special thanks go to the students of Math 174, 2003–2004, who suffered through early versions of these notes, which were riddled with (more) errors.

## Revision History

0.0 Transcription of course notes for Math 174, Fall 2003.

0.1 As used in Math 174, Fall 2004.

0.11 Added material on functional analysis and Orthogonal Least Squares.

## Todo

- More homework questions and example problems.
- Chapter on optimization.
- Chapters on basic finite difference and finite element methods?
- Section on root finding for functions of more than one variable.



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# Chapter 1

## Introduction

### 1.1 Taylor's Theorem

Recall from calculus the Taylor's series for a function,  $f(x)$ , expanded about some number,  $c$ , is written as

$$f(x) \sim a_0 + a_1(x - c) + a_2(x - c)^2 + \dots$$

Here the symbol  $\sim$  is used to denote a "formal series," meaning that convergence is not guaranteed in general. The constants  $a_i$  are related to the function  $f$  and its derivatives evaluated at  $c$ . When  $c = 0$ , this is a MacLaurin series.

For example we have the following Taylor's series (with  $c = 0$ ):

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots \quad (1.1)$$

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \dots \quad (1.2)$$

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \dots \quad (1.3)$$

**Theorem 1.1 (Taylor's Theorem).** If  $f(x)$  has derivatives of order  $0, 1, 2, \dots, n+1$  on the closed interval  $[a, b]$ , then for any  $x$  and  $c$  in this interval

$$f(x) = \sum_{k=0}^n \frac{f^{(k)}(c) (x - c)^k}{k!} + \frac{f^{(n+1)}(\xi) (x - c)^{n+1}}{(n + 1)!},$$

where  $\xi$  is some number between  $x$  and  $c$ , and  $f^k(x)$  is the  $k^{\text{th}}$  derivative of  $f$  at  $x$ .

We will use this theorem again and again in this class. The main usage is to approximate a function by the first few terms of its Taylor's series expansion; the theorem then tells us the approximation is "as good" as the final term, also known as the *error term*. That is, we can make the following manipulation:

$$\begin{aligned}
 f(x) &= \sum_{k=0}^n \frac{f^{(k)}(c)(x-c)^k}{k!} + \frac{f^{(n+1)}(\xi)(x-c)^{n+1}}{(n+1)!} \\
 f(x) - \sum_{k=0}^n \frac{f^{(k)}(c)(x-c)^k}{k!} &= \frac{f^{(n+1)}(\xi)(x-c)^{n+1}}{(n+1)!} \\
 \left| f(x) - \sum_{k=0}^n \frac{f^{(k)}(c)(x-c)^k}{k!} \right| &= \frac{|f^{(n+1)}(\xi)||x-c|^{n+1}}{(n+1)!}.
 \end{aligned}$$

On the left hand side is the difference between  $f(x)$  and its approximation by Taylor's series. We will then use our knowledge about  $f^{(n+1)}(\xi)$  on the interval  $[a, b]$  to find some constant  $M$  such that

$$\left| f(x) - \sum_{k=0}^n \frac{f^{(k)}(c)(x-c)^k}{k!} \right| = \frac{|f^{(n+1)}(\xi)||x-c|^{n+1}}{(n+1)!} \leq M|x-c|^{n+1}.$$

**Example Problem 1.2.** Find an approximation for  $f(x) = \sin x$ , expanded about  $c = 0$ , using  $n = 3$ .

*Solution:* Solving for  $f^{(k)}$  is fairly easy for this function. We find that

$$\begin{aligned}
 f(x) = \sin x &= \sin(0) + \frac{\cos(0)x}{1!} + \frac{-\sin(0)x^2}{2!} + \frac{-\cos(0)x^3}{3!} + \frac{\sin(\xi)x^4}{4!} \\
 &= x - \frac{x^3}{6} + \frac{\sin(\xi)x^4}{24},
 \end{aligned}$$

so

$$\left| \sin x - \left( x - \frac{x^3}{6} \right) \right| = \left| \frac{\sin(\xi)x^4}{24} \right| \leq \frac{x^4}{24},$$

because  $|\sin(\xi)| \leq 1$ . ◊

**Example Problem 1.3.** Apply Taylor's Theorem for the case  $n = 1$ .

*Solution:* Taylor's Theorem for  $n = 1$  states: Given a function,  $f(x)$  with a continuous derivative on  $[a, b]$ , then

$$f(x) = f(c) + f'(\xi)(x-c)$$

for some  $\xi$  between  $x, c$  when  $x, c$  are in  $[a, b]$ .

This is the Mean Value Theorem. As a one-liner, the MVT says that at some time during a trip, your velocity is the same as your average velocity for the trip. ◊

**Example Problem 1.4.** Apply Taylor's Theorem to expand  $f(x) = x^3 - 21x^2 + 17$  around  $c = 1$ .

*Solution:* Simple calculus gives us

$$\begin{aligned}
 f^{(0)}(x) &= x^3 - 21x^2 + 17, \\
 f^{(1)}(x) &= 3x^2 - 42x, \\
 f^{(2)}(x) &= 6x - 42, \\
 f^{(3)}(x) &= 6, \\
 f^{(k)}(x) &= 0.
 \end{aligned}$$

with the last holding for  $k > 3$ . Evaluating these at  $c = 1$  gives

$$f(x) = -3 + -39(x-1) + \frac{-36(x-1)^2}{2} + \frac{6(x-1)^3}{6}.$$

Note there is no error term, since the higher order derivatives are identically zero. By carrying out simple algebra, you will find that the above expansion is, in fact, the function  $f(x)$ .  $\dashv$

There is an alternative form of Taylor's Theorem, in this case substituting  $x + h$  for  $x$ , and  $x$  for  $c$  in the more general version. This gives

**Theorem 1.5 (Taylor's Theorem, Alternative Form).** If  $f(x)$  has derivatives of order  $0, 1, \dots, n+1$  on the closed interval  $[a, b]$ , then for any  $x$  in this interval and any  $h$  such that  $x + h$  is in this interval,

$$f(x+h) = \sum_{k=0}^n \frac{f^{(k)}(x) (h)^k}{k!} + \frac{f^{(n+1)}(\xi) (h)^{n+1}}{(n+1)!},$$

where  $\xi$  is some number between  $x$  and  $x + h$ .

We generally apply this form of the theorem with  $h \rightarrow 0$ . This leads to a discussion on the matter of *Orders of Convergence*. The following definition will suffice for this class

**Definition 1.6.** We say that a function  $f(h)$  is in the class  $\mathcal{O}(h^k)$  (pronounced "big-Oh of  $h^k$ ") if there is some constant  $C$  such that

$$|f(h)| \leq C |h|^k$$

for all  $h$  "sufficiently small," *i.e.*, smaller than some  $h^*$  in absolute value.

For a function  $f \in \mathcal{O}(h^k)$  we sometimes write  $f = \mathcal{O}(h^k)$ . We sometimes also write  $\mathcal{O}(h^k)$ , meaning some function which is a member of this class.

Roughly speaking, through use of the "Big-O" function we can write an expression without "sweating the small stuff." This can give us an intuitive understanding of how an approximation works, without losing too many of the details.

**Example 1.7.** Consider the Taylor expansion of  $\ln x$ :

$$\ln(x+h) = \ln x + \frac{(1/x)h}{1} + \frac{(-1/x^2)h^2}{2} + \frac{(2/\xi^3)h^3}{6}$$

Letting  $x = 1$ , we have

$$\ln(1+h) = h - \frac{h^2}{2} + \frac{1}{3\xi^3}h^3.$$

Using the fact that  $\xi$  is between 1 and  $1+h$ , as long as  $h$  is relatively small (say smaller than  $\frac{1}{2}$ ), the term  $\frac{1}{3\xi^3}$  can be bounded by a constant, and thus

$$\ln(1+h) = h - \frac{h^2}{2} + \mathcal{O}(h^3).$$

Thus we say that  $h - \frac{h^2}{2}$  is a  $\mathcal{O}(h^3)$  approximation to  $\ln(1+h)$ . For example

$$\ln(1+0.01) \approx 0.009950331 \approx 0.00995 = 0.01 - \frac{0.01^2}{2}.$$

## 1.2 Loss of Significance

Generally speaking, a computer stores a number  $x$  as a mantissa and exponent, that is  $x = \pm r \times 10^k$ , where  $r$  is a rational number of a given number of digits in  $[0.1, 1)$ , and  $k$  is an integer in a certain range.

The number of significant digits in  $r$  is usually determined by the user's input. Operations on numbers stored in this way follow a "lowest common denominator" type of rule, *i.e.*, precision cannot be gained but can be lost. Thus for example if you add the two quantities 0.171717 and 0.51, then the result should only have two significant digits; the precision of the first measurement is lost in the uncertainty of the second.

This is as it should be. However, a loss of significance can be incurred if two nearly equal quantities are subtracted from one another. Thus if I were to direct my computer to subtract 0.177241 from 0.177589, the result would be  $.348 \times 10^{-3}$ , and three significant digits have been lost. This loss is called *subtractive cancellation*, and can often be avoided by rewriting the expression. This will be made clearer by the examples below.

Errors can also occur when quantities of radically different magnitudes are summed. For example  $0.1234 + 5.6789 \times 10^{-20}$  might be rounded to 0.1234 by a system that keeps only 16 significant digits. This may lead to unexpected results.

The usual strategies for rewriting subtractive expressions are completing the square, factoring, or using the Taylor expansions, as the following examples illustrate.

**Example Problem 1.8.** Consider the stability of  $\sqrt{x+1} - 1$  when  $x$  is near 0. Rewrite the expression to rid it of subtractive cancellation.

*Solution:* Suppose that  $x = 1.2345678 \times 10^{-5}$ . Then  $\sqrt{x+1} \approx 1.000006173$ . If your computer (or calculator) can only keep 8 significant digits, this will be rounded to 1.0000062. When 1 is subtracted, the result is  $6.2 \times 10^{-6}$ . Thus 6 significant digits have been lost from the original.

To fix this, we *rationalize* the expression

$$\sqrt{x+1} - 1 = \sqrt{x+1} - 1 \frac{\sqrt{x+1} + 1}{\sqrt{x+1} + 1} = \frac{x+1-1}{\sqrt{x+1}+1} = \frac{x}{\sqrt{x+1}+1}.$$

This expression has no subtractions, and so is not subject to subtractive cancelling. When  $x = 1.2345678 \times 10^{-5}$ , this expression evaluates approximately as

$$\frac{1.2345678 \times 10^{-5}}{2.0000062} \approx 6.17281995 \times 10^{-6}$$

on a machine with 8 digits, there is no loss of precision. +

Note that nearly all modern computers and calculators store intermediate results of calculations in higher precision formats. This minimizes, but does not eliminate, problems like those of the previous example problem.

**Example Problem 1.9.** Write stable code to find the roots of the equation  $x^2 + bx + c = 0$ .

*Solution:* The usual quadratic formula is

$$x_{\pm} = \frac{-b \pm \sqrt{b^2 - 4c}}{2}$$

Supposing that  $b \gg c > 0$ , the expression in the square root might be rounded to  $b^2$ , giving two roots  $x_+ = 0$ ,  $x_- = -b$ . The latter root is nearly correct, while the former has no correct digits.

To correct this problem, multiply the numerator and denominator of  $x_+$  by  $-b - \sqrt{b^2 - 4c}$  to get

$$x_+ = \frac{2c}{-b - \sqrt{b^2 - 4c}}$$

Now if  $b \gg c > 0$ , this expression gives root  $x_+ = -c/b$ , which is nearly correct. This leads to the pair:

$$x_- = \frac{-b - \sqrt{b^2 - 4c}}{2}, \quad x_+ = \frac{2c}{-b - \sqrt{b^2 - 4c}}$$

Note that the two roots are nearly reciprocals, and if  $x_-$  is computed,  $x_+$  can easily be computed with little additional work.  $\dashv$

**Example Problem 1.10.** Rewrite  $e^x - \cos x$  to be stable when  $x$  is near 0.

*Solution:* Look at the Taylor's Series expansion for these functions:

$$\begin{aligned} e^x - \cos x &= \left[ 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \frac{x^5}{5!} + \dots \right] - \left[ 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots \right] \\ &= x + x^2 + \frac{x^3}{3!} + \mathcal{O}(x^5) \end{aligned}$$

This expression has no subtractions, and so is not subject to subtractive cancelling. Note that we propose calculating  $x + x^2 + x^3/6$  as an *approximation* of  $e^x - \cos x$ , which we cannot calculate exactly anyway. Since we assume  $x$  is nearly zero, the approximate should be good. If  $x$  is *very* close to zero, we may only have to take the first one or two terms. If  $x$  is not so close to zero, we may need to take all three terms, or even more terms of the expansion; if  $x$  is far from zero we should use some other technique.  $\dashv$

## 1.3 Vector Spaces, Inner Products, Norms

We explore some of the basics of functional analysis which may be useful in this text.

### 1.3.1 Vector Space

A vector space is a collection of objects together with a binary operator which is defined over an algebraic field.<sup>1</sup> The binary operator allows transparent algebraic manipulation of vectors.

**Definition 1.11.** A collection of vectors,  $\mathcal{V}$ , with a binary addition operator,  $+$ , defined over  $\mathcal{V}$ , and a scalar multiply over the real field  $\mathbb{R}$ , forms a *vector space* if

1. For each  $\mathbf{u}, \mathbf{v} \in \mathcal{V}$ , the sum  $\mathbf{u} + \mathbf{v}$  is a vector in  $\mathcal{V}$ . (*i.e.*, the space is “closed under addition.”)
2. Addition is commutative:  $\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}$  for each  $\mathbf{u}, \mathbf{v} \in \mathcal{V}$ .
3. For each  $\mathbf{u} \in \mathcal{V}$ , and each scalar  $\alpha \in \mathbb{R}$  the scalar product  $\alpha\mathbf{u}$  is a vector in  $\mathcal{V}$ . (*i.e.*, the space is “closed under scalar multiplication.”)
4. There is a zero vector  $\mathbf{0} \in \mathcal{V}$  such that for any  $\mathbf{u} \in \mathcal{V}$ ,  $0\mathbf{u} = \mathbf{0}$ , where 0 is the zero of  $\mathbb{R}$ .
5. For any  $\mathbf{u} \in \mathcal{V}$ ,  $1\mathbf{u} = \mathbf{u}$ , where 1 is the multiplicative identity of  $\mathbb{R}$ .
6. For any  $\mathbf{u}, \mathbf{v} \in \mathcal{V}$ , and scalars  $\alpha, \beta \in \mathbb{R}$ , both  $(\alpha +_{\mathbb{R}} \beta)\mathbf{u} = \alpha\mathbf{u} + \beta\mathbf{u}$  and  $\alpha(\mathbf{u} + \mathbf{v}) = \alpha\mathbf{u} + \alpha\mathbf{v}$  hold, where  $+_{\mathbb{R}}$  is addition in  $\mathbb{R}$ . (*i.e.*, scalar multiplication distributes in both ways.)

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<sup>1</sup>For the purposes of this text, this algebraic field will *always* be the real field,  $\mathbb{R}$ , though in the real world, the complex field,  $\mathbb{C}$ , has some currency.

**Example 1.12.** The most familiar example of a vector space is  $\mathbb{R}^n$ , which is the collection of  $n$ -tuples of real numbers. That is  $\mathbf{u} \in \mathbb{R}^n$  is of the form  $[u_1, u_2, \dots, u_n]^\top$ , where  $u_i \in \mathbb{R}$  for  $i = 1, 2, \dots, n$ . Addition and scalar multiplication over  $\mathbb{R}$  are defined pairwise:

$$\begin{aligned} [u_1, u_2, \dots, u_n]^\top + [v_1, v_2, \dots, v_n]^\top &= [u_1 + v_1, u_2 + v_2, \dots, u_n + v_n]^\top, \quad \text{and} \\ \alpha [u_1, u_2, \dots, u_n]^\top &= [\alpha u_1, \alpha u_2, \dots, \alpha u_n]^\top \end{aligned}$$

Note that some authors distinguish between *points* in  $n$ -dimensional space and *vectors* in  $n$ -dimensional space. We will use  $\mathbb{R}^n$  to refer to both of them, as in this text there is no need to distinguish them symbolically.

**Example 1.13.** Let  $X \subseteq \mathbb{R}^k$  be an closed, bounded set, and let  $H$  be the collection of all functions from  $X$  to  $\mathbb{R}$ . Then  $H$  forms a vector space under the “pointwise” defined addition and scalar multiplication over  $\mathbb{R}$ . That is, for  $u, v \in H$ ,  $u + v$  is the function in  $H$  defined by  $[u + v](x) = u(x) + v(x)$  for all  $x \in X$ . And for  $u \in H, \alpha \in \mathbb{R}$ ,  $\alpha u$  is the function in  $[ \alpha u ](x) = \alpha(u(x))$ .

**Example 1.14.** Let  $X \subseteq \mathbb{R}^k$  be a closed, bounded set, and let  $H_0$  be the collection of all functions from  $X$  to  $\mathbb{R}$  that take the value zero on  $\partial X$ . Then  $H_0$  forms a vector space under the “pointwise” defined addition and scalar multiplication over  $\mathbb{R}$ . The only difference between proving  $H_0$  is a vector space and the proof required for the previous example is in showing that  $H_0$  is indeed closed under addition and scalar multiplication. This is simple because if  $x \in \partial X$ , then  $[u + v](x) = u(x) + v(x) = 0 + 0$ , and thus  $u + v$  has the property that it takes value 0 on  $\partial X$ . Similarly for  $\alpha u$ . This would not have worked if the functions of  $H_0$  were required to take some other value on  $\partial X$ , like, say, 2 instead of 0.

**Example 1.15.** Let  $\mathcal{P}_n$  be the collection of all ‘formal’ polynomials of degree less than or equal to  $n$  with coefficients from  $\mathbb{R}$ . Then  $\mathcal{P}_n$  forms a vector space over  $\mathbb{R}$ .

**Example 1.16.** The collection of all real-valued  $m \times n$  matrices forms a vector space over the reals with the usual scalar multiplication and matrix addition. This space is denoted as  $\mathbb{R}^{m \times n}$ . Another way of viewing this space is it is the space of linear functions which carry vectors of  $\mathbb{R}^n$  to vectors of  $\mathbb{R}^m$ .

### 1.3.2 Inner Products

An inner product is a way of “multiplying” two vectors from a vector space together to get a scalar from the same field the space is defined over (*e.g.*, a real or a complex number). The inner product should have the following properties:

**Definition 1.17.** For a vector space,  $\mathcal{V}$ , defined over  $\mathbb{R}$ , a binary function,  $(,)$ , which takes two vectors of  $\mathcal{V}$  to  $\mathbb{R}$  is an *inner product* if

1. It is symmetric:  $(\mathbf{v}, \mathbf{u}) = (\mathbf{u}, \mathbf{v})$ .
2. It is linear in both its arguments:

$$\begin{aligned} (\alpha \mathbf{u} + \beta \mathbf{v}, \mathbf{w}) &= \alpha (\mathbf{u}, \mathbf{w}) + \beta (\mathbf{v}, \mathbf{w}) \quad \text{and} \\ (\mathbf{u}, \alpha \mathbf{v} + \beta \mathbf{w}) &= \alpha (\mathbf{u}, \mathbf{v}) + \beta (\mathbf{u}, \mathbf{w}). \end{aligned}$$

A binary function for which this holds is sometimes called a *bilinear form*.

3. It is positive:  $(\mathbf{v}, \mathbf{v}) \geq 0$ , with equality holding if and only if  $\mathbf{v}$  is the zero vector of  $\mathcal{V}$ .

**Example 1.18.** The most familiar example of an inner product is the  $L^2$  (pronounced “L two”) inner product on the vector space  $\mathbb{R}^n$ . If  $\mathbf{u} = [u_1, u_2, \dots, u_n]^\top$ , and  $\mathbf{v} = [v_1, v_2, \dots, v_n]^\top$ , then letting

$$(\mathbf{u}, \mathbf{v})_2 = \sum_i u_i v_i$$

gives an inner product. This inner product is the usual vector calculus dot product and is sometimes written as  $\mathbf{u} \cdot \mathbf{v}$  or  $\mathbf{u}^\top \mathbf{v}$ .

**Example 1.19.** Let  $H$  be the vector space of functions from  $X$  to  $\mathbb{R}$  from Example 1.13. Then for  $u, v \in H$ , letting

$$(u, v)_H = \int_X u(x)v(x) dx,$$

gives an inner product. This inner product is like the “limit case” of the  $L^2$  inner product on  $\mathbb{R}^n$  as  $n$  goes to infinity.

### 1.3.3 Norms

A norm is a way of measuring the “length” of a vector:

**Definition 1.20.** A function  $\|\cdot\|$  from a vector space,  $\mathcal{V}$ , to  $\mathbb{R}^+$  is called a *norm* if

1. It obeys the triangle inequality:  $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ .
2. It scales positively:  $\|\alpha\mathbf{x}\| = |\alpha| \|\mathbf{x}\|$ , for scalar  $\alpha$ .
3. It is positive:  $\|\mathbf{x}\| \geq 0$ , with equality only holding when  $\mathbf{x}$  is the zero vector.

The easiest way of constructing a norm is on top of an inner product. If  $(\cdot, \cdot)$  is an inner product on vector space  $\mathcal{V}$ , then letting

$$\|\mathbf{u}\| = \sqrt{(\mathbf{u}, \mathbf{u})}$$

gives a norm on  $\mathcal{V}$ . This is how we construct our most common norms:

**Example 1.21.** For vector  $\mathbf{x} \in \mathbb{R}^n$ , its  $L^2$  norm is defined

$$\|\mathbf{x}\|_2 = \left( \sum_{i=1}^n x_i^2 \right)^{\frac{1}{2}} = \left( \mathbf{x}^\top \mathbf{x} \right)^{\frac{1}{2}}.$$

This is constructed on top of the  $L^2$  inner product.

**Example 1.22.** The  $L^p$  norm on  $\mathbb{R}^n$  generalizes the  $L^2$  norm, and is defined, for  $p > 0$ , as

$$\|\mathbf{x}\|_p = \left( \sum_{i=1}^n |x_i|^p \right)^{1/p}.$$

**Example 1.23.** The  $L^\infty$  norm on  $\mathbb{R}^n$  is defined as

$$\|\mathbf{x}\|_\infty = \max_i |x_i|.$$

The  $L^\infty$  norm is somehow the “limit” of the  $L^p$  norm as  $p \rightarrow \infty$ .

## 1.4 Eigenvalues

It is assumed the reader has some familiarity with linear algebra. We review the topic of eigenvalues.

**Definition 1.24.** A nonzero vector  $\mathbf{x}$  is an *eigenvector* of a given matrix  $\mathbf{A}$ , with corresponding *eigenvalue*  $\lambda$  if

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

Subtracting the right hand side from the left and gathering terms gives

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}.$$

Since  $\mathbf{x}$  is assumed to be nonzero, the matrix  $\mathbf{A} - \lambda\mathbf{I}$  must be singular. A matrix is singular if and only if its determinant is zero. These steps are reversible, thus we claim  $\lambda$  is an eigenvalue if and only if

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0.$$

The left hand side can be expanded to a polynomial in  $\lambda$ , of degree  $n$  where  $\mathbf{A}$  is an  $n \times n$  matrix. This gives the so-called *characteristic equation*. Sometimes eigenvectors,-values are called characteristic vectors,-values.

**Example Problem 1.25.** Find the eigenvalues of

$$\begin{bmatrix} 1 & 1 \\ 4 & -2 \end{bmatrix}$$

*Solution:* The eigenvalues are roots of

$$0 = \det \begin{bmatrix} 1 - \lambda & 1 \\ 4 & -2 - \lambda \end{bmatrix} = (1 - \lambda)(-2 - \lambda) - 4 = \lambda^2 + \lambda - 6.$$

This equation has roots  $\lambda_1 = -3, \lambda_2 = 2$ . +

**Example Problem 1.26.** Find the eigenvalues of  $\mathbf{A}^2$ .

*Solution:* Let  $\lambda$  be an eigenvalue of  $\mathbf{A}$ , with corresponding eigenvector  $\mathbf{x}$ . Then

$$\mathbf{A}^2\mathbf{x} = \mathbf{A}(\mathbf{A}\mathbf{x}) = \mathbf{A}(\lambda\mathbf{x}) = \lambda\mathbf{A}\mathbf{x} = \lambda^2\mathbf{x}.$$
+

The eigenvalues of a matrix tell us, roughly, how the linear transform scales a given matrix; the eigenvectors tell us which directions are “purely scaled.” This will make more sense when we talk about norms of vectors and matrices.

### 1.4.1 Matrix Norms

Given a norm  $\|\cdot\|$  on the vector space,  $\mathbb{R}^n$ , we can define the matrix norm “subordinate” to it, as follows:

**Definition 1.27.** Given a norm  $\|\cdot\|$  on  $\mathbb{R}^n$ , we define the subordinate matrix norm on  $\mathbb{R}^{n \times n}$  by

$$\|\mathbf{A}\| = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{x}\|}{\|\mathbf{x}\|}.$$



We will use the subordinate two-norm for matrices. From the definition of the subordinate norm as a max, we conclude that if  $\mathbf{x}$  is a nonzero vector then

$$\begin{aligned}\frac{\|\mathbf{Ax}\|_2}{\|\mathbf{x}\|_2} &\leq \|\mathbf{A}\|_2 \quad \text{thus,} \\ \|\mathbf{Ax}\|_2 &\leq \|\mathbf{A}\|_2 \|\mathbf{x}\|_2.\end{aligned}$$

**Example 1.28.** Strange but true: If  $\Lambda$  is the set of eigenvalues of  $\mathbf{A}$ , then

$$\|\mathbf{A}\|_2 = \max_{\lambda \in \Lambda} |\lambda|.$$

**Example Problem 1.29.** Prove that

$$\|\mathbf{AB}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{B}\|_2.$$

*Solution:*

$$\|\mathbf{AB}\|_2 =_{\text{df}} \max_{\mathbf{x} \neq \mathbf{0}} \frac{\|\mathbf{ABx}\|_2}{\|\mathbf{x}\|_2} \leq \max_{\mathbf{x} \neq \mathbf{0}} \frac{\|\mathbf{A}\|_2 \|\mathbf{Bx}\|_2}{\|\mathbf{x}\|_2} = \|\mathbf{A}\|_2 \|\mathbf{B}\|_2.$$

†

## EXERCISES

- (1.1) Suppose  $f \in \mathcal{O}(h^k)$ . Show that  $f \in \mathcal{O}(h^m)$  for any  $m$  with  $0 < m < k$ . (*Hint:* Take  $h^* < 1$ .) Note this may appear counterintuitive, unless you remember that  $\mathcal{O}(h^k)$  is a *better* approximation than  $\mathcal{O}(h^m)$  when  $m < k$ .
- (1.2) Suppose  $f \in \mathcal{O}(h^k)$ , and  $g \in \mathcal{O}(h^m)$ . Show that  $fg \in \mathcal{O}(h^{k+m})$ .
- (1.3) Suppose  $f \in \mathcal{O}(h^k)$ , and  $g \in \mathcal{O}(h^m)$ , with  $m < k$ . Show that  $f + g \in \mathcal{O}(h^m)$ .
- (1.4) Prove that  $f(h) = -3h^5$  is in  $\mathcal{O}(h^5)$ .
- (1.5) Prove that  $f(h) = h^2 + 5h^{17}$  is in  $\mathcal{O}(h^2)$ .
- (1.6) Prove that  $f(h) = h^3$  is *not* in  $\mathcal{O}(h^4)$  (*Hint:* Proof by contradiction.)
- (1.7) Prove that  $\sin(h)$  is in  $\mathcal{O}(h)$ .
- (1.8) Find a  $\mathcal{O}(h^3)$  approximation to  $\sin h$ .
- (1.9) Find a  $\mathcal{O}(h^4)$  approximation to  $\ln(1+h)$ . Compare the approximate value to the actual when  $h = 0.1$ . How does this approximation compare to the  $\mathcal{O}(h^3)$  approximate from Example 1.7 for  $h = 0.1$ ?
- (1.10) Suppose that  $f \in \mathcal{O}(h^k)$ . Can you show that  $f' \in \mathcal{O}(h^{k-1})$ ?
- (1.11) Rewrite  $\sqrt{x+1} - \sqrt{1}$  to get rid of subtractive cancellation when  $x \approx 0$ .
- (1.12) Rewrite  $\sqrt{x+1} - \sqrt{x}$  to get rid of subtractive cancellation when  $x$  is very large.
- (1.13) Use a Taylor's expansion to rid the expression  $1 - \cos x$  of subtractive cancellation for  $x$  small. Use a  $\mathcal{O}(x^5)$  approximate.
- (1.14) Use a Taylor's expansion to rid the expression  $1 - \cos^2 x$  of subtractive cancellation for  $x$  small. Use a  $\mathcal{O}(x^6)$  approximate.
- (1.15) Calculate  $\cos(\pi/2 + 0.001)$  to within 8 decimal places by using the Taylor's expansion.
- (1.16) Prove that if  $\mathbf{x}$  is an eigenvector of  $\mathbf{A}$  then  $\alpha\mathbf{x}$  is also an eigenvector of  $\mathbf{A}$ , for the same eigenvalue. Here  $\alpha$  is a nonzero real number.
- (1.17) Prove, by induction, that if  $\lambda$  is an eigenvalue of  $\mathbf{A}$  then  $\lambda^k$  is an eigenvalue of  $\mathbf{A}^k$  for integer  $k > 1$ . The base case was done in Example Problem 1.26.
- (1.18) Let  $\mathbf{B} = \sum_{i=0}^k \alpha_i \mathbf{A}^i$ , where  $\mathbf{A}^0 = \mathbf{I}$ . Prove that if  $\lambda$  is an eigenvalue of  $\mathbf{A}$ , then  $\sum_{i=0}^k \alpha_i \lambda^i$  is an eigenvalue of  $\mathbf{B}$ . Thus for polynomial  $p(x)$ ,  $p(\lambda)$  is an eigenvalue of  $p(\mathbf{A})$ .
- (1.19) Suppose  $\mathbf{A}$  is an invertible matrix with eigenvalue  $\lambda$ . Prove that  $\lambda^{-1}$  is an eigenvalue for  $\mathbf{A}^{-1}$ .
- (1.20) Suppose that the eigenvalues of  $\mathbf{A}$  are 1, 10, 100. Give the eigenvalues of  $\mathbf{B} = 3\mathbf{A}^3 - 4\mathbf{A}^2 + \mathbf{I}$ . Show that  $\mathbf{B}$  is singular.
- (1.21) Show that if  $\|\mathbf{x}\|_2 = r$ , then  $\mathbf{x}$  is on a sphere centered at the origin of radius  $r$ , in  $\mathbb{R}^n$ .
- (1.22) If  $\|\mathbf{x}\|_2 = 0$ , what does this say about vector  $\mathbf{x}$ ?
- (1.23) Letting  $\mathbf{x} = [3 \ 4 \ 12]^\top$ , what is  $\|\mathbf{x}\|_2$ ?
- (1.24) What is the norm of

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1/2 & 0 & \cdots & 0 \\ 0 & 0 & 1/3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1/n \end{bmatrix} ?$$

- (1.25) Show that  $\|\mathbf{A}\|_2 = 0$  implies that  $\mathbf{A}$  is the matrix of all zeros.
- (1.26) Show that  $\|\mathbf{A}^{-1}\|_2$  equals  $(1/|\lambda_{\min}|)$ , where  $\lambda_{\min}$  is the smallest, in absolute value, eigenvalue of  $\mathbf{A}$ .
- (1.27) Suppose there is some  $\mu > 0$  such that, for a given  $\mathbf{A}$ ,

$$\|\mathbf{A}\mathbf{v}\|_2 \geq \mu\|\mathbf{v}\|_2,$$

for all vectors  $\mathbf{v}$ .

- (a) Show that  $\mu \leq \|\mathbf{A}\|_2$ . (Should be very simple.)
  - (b) Show that  $\mathbf{A}$  is nonsingular. (*Recall:*  $\mathbf{A}$  is singular if there is some  $\mathbf{x} \neq \mathbf{0}$  such that  $\mathbf{Ax} = \mathbf{0}$ .)
  - (c) Show that  $\|\mathbf{A}^{-1}\|_2 \leq (1/\mu)$ .
- (1.28) If  $\mathbf{A}$  is singular, is it necessarily the case that  $\|\mathbf{A}\|_2 = 0$ ?
- (1.29) If  $\|\mathbf{A}\|_2 \geq \mu > 0$  does it follow that  $\mathbf{A}$  is nonsingular?
- (1.30) Towards proving the equality in Example Problem 1.28, prove that if  $\Lambda$  is the set of eigenvalues of  $\mathbf{A}$ , then

$$\|\mathbf{A}\| \geq \max_{\lambda \in \Lambda} |\lambda|,$$

where  $\|\cdot\|$  is *any* subordinate matrix norm. The inequality in the other direction holds when the norm is  $\|\cdot\|_2$ , but is difficult to prove.



## Chapter 2

# A “Crash” Course in octave/Matlab

### 2.1 Getting Started

Matlab is a software package that allows you to program the mathematics of an algorithm without getting too bogged down in the details of data structures, pointers, and reinventing the wheel. It also includes graphing capabilities, and there are numerous packages available for all kinds of functions, enabling relatively high-level programming. Unfortunately, it also costs quite a bit of money, which is why I recommend the free Matlab clone, octave, available under the GPL<sup>1</sup>, freely downloadable from <http://www.octave.org>.

In a lame attempt to retain market share, Mathworks continues to tinker with Matlab to make it noncompatible with octave; this has the side effect of obsoletizing old Matlab code. I will try to focus on the intersection of the two systems, except where explicitly noted otherwise. What follows, then, is an introduction to octave; Matlab users will have to make some changes.

You can find a number of octave/Matlab tutorials for free on the web; many of them are certainly better than this one. A brief web search reveals the following excellent tutorials:

- <http://www.math.mtu.edu/~msgocken/intro/intro.html>
- <http://www.cyclismo.org/tutorial/matlab/vector.html>
- <http://web.ew.usna.edu/~mecheng/DESIGN/CAD/MATLAB/usna.html>

Matlab has some demo programs covering a number of topics— from the most basic functionality to the more arcane toolboxes. In Matlab, simply type `demo`.

What follows is a lame demo for octave. Start up octave. You should get something like:

```
GNU Octave, version 2.1.44 (i686-pc-linux-gnu).
Copyright (C) 1996, 1997, 1998, 1999, 2000, 2001, 2002, 2003 John W. Eaton.
This is free software; see the source code for copying conditions.
There is ABSOLUTELY NO WARRANTY; not even for MERCHANTABILITY or
FITNESS FOR A PARTICULAR PURPOSE. For details, type 'warranty'.
```

Please contribute if you find this software useful.

For more information, visit <http://www.octave.org/help-wanted.html>

Report bugs to <[bug-octave@bevo.che.wisc.edu](mailto:bug-octave@bevo.che.wisc.edu)>.

```
octave:1>
```

---

<sup>1</sup>Gnu Public License. See <http://www.gnu.org/copyleft/gpl.html>.

You now have a command line. The basic octavian data structure is a matrix; a scalar is a  $1 \times 1$  matrix, a vector is an  $n \times 1$  matrix. Some simple matrix constructions are as follows:

```
octave:2> a = [1 2 3]
a =
```

```
1 2 3
```

```
octave:3> b = [5;4;3]
b =
```

```
5
4
3
```

```
octave:4> c = a'
c =
```

```
1
2
3
```

```
octave:5> d = 5*c - 2 * b
d =
```

```
-5
2
9
```

You should notice that octave “echoes” the lvalues it creates. This is either a feature or an annoyance. It can be prevented by appending a semicolon at the end of a command. Thus the previous becomes

```
octave:5> d = 5*c - 2 * b;
octave:6>
```

For illustration purposes, I am leaving the semicolon off. To access an entry or entries of a matrix, use parentheses. In the case where the variable is a vector, you only need give a single index, as shown below; when the variable is a matrix, you need give both indices. You can also give a range of indices, as in what follows.

**WARNING:** vectors and matrices in octave/Matlab are indexed starting from 1, and *not* from 0, as is more common in modern programming languages. You are warned! Moreover, the last index of a vector is denoted by the special symbol `end`.

```
octave:6> a(1) = 77
a =
```

```
77 2 3
```

```
octave:7> a(end) = -400
a =
```

```
77 2 -400
```

```
octave:8> a(2:3) = [22 333]
```

```
a =  
    77    22   333
```

```
octave:9> M = diag(a)
```

```
M =  
    77     0     0  
     0    22     0  
     0     0   333
```

```
octave:10> M(2,1) = 14
```

```
M =  
    77     0     0  
    14    22     0  
     0     0   333
```

```
octave:11> M(1:2,1:2) = [1 2;3 4]
```

```
M =  
     1     2     0  
     3     4     0  
     0     0   333
```

The command `diag(v)` returns a matrix with `v` as the diagonal, if `v` is a vector. `diag(M)` returns the diagonal of matrix `M` as a vector.

The form `c:d` gives returns a row vector of the integers between `a` and `d`, as we will examine later. First we look at matrix manipulation:

```
octave:12> j = M * b
```

```
j =  
    13  
    31  
   999
```

```
octave:13> N = rand(3,3)
```

```
N =  
    0.166880    0.027866    0.087402  
    0.706307    0.624716    0.067067  
    0.911833    0.769423    0.938714
```

```
octave:14> L = M + N
```

```
L =  
    1.166880    2.027866    0.087402  
    3.706307    4.624716    0.067067  
    0.911833    0.769423   333.938714
```

```
octave:15> P = L * M
```

```
P =
```

```

7.2505e+00  1.0445e+01  2.9105e+01
1.7580e+01  2.5911e+01  2.2333e+01
3.2201e+00  4.9014e+00  1.1120e+05

```

```
octave:16> P = L .* M
```

```
P =
```

```

1.1669e+00  4.0557e+00  0.0000e+00
1.1119e+01  1.8499e+01  0.0000e+00
0.0000e+00  0.0000e+00  1.1120e+05

```

```
octave:17> x = M \ b
```

```
x =
```

```

-6.0000000
 5.5000000
 0.0090090

```

```
octave:18> err = M * x - b
```

```
err =
```

```

0
0
0

```

Note the difference between  $L * M$  and  $L .* M$ ; the former is matrix multiplication, the latter is *element by element* multiplication, *i.e.*,

$$(L .* M)_{i,j} = L_{i,j} M_{i,j}.$$

The command `rand(m,n)` gives an  $m \times n$  matrix with each element “uniformly distributed” on  $[0, 1]$ . For a zero mean normal distribution with unit variance, use `randn(m,n)`.

In line 17 we asked octave to solve the linear system

$$Mx = b,$$

by setting

$$x = M \backslash b = M^{-1}b.$$

Note that you can construct matrices directly as you did vectors:

```
octave:19> B = [1 3 4 5; 2 -2 2 -2]
```

```
B =
```

```

 1  3  4  5
 2 -2  2 -2

```

You can also create row vectors as a sequence, either using the form `c:d` or the form `c:e:d`, which give, respectively,  $c, c+1, \dots, d$ , and  $c, c+e, \dots, d$ , (or something like it if  $e$  does not divide  $d-c$ ) as follows:

```
octave:20> z = 1:5
```

```
z =
```

```

1  2  3  4  5

```



```
octave:21> z = 5:(-1):1
```

```
z =
  5  4  3  2  1
```

```
octave:22> z = 5:(-2):1
```

```
z =
  5  3  1
```

```
octave:23> z = 2:3:11
```

```
z =
  2  5  8  11
```

```
octave:24> z = 2:3:10
```

```
z =
  2  5  8
```

Matrices and vectors can be constructed “blockwise.” Blocks in the same row are separated by a comma, those in the same column by a semicolon. Thus

```
octave:2> y=[2 7 9]
```

```
y =
  2  7  9
```

```
octave:3> m = [z;y]
```

```
m =
  2  5  8
  2  7  9
```

```
octave:4> k = [(3:4)', m]
```

```
k =
  3  2  5  8
  4  2  7  9
```

## 2.2 Useful Commands

Here’s a none too complete listing of useful commands in octave:

- `help` is the most useful command.
- `floor(X)` returns the largest integer not greater than  $X$ . If  $X$  is a vector or matrix, it computes the floor element-wise. This behavior is common in octave: many functions which we normally think of as applicable to scalars can be applied to matrices, with the result computed element-wise.
- `ceil(X)` returns the smallest integer not less than  $X$ , computed element-wise.
- `sin(X)`, `cos(X)`, `tan(X)`, `atan(X)`, `sqrt(X)`, returns the sine, cosine, tangent, arctangent, square root of  $X$ , computed elementwise.
- `exp(X)` returns  $e^X$ , elementwise.
- `abs(X)` returns  $|X|$ , elementwise.

- `norm(X)` returns the norm of `X`; if `X` is a vector, this is the  $L^2$  norm:

$$\|X\|_2 = \left( \sum_i X_i^2 \right)^{1/2},$$

if `X` is a matrix, it is the matrix norm subordinate to the  $L^2$  norm.

You can compute other norms with `norm(X,p)` where `p` is a number, to get the  $L^p$  norm, or with `p` one of `Inf`, `-Inf`, etc.

- `zeros(m,n)` returns an  $m \times n$  matrix of all zeros.
- `eye(m)` returns the  $m \times m$  identity matrix.
- `[m,n] = size(A)` returns the number of rows, columns of `A`. Similarly the functions `rows(A)` and `columns(A)` return the number of rows and columns, respectively.
- `length(v)` returns the length of vector `v`, or the larger dimension if `v` is a matrix.
- `find(M)` returns the indices of the nonzero elements of `N`. This may not seem helpful at first, but it can be very useful for selecting subsets of data because the indices can be used for selection. Thus, for example, in this code
 

```
octave:1> v = round(20*randn(400,3));
octave:2> selectv = v(find(v(:,2) == 7),:)
```

 we have selected the rows of `v` where the element in the second column equals 7. Now you see why leading computer scientists refer to octave/Matlab as “semantically suspect.” It is a very useful language nonetheless, and you should try to learn its quirks rather than resist them.
- `diag(v)` returns the diagonal matrix with vector `v` as diagonal. `diag(M)` returns as a vector, the diagonal of matrix `v`. Thus `diag(diag(v))` is `v` for vector `v`, but `diag(diag(M))` is the diagonal part of matrix `M`.
- `toeplitz(v)` returns the Toeplitz matrix associated with vector `v`. That is

$$\text{toeplitz}(v) = \begin{bmatrix} v(1) & v(2) & v(3) & \cdots & v(n) \\ v(2) & v(1) & v(2) & \cdots & v(n-1) \\ v(3) & v(2) & v(1) & \cdots & v(n-2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ v(n) & v(n-1) & v(n-2) & \cdots & v(1) \end{bmatrix}$$

In the more general form, `toeplitz(c,r)` can be used to return a assymmetric Toeplitz matrix.

A matrix which is banded on the cross diagonals is evidently called a “Hankel” matrix:

$$\text{hankel}(u,v) = \begin{bmatrix} u(1) & u(2) & u(3) & \cdots & u(n) \\ u(2) & u(3) & u(4) & \cdots & v(2) \\ u(3) & u(4) & u(5) & \cdots & v(3) \\ \vdots & \vdots & \vdots & & \vdots \\ u(n) & v(2) & v(3) & \cdots & v(n) \end{bmatrix}$$

- `eig(M)` returns the eigenvalues of `M`. `[V, LAMBDA] = eig(M)` returns the eigenvectors, and eigenvalues of `M`.
- `kron(M,N)` returns the Kronecker product of the two matrices. This is a block construction which returns a matrix where each block is an element of `M` as a scalar multiplied by the whole matrix `N`.
- `flipud(N)` flips the vector or matrix `N` so that its first row is last and *vice versa*. Similarly `fliplr(N)` flips left/right.

## 2.3 Programming and Control

If you are going to do any serious programming in octave, you should keep your commands in a file. octave loads commands from '.m' files.<sup>2</sup> If you have the following in a file called `myfunc.m`:

```
function [y1,y2] = myfunc(x1,x2)
% comments start with a '%'
% this function is useless, except as an example of functions.
% input:
% x1 a number
% x2 another number
% output:
% y1 some output
% y2 some output
```

```
y1 = cos(x1) .* sin(x2);
y2 = norm(y1);
```

then you can call this function from octave, as follows:

```
octave:1> myfunc(2,3)
ans = -0.058727
octave:2> [a,b] = myfunc(2,3)
a = -0.058727
b = 0.058727
octave:3> [a,b] = myfunc([1 2 3 4],[1 2 3 4])
a =
```

```
    0.45465   -0.37840   -0.13971    0.49468
```

```
b = 0.78366
```

Note this silly function will throw an error if `x1` and `x2` are not of the same size.

It is recommended that you write your functions so that they can take scalar and vector input where appropriate. For example, the octave builtin sine function can take a scalar and output a scalar, or take a vector and output a vector which is, elementwise, the sine of the input. It is not too difficult to write functions this way, it often only requires judicious use of `.*` multiplies instead of `*` multiplies. For example, if the file `myfunc.m` were changed to read

```
y1 = cos(x1) * sin(x2);
```

it could easily crash if `x1` and `x2` were vectors of the same size because matrix multiplication is not defined for an  $n \times 1$  matrix times another  $n \times 1$  matrix.

An .m file does not have to contain a function, it can merely contain some octave commands. For example, putting the following into `runner.m`:

```
x1 = rand(4,3);
x2 = rand(size(x1));
[a,b] = myfunc(x1,x2)
```

---

<sup>2</sup>The 'm' stands for 'octave.'

octave allows you to call this script without arguments:

```
octave:4> runner
a =

    0.245936    0.478054    0.535323
    0.246414    0.186454    0.206279
    0.542728    0.419457    0.083917
    0.257607    0.378558    0.768188

b = 1.3135
```

octave has to know where your .m file is. It will look in the directory from which it was called. You can set this to something else with `cd` or `chdir`.

You can also use the octave builtin function `feval` to evaluate a function by name. For example, the following is a different way of calling `myfunc.m`:

```
octave:5> [a,b] = feval("myfunc",2,3)
a = -0.058727
b = 0.058727
```

In this form `feval` seems like a way of using more keystrokes to get the same result. However, you can pass a variable function name as well:

```
octave:6> fname = "myfunc"
fname = myfunc
octave:7> [a,b] = feval(fname,2,3)
a = -0.058727
b = 0.058727
```

This allows you to effectively pass functions to other functions.

### 2.3.1 Logical Forks and Control

octave has the regular assortment of ‘if-then-else’ and ‘for’ and ‘while’ loops. These take the following form:

```
if expr1
    statements
elseif expr2
    statements
elsif expr3
    statements
...
else
    statements
end
for var=vector
    statements
end
while expr
```

```

statements
end

```

Note that the word `end` is one of the most overloaded in octave/Matlab. It stands for the last index of a vector of matrix, as well as the exit point for for loops, if statements, switches, etc. To simplify debugging, it is also permissible to use `endif` to end an `if` statement, `endfor` to end a for loop, *etc.*.

The test expressions may use the logical conditionals: `>`, `<`, `>=`, `<=`, `==`, `~=`. Do *not* use the assignment operator `=` as a conditional, as this can lead to disastrous results, as in C.

Here are some examples:

```

%compute the sign of x
if x > 0
    s = 1;
elseif x == 0
    s = 0;
else
    s = -1;
end

```

```

%a 'regular' for loop
for i=1:10
    sm = sm + i;
end

```

```

%an 'irregular' for loop
for i=[1 2 3 5 8 13 21 34]
    fsm = fsm + i;
end

```

```

while (sin(x) > 0)
    x = x * pi;
end

```

## 2.4 Plotting

Plotting is one area in which there are some noticeable differences between octave and Matlab. The commands and examples given herein are for octave, but the commands for Matlab are not too different. octave ships its plotting commands to Gnuplot.

The main plot command is `plot`. You may also use `semilogx`, `semilogy`, `loglog` for 2D plots with log axes, and `contour` and `mesh` for 3D plots. Use the `help` command to get the specific syntax for each command. We present some examples:

```

n = 100;
X = pi .* ((1:n) ./ n);
Y = sin(X);
%just plot Y
plot(Y);

```

```
%plot Y, but with the 'right' X axis labels
plot(X,Y);
```

```
W = sqrt(Y);
plot(W);
%plot W, but with the 'right' X axis labels
plot(Y,W);
```

The output from these commands is seen in Figure 2.1. In particular, you should note the difference between plotting a vector, as in Figure 2.1(c) versus plotting the same vector but with the appropriate abscissa values, as in Figure 2.1(d).

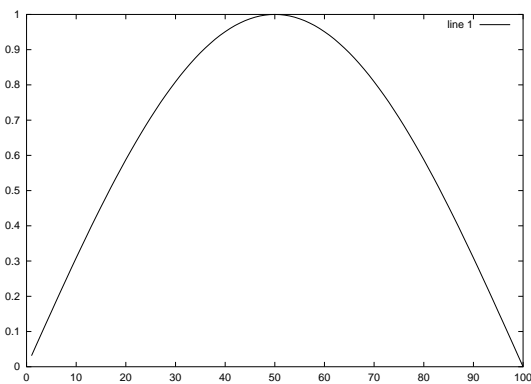
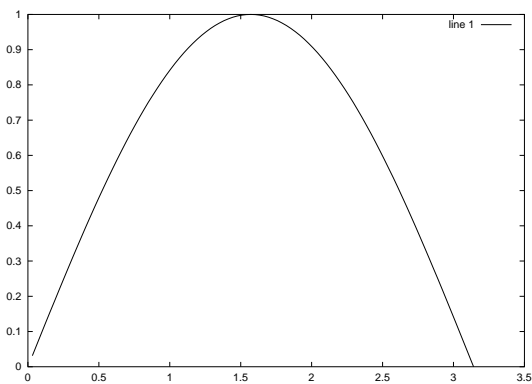
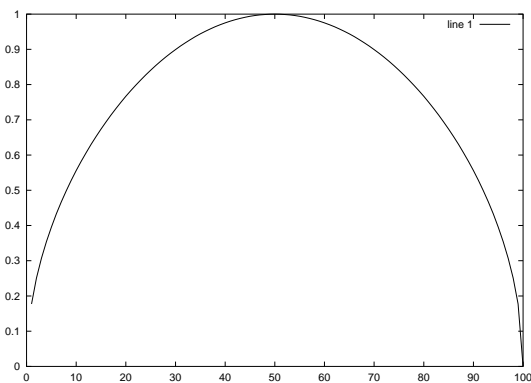
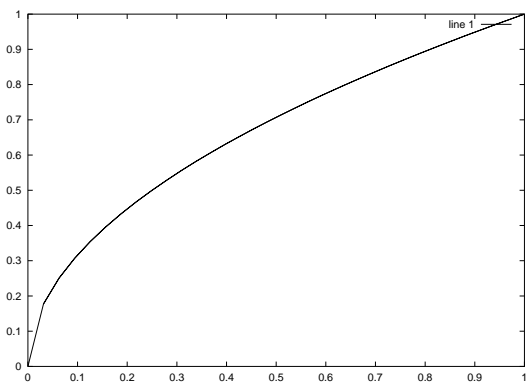
(a)  $Y = \sin(X)$ (b)  $Y$  versus  $X$ (c)  $W = \sqrt{Y}$ (d)  $W$  versus  $Y$ 

Figure 2.1: Four plots from octave.

Some magic commands are required to plot to a file. For octave, I recommend the following magic formula, which replots the figure to a file:

```
%call the plot commands before this line
gset term postscript color;
```

```
gset output "filename.ps";  
replot;  
gset term x11;  
gset output "/dev/null";
```

In Matlab, the commands are something like this:

```
%call the plot commands before this line  
print(gcf, '-deps', 'filename.eps');
```

## EXERCISES

(2.1) What do the following pieces of octave/Matlab code accomplish?

- (a) `x = (0:40) ./ 40;`  
 (b) `a = 2;`  
     `b = 5;`  
     `x = a + (b-a) .* (0:40) ./ 40;`  
 (c) `x = a + (b-a) .* (0:40) ./ 40;`  
     `y = sin(x);`  
     `plot(x,y);`

(2.2) Implement the naïve quadratic formula to find the roots of  $x^2 + bx + c = 0$ , for real  $b, c$ . Your code should return

$$\frac{-b \pm \sqrt{b^2 - 4c}}{2}.$$

Your m-file should have header line like:

```
function [x1,x2] = naivequad(b,c)
```

Test your code for  $(b, c) = (1 \times 10^{15}, 1)$ . Do you get a spurious root?

(2.3) Implement a robust quadratic formula (*cf.* Example Problem 1.9) to find the roots of  $x^2 + bx + c = 0$ . Your m-file should have header line like:

```
function [x1,x2] = robustquad(b,c)
```

Test your code for  $(b, c) = (1 \times 10^{15}, 1)$ . Do you get a spurious root?

(2.4) Write octave/Matlab code to find a fixed point for the cosine, *i.e.*, some  $x$  such that  $x = \cos(x)$ . Do this as follows: pick some initial value  $x_0$ , then let  $x_{i+1} = \cos(x_i)$  for  $i = 0, 1, \dots, n$ . Pick  $n$  to be reasonably large, or choose some convergence criterion (*i.e.*, terminate if  $|x_{i+1} - x_i| < 1 \times 10^{-10}$ ). Does your code always converge?

(2.5) Write code to implement the factorial function for integers:

```
function [nfact] = factorial(n)
```

where  $n$  factorial is equal to  $1 \cdot 2 \cdot 3 \cdots (n-1) \cdot n$ . Either use a ‘for’ loop, or write the function to recursively call itself.



## Chapter 3

# Solving Linear Systems

A number of problems in numerical analysis can be reduced to, or approximated by, a system of linear equations.

### 3.1 Gaussian Elimination with Naïve Pivoting

Our goal is the automatic solution of systems of linear equations:

$$\begin{array}{cccccc} a_{11}x_1 & + & a_{12}x_2 & + & a_{13}x_3 & + \cdots & + & a_{1n}x_n & = & b_1 \\ a_{21}x_1 & + & a_{22}x_2 & + & a_{23}x_3 & + \cdots & + & a_{2n}x_n & = & b_2 \\ a_{31}x_1 & + & a_{32}x_2 & + & a_{33}x_3 & + \cdots & + & a_{3n}x_n & = & b_3 \\ \vdots & & \vdots & & \vdots & & \ddots & \vdots & & \vdots \\ a_{n1}x_1 & + & a_{n2}x_2 & + & a_{n3}x_3 & + \cdots & + & a_{nn}x_n & = & b_n \end{array}$$

In these equations, the  $a_{ij}$  and  $b_i$  are given real numbers. We also write this as

$$\mathbf{Ax} = \mathbf{b},$$

where  $\mathbf{A}$  is a matrix, whose element in the  $i^{\text{th}}$  row and  $j^{\text{th}}$  column is  $a_{ij}$ , and  $\mathbf{b}$  is a column vector, whose  $i^{\text{th}}$  entry is  $b_i$ .

This gives the easier way of writing this equation:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix} \quad (3.1)$$

#### 3.1.1 Elementary Row Operations

You may remember that one way to solve linear equations is by applying *elementary row operations* to a given equation of the system. For example, if we are trying to solve the given system of equations, they should have the same solution as the following system:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \kappa a_{i1} & \kappa a_{i2} & \kappa a_{i3} & \cdots & \kappa a_{in} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_i \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ \kappa b_i \\ \vdots \\ b_n \end{bmatrix}$$

where  $\kappa$  is some given number which is *not zero*. It suffices to solve this system of linear equations, as it has the same solution(s) as our original system. Multiplying a row of the system by a nonzero constant is one of the elementary row operations.

The second elementary row operation is to replace a row by the sum of that row and a constant times another. Thus, for example, the following system of equations has the same solution as the original system:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{(i-1)1} & a_{(i-1)2} & a_{(i-1)3} & \cdots & a_{(i-1)n} \\ a_{i1} + \beta a_{j1} & a_{i2} + \beta a_{j2} & a_{i3} + \beta a_{j3} & \cdots & a_{in} + \beta a_{jn} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{(i-1)} \\ x_i \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_{(i-1)} \\ b_i + \beta b_j \\ \vdots \\ b_n \end{bmatrix}$$

We have replaced the  $i^{\text{th}}$  row by the  $i^{\text{th}}$  row plus  $\beta$  times the  $j^{\text{th}}$  row. The third elementary row operation is to switch rows:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_3 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

We have here switched the second and third rows. The purpose of this e.r.o. is mainly to make things look nice.

Note that none of the e.r.o.'s change the structure of the solution vector  $\mathbf{x}$ . For this reason, it is customary to drop the solution vector entirely and to write the matrix  $\mathbf{A}$  and the vector  $\mathbf{b}$  together in *augmented form*:

$$\left( \begin{array}{cccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} & b_2 \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} & b_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} & b_n \end{array} \right)$$

The idea of Gaussian Elimination is to use the elementary row operations to put a system into *upper triangular form* then use *back substitution*. We'll give an example here:

**Example Problem 3.1.** Solve the set of linear equations:

$$\begin{aligned}x_1 + x_2 - x_3 &= 2 \\ -3x_1 - 4x_2 + 4x_3 &= -7 \\ 2x_1 + 1x_2 + 1x_3 &= 7\end{aligned}$$

*Solution:* We start by rewriting in the augmented form:

$$\left( \begin{array}{ccc|c} 1 & 1 & -1 & 2 \\ -3 & -4 & 4 & -7 \\ 2 & 1 & 1 & 7 \end{array} \right)$$

We add 3 times the first row to the second, and  $-2$  times the first row to the third to get:

$$\left( \begin{array}{ccc|c} 1 & 1 & -1 & 2 \\ 0 & -1 & 1 & -1 \\ 0 & -1 & 3 & 3 \end{array} \right)$$

We now add  $-1$  times the second row to the third row to get:

$$\left( \begin{array}{ccc|c} 1 & 1 & -1 & 2 \\ 0 & -1 & 1 & -1 \\ 0 & 0 & 2 & 4 \end{array} \right)$$

The matrix is now in upper triangular form: there are no nonzero entries below the diagonal. This corresponds to the set of equations:

$$\begin{aligned}x_1 + x_2 - x_3 &= 2 \\ -x_2 + x_3 &= -1 \\ 2x_3 &= 4\end{aligned}$$

We now solve this by back substitution. Because the matrix is in upper triangular form, we can solve  $x_3$  by looking only at the last equation; namely  $x_3 = 2$ . However, once  $x_3$  is known, the second equation involves only one unknown,  $x_2$ , and can be solved only by  $x_2 = 3$ . Then the first equation has only one unknown, and is solved by  $x_1 = 1$ .  $\dashv$

All sorts of funny things can happen when you attempt Gaussian Elimination: it may turn out that your system has no solution, or has a single solution (as above), or an infinite number of solutions. We should expect that an algorithm for automatic solution of systems of equations should detect these problems.

### 3.1.2 Algorithm Terminology

The method outlined above is fine for solving small systems. We should like to devise an algorithm for doing the same thing which can be applied to large systems of equations. The algorithm will take the system (in augmented form):

$$\left( \begin{array}{cccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} & b_2 \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} & b_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} & b_n \end{array} \right)$$

The algorithm then selects the first row as the *pivot equation* or *pivot row*, and the first element of the first row,  $a_{11}$  is the *pivot element*. The algorithm then *pivots* on the pivot element to get the system:

$$\left( \begin{array}{cccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & b_1 \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} & b'_2 \\ 0 & a'_{32} & a'_{33} & \cdots & a'_{3n} & b'_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \\ 0 & a'_{n2} & a'_{n3} & \cdots & a'_{nn} & b'_n \end{array} \right)$$

Where

$$\left. \begin{aligned} a'_{ij} &= a_{ij} - \left( \frac{a_{i1}}{a_{11}} \right) a_{1j} \\ b'_i &= b_i - \left( \frac{a_{i1}}{a_{11}} \right) b_1 \end{aligned} \right\} \quad (2 \leq i \leq n, 1 \leq j \leq n)$$

Effectively we are carrying out the e.r.o. of replacing the  $i^{\text{th}}$  row by the  $i^{\text{th}}$  row minus  $\left( \frac{a_{i1}}{a_{11}} \right)$  times the first row. The quantity  $\left( \frac{a_{i1}}{a_{11}} \right)$  is the *multiplier* for the  $i^{\text{th}}$  row.

Hereafter the algorithm will not alter the first row or first column of the system. Thus, the algorithm could be written recursively. By pivoting on the second row, the algorithm then generates the system:

$$\left( \begin{array}{cccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & b_1 \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} & b'_2 \\ 0 & 0 & a''_{33} & \cdots & a''_{3n} & b''_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \\ 0 & 0 & a''_{n3} & \cdots & a''_{nn} & b''_n \end{array} \right)$$

In this case

$$\left. \begin{aligned} a''_{ij} &= a'_{ij} - \left( \frac{a'_{i2}}{a'_{22}} \right) a'_{2j} \\ b''_i &= b'_i - \left( \frac{a'_{i2}}{a'_{22}} \right) b'_2 \end{aligned} \right\} \quad (3 \leq i \leq n, 1 \leq j \leq n)$$

### 3.1.3 Algorithm Problems

The pivoting strategy we examined in this section is called ‘naïve’ because a real algorithm is a bit more complicated. The algorithm we have outlined is far too rigid—it always chooses to pivot on the  $k^{\text{th}}$  row during the  $k^{\text{th}}$  step. This would be bad if the pivot element were zero; in this case all the multipliers  $\frac{a_{ik}}{a_{kk}}$  are not defined.

Bad things can happen if  $a_{kk}$  is merely small instead of zero. Consider the following example:

**Example 3.2.** Solve the system of equations given by the augmented form:

$$\left( \begin{array}{cc|c} -0.0590 & 0.2372 & -0.3528 \\ 0.1080 & -0.4348 & 0.6452 \end{array} \right)$$

Note that the exact solution of this system is  $x_1 = 10$ ,  $x_2 = 1$ . Suppose, however, that the algorithm uses only 4 significant figures for its calculations. The algorithm, naïvely, pivots on the first equation. The multiplier for the second row is

$$\frac{0.1080}{-0.0590} \approx -1.830508\dots,$$

which will be rounded to  $-1.831$  by the algorithm.

The second entry in the matrix is replaced by

$$-0.4348 - (-1.831)(0.2372) = -0.4348 + 0.4343 = -0.0005,$$

where the arithmetic is rounded to four significant figures each time. There is some serious subtractive cancellation going on here. We have lost three figures with this subtraction. The errors get worse from here. Similarly, the second vector entry becomes:

$$0.6452 - (-1.831)(-0.3528) = 0.6452 - 0.6460 = -0.0008,$$

where, again, intermediate steps are rounded to four significant figures, and again there is subtractive cancelling. This puts the system in the form

$$\left( \begin{array}{cc|c} -0.0590 & 0.2372 & -0.3528 \\ 0 & -0.0005 & -0.0008 \end{array} \right)$$

When the algorithm attempts back substitution, it gets the value

$$x_2 = \frac{-0.0008}{-0.0005} = 1.6.$$

This is a bit off from the actual value of 1. The algorithm now finds

$$x_1 = (-0.3528 - 0.2372 \cdot 1.6) / -0.059 = (-0.3528 - 0.3795) / -0.059 = (-0.7323) / -0.059 = 12.41,$$

where each step has rounding to four significant figures. This is also a bit off.

## 3.2 Pivoting Strategies for Gaussian Elimination

Gaussian Elimination can fail when performed in the wrong order. If the algorithm selects a zero pivot, the multipliers are undefined, which is no good. We also saw that a pivot small in magnitude can cause failure. As here:

$$\begin{aligned} \epsilon x_1 + x_2 &= 1 \\ x_1 + x_2 &= 2 \end{aligned}$$

The naïve algorithm solves this as

$$\begin{aligned} x_2 &= \frac{2 - \frac{1}{\epsilon}}{1 - \frac{1}{\epsilon}} = 1 - \frac{\epsilon}{1 - \epsilon} \\ x_1 &= \frac{1 - x_2}{\epsilon} = \frac{1}{1 - \epsilon} \end{aligned}$$

If  $\epsilon$  is very small, then  $\frac{1}{\epsilon}$  is enormous compared to both 1 and 2. With poor rounding, the algorithm solves  $x_2$  as 1. Then it solves  $x_1 = 0$ . This is nearly correct for  $x_2$ , but is an awful approximation for  $x_1$ . Note that this choice of  $x_1, x_2$  satisfies the first equation, but not the second.

Now suppose the algorithm changed the order of the equations, then solved:

$$\begin{aligned} x_1 + x_2 &= 2 \\ \epsilon x_1 + x_2 &= 1 \end{aligned}$$

The algorithm solves this as

$$\begin{aligned}x_2 &= \frac{1 - 2\epsilon}{1 - \epsilon} \\x_1 &= 2 - x_2\end{aligned}$$

There's no problem with rounding here.

The problem is not the small entry *per se*: Suppose we use an e.r.o. to scale the first equation, then use naïve G.E.:

$$\begin{aligned}x_1 + \frac{1}{\epsilon}x_2 &= \frac{1}{\epsilon} \\x_1 + x_2 &= 2\end{aligned}$$

This is still solved as

$$\begin{aligned}x_2 &= \frac{2 - \frac{1}{\epsilon}}{1 - \frac{1}{\epsilon}} \\x_1 &= \frac{1 - x_2}{\epsilon},\end{aligned}$$

and rounding is still a problem.

### 3.2.1 Scaled Partial Pivoting

The naïve G.E. algorithm uses the rows 1, 2, ..., n-1 in order as pivot equations. As shown above, this can cause errors. Better is to pivot first on row  $\ell_1$ , then row  $\ell_2$ , etc, until finally pivoting on row  $\ell_{n-1}$ , for some permutation  $\{\ell_i\}_{i=1}^n$  of the integers 1, 2, ..., n. The strategy of *scaled partial pivoting* is to compute this permutation so that G.E. works well.

In light of our example, we want to pivot on an element which is not small compared to other elements in its row. So our algorithm first determines “smallness” by calculating a scale, row-wise:

$$s_i = \max_{1 \leq j \leq n} |a_{ij}|.$$

The scales are only computed once.

Then the first pivot,  $\ell_1$ , is chosen to be the  $i$  such that

$$\frac{|a_{i,1}|}{s_i}$$

is maximized. The algorithm pivots on row  $\ell_1$ , producing a bunch of zeros in the first column. Note that the algorithm should *not* rearrange the matrix—this takes too much work.

The second pivot,  $\ell_2$ , is chosen to be the  $i$  such that

$$\frac{|a_{i,2}|}{s_i}$$

is maximized, but without choosing  $\ell_2 = \ell_1$ . The algorithm pivots on row  $\ell_2$ , producing a bunch of zeros in the second column.

In the  $k^{\text{th}}$  step  $\ell_k$  is chosen to be the  $i$  not among  $\ell_1, \ell_2, \dots, \ell_{k-1}$  such that

$$\frac{|a_{i,k}|}{s_i}$$

is maximized. The algorithm pivots on row  $\ell_k$ , producing a bunch of zeros in the  $k^{\text{th}}$  column.

The slick way to implement this is to first set  $\ell_i = i$  for  $i = 1, 2, \dots, n$ . Then rearrange this vector in a kind of “bubble sort”: when you find the index that should be  $\ell_1$ , swap them, *i.e.*, find the  $j$  such that  $\ell_j$  should be the first pivot and switch the values of  $\ell_1, \ell_j$ .

Then at the  $k^{\text{th}}$  step, search only those indices in the tail of this vector: *i.e.*, only among  $\ell_j$  for  $k \leq j \leq n$ , and perform a swap.

### 3.2.2 An Example

We present an example of using scaled partial pivoting with G.E. It’s hard to come up with an example where the numbers do not come out as ugly fractions. We’ll look at a homework question.

$$\left( \begin{array}{cccc|c} 2 & -1 & 3 & 7 & 15 \\ 4 & 4 & 0 & 7 & 11 \\ 2 & 1 & 1 & 3 & 7 \\ 6 & 5 & 4 & 17 & 31 \end{array} \right)$$

The scales are as follows:  $s_1 = 7, s_2 = 7, s_3 = 3, s_4 = 17$ .

We pick  $\ell_1$ . It should be the index which maximizes  $|a_{i1}|/s_i$ . These values are:

$$\frac{2}{7}, \frac{4}{7}, \frac{2}{3}, \frac{6}{17}.$$

We pick  $\ell_1 = 3$ , and pivot:

$$\left( \begin{array}{cccc|c} 0 & -2 & 2 & 4 & 8 \\ 0 & 2 & -2 & 1 & -3 \\ 2 & 1 & 1 & 3 & 7 \\ 0 & 2 & 1 & 8 & 10 \end{array} \right)$$

We pick  $\ell_2$ . It should *not* be 3, and should be the index which maximizes  $|a_{i2}|/s_i$ . These values are:

$$\frac{2}{7}, \frac{2}{7}, \frac{2}{17}.$$

We have a tie. In this case we pick the second row, *i.e.*,  $\ell_2 = 2$ . We pivot:

$$\left( \begin{array}{cccc|c} 0 & 0 & 0 & 5 & 5 \\ 0 & 2 & -2 & 1 & -3 \\ 2 & 1 & 1 & 3 & 7 \\ 0 & 0 & 3 & 7 & 13 \end{array} \right)$$

The matrix is in permuted upper triangular form. We could proceed, but would get a zero multiplier, and no changes would occur.

If we did proceed we would have  $\ell_3 = 4$ . Then  $\ell_4 = 1$ . Our row permutation is 3, 2, 4, 1. When we do back substitution, we work in this order *reversed* on the rows, solving  $x_4$ , then  $x_3, x_2, x_1$ .

We get  $x_4 = 1$ , so

$$\begin{aligned} x_3 &= \frac{1}{3}(13 - 7 * 1) = 2 \\ x_2 &= \frac{1}{2}(-3 - 1 * 1 + 2 * 2) = 0 \\ x_1 &= \frac{1}{2}(7 - 3 * 1 - 1 * 2 - 1 * 0) = 1 \end{aligned}$$

### 3.2.3 Another Example and A Real Algorithm

Sometimes we want to solve

$$A\mathbf{x} = \mathbf{b}$$

for a number of different vectors  $\mathbf{b}$ . It turns out we can run G.E. on the matrix  $A$  alone and come up with all the multipliers, which can then be used multiple times on different vectors  $\mathbf{b}$ . We illustrate with an example:

$$M_0 = \begin{pmatrix} 1 & 2 & 4 & 1 \\ 4 & 2 & 1 & 2 \\ 2 & 1 & 2 & 3 \\ 1 & 3 & 2 & 1 \end{pmatrix}, \quad \boldsymbol{\ell} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}.$$

The scale vector is  $\mathbf{s} = [4 \ 4 \ 3 \ 3]^\top$ .

Our scale choices are  $\frac{1}{4}, \frac{4}{4}, \frac{2}{3}, \frac{1}{3}$ . We choose  $\ell_1 = 2$ , and swap  $\ell_1, \ell_2$ . In the places where there would be zeros in the real matrix, we will put the multipliers. We will illustrate them here boxed:

$$M_1 = \begin{pmatrix} \boxed{\frac{1}{4}} & \frac{3}{2} & \frac{15}{4} & \frac{1}{2} \\ 4 & 2 & 1 & 2 \\ \boxed{\frac{1}{2}} & 0 & \frac{3}{2} & 2 \\ \boxed{\frac{1}{4}} & \frac{5}{2} & \frac{7}{4} & \frac{1}{2} \end{pmatrix}, \quad \boldsymbol{\ell} = \begin{bmatrix} 2 \\ 1 \\ 3 \\ 4 \end{bmatrix}.$$

Our scale choices are  $\frac{3}{8}, \frac{0}{3}, \frac{5}{6}$ . We choose  $\ell_2 = 4$ , and so swap  $\ell_2, \ell_4$ :

$$M_2 = \begin{pmatrix} \boxed{\frac{1}{4}} & \boxed{\frac{3}{5}} & \frac{27}{10} & \frac{1}{5} \\ 4 & 2 & 1 & 2 \\ \boxed{\frac{1}{2}} & \boxed{0} & \frac{3}{2} & 2 \\ \boxed{\frac{1}{4}} & \frac{5}{2} & \frac{7}{4} & \frac{1}{2} \end{pmatrix}, \quad \boldsymbol{\ell} = \begin{bmatrix} 2 \\ 4 \\ 3 \\ 1 \end{bmatrix}.$$

Our scale choices are  $\frac{27}{40}, \frac{1}{2}$ . We choose  $\ell_3 = 1$ , and so swap  $\ell_3, \ell_4$ :

$$M_3 = \begin{pmatrix} \boxed{\frac{1}{4}} & \boxed{\frac{3}{5}} & \frac{27}{10} & \frac{1}{5} \\ 4 & 2 & 1 & 2 \\ \boxed{\frac{1}{2}} & \boxed{0} & \boxed{\frac{5}{9}} & \frac{17}{9} \\ \boxed{\frac{1}{4}} & \frac{5}{2} & \frac{7}{4} & \frac{1}{2} \end{pmatrix}, \quad \boldsymbol{\ell} = \begin{bmatrix} 2 \\ 4 \\ 1 \\ 3 \end{bmatrix}.$$

Now suppose we had to solve the linear system for  $\mathbf{b} = [-1 \ 8 \ 2 \ 1]^\top$ .

We scale  $\mathbf{b}$  by the multipliers in order:  $\ell_1 = 2$ , so, we sweep through the first column of  $M_3$ , picking off the boxed numbers (your computer doesn't really have boxed variables), and scaling  $\mathbf{b}$



appropriately:

$$\begin{bmatrix} -1 \\ 8 \\ 2 \\ 1 \end{bmatrix} \Rightarrow \begin{bmatrix} -3 \\ 8 \\ -2 \\ -1 \end{bmatrix}$$

This continues:

$$\begin{bmatrix} -3 \\ 8 \\ -2 \\ -1 \end{bmatrix} \Rightarrow \begin{bmatrix} -\frac{12}{5} \\ 8 \\ -2 \\ -1 \end{bmatrix} \Rightarrow \begin{bmatrix} -\frac{12}{5} \\ 8 \\ -\frac{2}{3} \\ -1 \end{bmatrix}$$

We then perform a permuted backwards substitution on the augmented system

$$\left( \begin{array}{cccc|c} 0 & 0 & \frac{27}{10} & \frac{1}{5} & -\frac{12}{5} \\ 4 & 2 & 1 & 2 & 8 \\ 0 & 0 & 0 & \frac{17}{9} & -\frac{2}{3} \\ 0 & \frac{5}{2} & \frac{7}{4} & \frac{1}{2} & -1 \end{array} \right)$$

This proceeds as

$$\begin{aligned} x_4 &= \frac{-2}{3} \frac{9}{17} = \frac{-6}{17} \\ x_3 &= \frac{10}{27} \left( -\frac{12}{5} - \frac{1}{5} \frac{-6}{17} \right) = \dots \\ x_2 &= \frac{2}{5} \left( -1 - \frac{1}{2} \frac{-6}{17} - \frac{7}{4} x_3 \right) = \dots \\ x_1 &= \frac{1}{4} \left( 8 - 2 \frac{-6}{17} - x_3 - 2x_2 \right) = \dots \end{aligned}$$

Fill in your own values here.

### 3.3 LU Factorization

We examined G.E. to solve the system

$$\mathbf{Ax} = \mathbf{b},$$

where  $\mathbf{A}$  is a matrix:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix}.$$

We want to show that G.E. actually factors  $\mathbf{A}$  into lower and upper triangular parts, that is  $\mathbf{A} = \mathbf{LU}$ , where

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{bmatrix}, \quad \mathbf{U} = \begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix}.$$

We call this a *LU Factorization* of  $\mathbf{A}$ .

### 3.3.1 An Example

We consider solution of the following augmented form:

$$\left( \begin{array}{cccc|c} 2 & 1 & 1 & 3 & 7 \\ 4 & 4 & 0 & 7 & 11 \\ 6 & 5 & 4 & 17 & 31 \\ 2 & -1 & 0 & 7 & 15 \end{array} \right) \quad (3.2)$$

The naïve G.E. reduces this to

$$\left( \begin{array}{cccc|c} 2 & 1 & 1 & 3 & 7 \\ 0 & 2 & -2 & 1 & -3 \\ 0 & 0 & 3 & 7 & 13 \\ 0 & 0 & 0 & 12 & 18 \end{array} \right)$$

We are going to run the naïve G.E., and see how it is a LU Factorization. Since this is the naïve version, we first pivot on the first row. Our multipliers are 2, 3, 1. We pivot to get

$$\left( \begin{array}{cccc|c} 2 & 1 & 1 & 3 & 7 \\ 0 & 2 & -2 & 1 & -3 \\ 0 & 2 & 1 & 8 & 10 \\ 0 & -2 & -1 & 4 & 8 \end{array} \right)$$

Careful inspection shows that we've merely multiplied  $A$  and  $\mathbf{b}$  by a lower triangular matrix  $M_1$ :

$$M_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ -3 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}$$

The entries in the first column are the negative e.r.o. multipliers for each row. Thus after the first pivot, it is like we are solving the system

$$M_1 A \mathbf{x} = M_1 \mathbf{b}.$$

We pivot on the second row to get:

$$\left( \begin{array}{cccc|c} 2 & 1 & 1 & 3 & 7 \\ 0 & 2 & -2 & 1 & -3 \\ 0 & 0 & 3 & 7 & 13 \\ 0 & 0 & -3 & 5 & 5 \end{array} \right)$$

The multipliers are 1,  $-1$ . We can view this pivot as a multiplication by  $M_2$ , with

$$M_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

We are now solving

$$M_2 M_1 A \mathbf{x} = M_2 M_1 \mathbf{b}.$$

We pivot on the third row, with a multiplier of  $-1$ . Thus we get

$$\left( \begin{array}{cccc|c} 2 & 1 & 1 & 3 & 7 \\ 0 & 2 & -2 & 1 & -3 \\ 0 & 0 & 3 & 7 & 13 \\ 0 & 0 & 0 & 12 & 18 \end{array} \right)$$

We have multiplied by  $M_3$  :

$$M_3 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

We are now solving

$$M_3 M_2 M_1 A x = M_3 M_2 M_1 b.$$

But we have an upper triangular form, that is, if we let

$$U = \begin{bmatrix} 2 & 1 & 1 & 3 \\ 0 & 2 & -2 & 1 \\ 0 & 0 & 3 & 7 \\ 0 & 0 & 0 & 12 \end{bmatrix}$$

Then we have

$$\begin{aligned} M_3 M_2 M_1 A &= U, \\ A &= (M_3 M_2 M_1)^{-1} U, \\ A &= M_1^{-1} M_2^{-1} M_3^{-1} U, \\ A &= LU. \end{aligned}$$

We are hoping that  $L$  is indeed lower triangular, and has ones on the diagonal. It turns out that the inverse of each  $M_i$  matrix has a nice form (See Exercise (3.6)). We write them here:

$$\begin{aligned} L &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 3 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 3 & 1 & 1 & 0 \\ 1 & -1 & -1 & 1 \end{bmatrix} \end{aligned}$$

This is really crazy: the matrix  $L$  looks to be composed of ones on the diagonal and multipliers under the diagonal.

Now we check to see if we made any mistakes:

$$\begin{aligned} LU &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 3 & 1 & 1 & 0 \\ 1 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 3 \\ 0 & 2 & -2 & 1 \\ 0 & 0 & 3 & 7 \\ 0 & 0 & 0 & 12 \end{bmatrix} \\ &= \begin{bmatrix} 2 & 1 & 1 & 3 \\ 4 & 4 & 0 & 7 \\ 6 & 5 & 4 & 17 \\ 2 & -1 & 0 & 7 \end{bmatrix} = A. \end{aligned}$$

### 3.3.2 Using LU Factorizations

We see that the G.E. algorithm can be used to actually calculate the LU factorization. We will look at this in more detail in another example. We now examine how we can use the LU factorization to solve the equation

$$A\mathbf{x} = \mathbf{b},$$

Since we have  $A = LU$ , we first solve

$$L\mathbf{z} = \mathbf{b},$$

then solve

$$U\mathbf{x} = \mathbf{z}.$$

Since  $L$  is lower triangular, we can solve for  $\mathbf{z}$  with a *forward* substitution. Similarly, since  $U$  is upper triangular, we can solve for  $\mathbf{x}$  with a back substitution. We drag out the previous example (which we never got around to solving):

$$\left( \begin{array}{cccc|c} 2 & 1 & 1 & 3 & 7 \\ 4 & 4 & 0 & 7 & 11 \\ 6 & 5 & 4 & 17 & 31 \\ 2 & -1 & 0 & 7 & 15 \end{array} \right)$$

We had found the LU factorization of  $A$  as

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 3 & 1 & 1 & 0 \\ 1 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 3 \\ 0 & 2 & -2 & 1 \\ 0 & 0 & 3 & 7 \\ 0 & 0 & 0 & 12 \end{bmatrix}$$

So we solve

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 3 & 1 & 1 & 0 \\ 1 & -1 & -1 & 1 \end{bmatrix} \mathbf{z} = \begin{bmatrix} 7 \\ 11 \\ 31 \\ 15 \end{bmatrix}$$

We get

$$\mathbf{z} = \begin{bmatrix} 7 \\ -3 \\ 13 \\ 18 \end{bmatrix}$$

Now we solve

$$\begin{bmatrix} 2 & 1 & 1 & 3 \\ 0 & 2 & -2 & 1 \\ 0 & 0 & 3 & 7 \\ 0 & 0 & 0 & 12 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 7 \\ -3 \\ 13 \\ 18 \end{bmatrix}$$

We get the ugly solution

$$\mathbf{z} = \begin{bmatrix} \frac{37}{12} \\ \frac{24}{12} \\ \frac{-17}{12} \\ \frac{18}{12} \\ \frac{13}{6} \\ \frac{3}{2} \end{bmatrix}$$

### 3.3.3 Some Theory

We aren't doing much proving here. The following theorem has an ugly proof in the Cheney & Kincaid [7].

**Theorem 3.3.** If  $A$  is an  $n \times n$  matrix, and naïve Gaussian Elimination does not encounter a zero pivot, then the algorithm generates a LU factorization of  $A$ , where  $L$  is the lower triangular part of the output matrix, and  $U$  is the upper triangular part.

This theorem relies on us using the fancy version of G.E., which saves the multipliers in the spots where there should be zeros. If correctly implemented, then,  $L$  is the lower triangular part but with ones put on the diagonal.

This theorem is proved in Cheney & Kincaid [7]. This appears to me to be a case of something which can be better illustrated with an example or two and some informal investigation. The proof is an unilluminating index-chase—read it at your own risk.

### 3.3.4 Computing Inverses

We consider finding the inverse of  $A$ . Since

$$AA^{-1} = I,$$

then the  $j^{\text{th}}$  column of the inverse  $A^{-1}$  solves the equation

$$A\mathbf{x} = \mathbf{e}_j,$$

where  $\mathbf{e}_j$  is the column matrix of all zeros, but with a one in the  $j^{\text{th}}$  position.

Thus we can find the inverse of  $A$  by running  $n$  linear solves. Obviously we are only going to run G.E. once, to put the matrix in LU form, then run  $n$  solves using forward and backward substitutions.

## 3.4 Iterative Solutions

Recall we are trying to solve

$$A\mathbf{x} = \mathbf{b}.$$

We examine the computational cost of Gaussian Elimination to motivate the search for an alternative algorithm.

### 3.4.1 An Operation Count for Gaussian Elimination

We consider the number of floating point operations (“flops”) required to solve the system  $A\mathbf{x} = \mathbf{b}$ . Gaussian Elimination first uses row operations to transform the problem into an equivalent problem of the form  $U\mathbf{x} = \mathbf{b}'$ , where  $U$  is upper triangular. Then back substitution is used to solve for  $\mathbf{x}$ .

First we look at how many floating point operations are required to reduce

$$\left( \begin{array}{cccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} & b_2 \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} & b_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} & b_n \end{array} \right)$$

to

$$\left( \begin{array}{cccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & b_1 \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} & b'_2 \\ 0 & a'_{32} & a'_{33} & \cdots & a'_{3n} & b'_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & a'_{n2} & a'_{n3} & \cdots & a'_{nn} & b'_n \end{array} \right)$$

First a multiplier is computed for each row. Then in each row the algorithm performs  $n$  multiplies and  $n$  adds. This gives a total of  $(n-1) + (n-1)n$  multiplies (counting in the computing of the multiplier in each of the  $(n-1)$  rows) and  $(n-1)n$  adds. In total this is  $2n^2 - n - 1$  floating point operations to do a single pivot on the  $n$  by  $n$  system.

Then this has to be done recursively on the lower right subsystem, which is an  $(n-1)$  by  $(n-1)$  system. This requires  $2(n-1)^2 - (n-1) - 1$  operations. Then this has to be done on the next subsystem, requiring  $2(n-2)^2 - (n-2) - 1$  operations, and so on.

In total, then, we use  $I_n$  total floating point operations, with

$$I_n = 2 \sum_{j=1}^n j^2 - \sum_{j=1}^n j - \sum_{j=1}^n 1.$$

Recalling that

$$\sum_{j=1}^n j^2 = \frac{1}{6}(n)(n+1)(2n+1), \quad \text{and} \quad \sum_{j=1}^n j = \frac{1}{2}(n)(n+1),$$

We find that

$$I_n = \frac{1}{6}(4n-1)n(n+1) - n \approx \frac{2}{3}n^3.$$

Now consider the costs of back substitution. To solve

$$\left( \begin{array}{cccc|c} a_{11} & \cdots & a_{1,n-2} & a_{1,n-1} & a_{1n} & b_1 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & a_{n-2,n-2} & a_{n-2,n-1} & a_{n-2,n} & b_{n-2} \\ 0 & \cdots & 0 & a_{n-1,n-1} & a_{n-1,n} & b_{n-1} \\ 0 & \cdots & 0 & 0 & a_{nn} & b_n \end{array} \right)$$

for  $x_n$  requires only a single division. Then to solve for  $x_{n-1}$  we compute

$$x_{n-1} = \frac{1}{a_{n-1,n-1}} [b_{n-1} - a_{n-1,n}x_n],$$

and requires 3 flops. Similarly, solving for  $x_{n-2}$  requires 5 flops. Thus in total back substitution requires  $B_n$  total floating point operations with

$$B_n = \sum_{j=1}^n 2j - 1 = n(n-1) - n = n(n-2) \approx n^2$$

### 3.4.2 Dividing by Multiplying

We saw that Gaussian Elimination requires around  $\frac{2}{3}n^3$  operations just to find the LU factorization, then about  $n^2$  operations to solve the system, when  $\mathbf{A}$  is  $n \times n$ . When  $n$  is large, this may take too long to be practical. Additionally, if  $\mathbf{A}$  is sparse (has few nonzero elements per row), we would like the complexity of our computations to scale with the sparsity of  $\mathbf{A}$ . Thus we look for an alternative algorithm.

First we consider the simplest case,  $n = 1$ . Suppose we are to solve the equation

$$Ax = b.$$

for scalars  $A, b$ . We solve this by

$$x = \frac{1}{A}b = \frac{1}{\omega A}\omega b = \frac{1}{1 - (1 - \omega A)}\omega b = \frac{1}{1 - r}\omega b,$$

where  $\omega \neq 0$  is some real number chosen to “weight” the problem appropriately, and  $r = 1 - \omega A$ . Now suppose that  $\omega$  is chosen such that  $|r| < 1$ . This can be done so long as  $A \neq 0$ , which would have been a problem anyway. Now use the geometric expansion:

$$\frac{1}{1 - r} = 1 + r + r^2 + r^3 + \dots$$

Because of the assumption  $|r| < 1$ , the terms  $r^n$  converge to zero as  $n \rightarrow \infty$ . This gives the approximate solution to our one dimensional problem as

$$\begin{aligned} x &\approx \left[1 + r + r^2 + r^3 + \dots + r^k\right] \omega b \\ &= \omega b + \left[r + r^2 + r^3 + \dots + r^k\right] \omega b \\ &= \omega b + r \left[1 + r + r^2 + \dots + r^{k-1}\right] \omega b \end{aligned}$$

This suggests an *iterative* approach to solving  $Ax = b$ . First let  $x^{(0)} = \omega b$ , then let

$$x^{(k)} = \omega b + r x^{(k-1)}.$$

The iterates  $x^{(k)}$  will converge to the solution of  $Ax = b$  if  $|r| < 1$ .

You should now convince yourself that because  $r^n \rightarrow 0$ , that the choice of the initial iterate  $x^{(0)}$  was immaterial, *i.e.*, that under *any* choice of initial iterate convergence is guaranteed.

We now translate this scalar result into the vector case. The algorithm proceeds as follows: first fix some initial estimate of the solution,  $\mathbf{x}^{(0)}$ . A good choice might be  $\omega \mathbf{b}$ , but this is not necessary. Then calculate successive approximations to the actual solution by updates of the form

$$\mathbf{x}^{(k)} = \omega \mathbf{b} + (1 - \omega A) \mathbf{x}^{(k-1)}.$$

It turns out that we can consider a slightly more general form of the algorithm, one in which successive iterates are defined *implicitly*. That is we consider iterates of the form

$$\boxed{\mathbf{Q}\mathbf{x}^{(k+1)} = (\mathbf{Q} - \omega \mathbf{A}) \mathbf{x}^{(k)} + \omega \mathbf{b},} \quad (3.3)$$

for some matrix  $\mathbf{Q}$ , and some scaling factor  $\omega$ . Note that this update relies on vector additions and possibly by premultiplication of a vector by  $\mathbf{A}$  or  $\mathbf{Q}$ . In the case where these two matrices are sparse, such an update can be relatively cheap.

Now suppose that as  $k \rightarrow \infty$ ,  $\mathbf{x}^{(k)}$  converges to some vector  $\mathbf{x}^*$ , which is a fixed point of the iteration. Then

$$\begin{aligned} \mathbf{Q}\mathbf{x}^* &= (\mathbf{Q} - \omega\mathbf{A})\mathbf{x}^* + \omega\mathbf{b}, \\ \mathbf{Q}\mathbf{x}^* &= \mathbf{Q}\mathbf{x}^* - \omega\mathbf{A}\mathbf{x}^* + \omega\mathbf{b}, \\ \omega\mathbf{A}\mathbf{x}^* &= \omega\mathbf{b}, \\ \mathbf{A}\mathbf{x}^* &= \mathbf{b}. \end{aligned}$$

We have some freedom in choosing  $\mathbf{Q}$ , but there are two considerations we should keep in mind:

1. Choice of  $\mathbf{Q}$  affects convergence and speed of convergence of the method. In particular, we want  $\mathbf{Q}$  to be similar to  $\mathbf{A}$ .
2. Choice of  $\mathbf{Q}$  affects ease of computing the update. That is, given

$$\mathbf{z} = (\mathbf{Q} - \mathbf{A})\mathbf{x}^{(k)} + \mathbf{b},$$

we should pick  $\mathbf{Q}$  such that the equation

$$\mathbf{Q}\mathbf{x}^{(k+1)} = \mathbf{z}$$

is easy to solve exactly.

These two goals conflict with each other. At one end of the spectrum is the so-called “impossible iteration,” at the other is the Richardson’s.

### 3.4.3 Impossible Iteration

I made up the term “impossible iteration.” But consider the method which takes  $\mathbf{Q}$  to be  $\mathbf{A}$ . This seems to be the best choice for satisfying the first goal. Letting  $\omega = 1$ , our method becomes

$$\mathbf{A}\mathbf{x}^{(k+1)} = (\mathbf{A} - \mathbf{A})\mathbf{x}^{(k)} + \mathbf{b} = \mathbf{b}.$$

This method should clearly converge in one step. However, the second goal is totally ignored. Indeed, we are considering iterative methods because we cannot easily solve this linear equation in the first place.

### 3.4.4 Richardson Iteration

At the other end of the spectrum is the Richardson Iteration, which chooses  $\mathbf{Q}$  to be the identity matrix. Solving the system

$$\mathbf{Q}\mathbf{x}^{(k+1)} = \mathbf{z}$$

is trivial: we just have  $\mathbf{x}^{(k+1)} = \mathbf{z}$ .

**Example Problem 3.4.** Use Richardson Iteration with  $\omega = 1$  on the system

$$\mathbf{A} = \begin{bmatrix} 6 & 1 & 1 \\ 2 & 4 & 0 \\ 1 & 2 & 6 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 12 \\ 0 \\ 6 \end{bmatrix}.$$

*Solution:* We let

$$\mathbf{Q} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (\mathbf{Q} - \mathbf{A}) = \begin{bmatrix} -5 & -1 & -1 \\ -2 & -3 & 0 \\ -1 & -2 & -5 \end{bmatrix}.$$



We start with an arbitrary  $\mathbf{x}^{(0)}$ , say  $\mathbf{x}^{(0)} = [2 \ 2 \ 2]^\top$ . We get  $\mathbf{x}^{(1)} = [-2 \ -10 \ -10]^\top$ , and  $\mathbf{x}^{(2)} = [42 \ 34 \ 78]^\top$ .

Note the real solution is  $\mathbf{x} = [2 \ -1 \ 1]^\top$ . The Richardson Iteration does not appear to converge for this example, unfortunately.  $\dashv$

**Example Problem 3.5.** Apply Richardson Iteration with  $\omega = 1/6$  on the previous system.

*Solution:* Our iteration becomes

$$\mathbf{x}^{(k+1)} = \begin{bmatrix} 0 & -1/6 & -1/6 \\ -1/3 & 1/3 & 0 \\ -1/6 & -1/3 & 0 \end{bmatrix} \mathbf{x}^{(k)} + \begin{bmatrix} 2 \\ 0 \\ 1 \end{bmatrix}.$$

We start with the same  $\mathbf{x}^{(0)}$  as previously,  $\mathbf{x}^{(0)} = [2 \ 2 \ 2]^\top$ . We get  $\mathbf{x}^{(1)} = [4/3 \ 0 \ 0]^\top$ ,  $\mathbf{x}^{(2)} = [2 \ -4/9 \ 7/9]^\top$ , and finally  $\mathbf{x}^{(12)} = [2 \ -0.99998 \ 0.99998]^\top$ .

Thus, the choice of  $\omega$  has some affect on convergence.  $\dashv$

We can rethink the Richardson Iteration as

$$\mathbf{x}^{(k+1)} = (1 - \omega\mathbf{A})\mathbf{x}^{(k)} + \omega\mathbf{b} = \mathbf{x}^{(k)} + \omega(\mathbf{b} - \mathbf{A}\mathbf{x}^{(k)}).$$

Thus at each step we are adding some scaled version of the *residual*, defined as  $\mathbf{b} - \mathbf{A}\mathbf{x}^{(k)}$ , to the iterate.

### 3.4.5 Jacobi Iteration

The Jacobi Iteration chooses  $\mathbf{Q}$  to be the matrix consisting of the diagonal of  $\mathbf{A}$ . This is more similar to  $\mathbf{A}$  than the identity matrix, but nearly as simple to invert.

**Example Problem 3.6.** Use Jacobi Iteration, with  $\omega = 1$ , to solve the system

$$\mathbf{A} = \begin{bmatrix} 6 & 1 & 1 \\ 2 & 4 & 0 \\ 1 & 2 & 6 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 12 \\ 0 \\ 6 \end{bmatrix}.$$

*Solution:* We let

$$\mathbf{Q} = \begin{bmatrix} 6 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 6 \end{bmatrix}, \quad (\mathbf{Q} - \mathbf{A}) = \begin{bmatrix} 0 & -1 & -1 \\ -2 & 0 & 0 \\ -1 & -2 & 0 \end{bmatrix}, \quad \mathbf{Q}^{-1} = \begin{bmatrix} \frac{1}{6} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{6} \end{bmatrix}.$$

We start with an arbitrary  $\mathbf{x}^{(0)}$ , say  $\mathbf{x}^{(0)} = [2 \ 2 \ 2]^\top$ . We get  $\mathbf{x}^{(1)} = [\frac{4}{3} \ -1 \ 0]^\top$ . Then  $\mathbf{x}^{(2)} = [\frac{13}{6} \ -\frac{2}{3} \ \frac{10}{9}]^\top$ . Continuing, we find that  $\mathbf{x}^{(5)} \approx [1.987 \ -1.019 \ 0.981]^\top$ .

Note the real solution is  $\mathbf{x} = [2 \ -1 \ 1]^\top$ .  $\dashv$

There is an alternative way to describe the Jacobi Iteration for  $\omega = 1$ . By considering the update elementwise, we see that the operation can be described by

$$\mathbf{x}_j^{(k+1)} = \frac{1}{a_{jj}} \left( b_j - \sum_{i=1, i \neq j}^n a_{ji} \mathbf{x}_i^{(k)} \right).$$

Thus an update takes less than  $2n^2$  operations. In fact, if  $\mathbf{A}$  is sparse, with less than  $k$  nonzero entries per row, the update should take less than  $2nk$  operations.

### 3.4.6 Gauss Seidel Iteration

The Gauss Seidel Iteration chooses  $\mathbf{Q}$  to be lower triangular part of  $\mathbf{A}$ , including the diagonal. In this case solving the system

$$\mathbf{Q}\mathbf{x}^{(k+1)} = \mathbf{z}$$

is performed by forward substitution. Here the  $\mathbf{Q}$  is more like  $\mathbf{A}$  than for Jacobi Iteration, but involves more work for inverting.

**Example Problem 3.7.** Use Gauss Seidel Iteration to again solve for

$$\mathbf{A} = \begin{bmatrix} 6 & 1 & 1 \\ 2 & 4 & 0 \\ 1 & 2 & 6 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 12 \\ 0 \\ 6 \end{bmatrix}.$$

*Solution:* We let

$$\mathbf{Q} = \begin{bmatrix} 6 & 0 & 0 \\ 2 & 4 & 0 \\ 1 & 2 & 6 \end{bmatrix}, \quad (\mathbf{Q} - \mathbf{A}) = \begin{bmatrix} 0 & -1 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

We start with an arbitrary  $\mathbf{x}^{(0)}$ , say  $\mathbf{x}^{(0)} = [2\ 2\ 2]^\top$ . We get  $\mathbf{x}^{(1)} = [\frac{4}{3} \ -\frac{2}{3}\ 1]^\top$ . Then  $\mathbf{x}^{(2)} = [\frac{35}{18} \ -\frac{35}{36}\ 1]^\top$ .

Already this is fairly close to the actual solution  $\mathbf{x} = [2 \ -1\ 1]^\top$ . ←

Just as with Jacobi Iteration, there is an easier way to describe the Gauss Seidel Iteration. In this case we will keep a single vector  $\mathbf{x}$  and overwrite it, element by element. Thus for  $j = 1, 2, \dots, n$ , we set

$$x_j \leftarrow \frac{1}{a_{jj}} \left( b_j - \sum_{i=1, i \neq j}^n a_{ji} x_i \right).$$

This looks exactly like the Jacobi update. However, in the sum on the right there are some “old” values of  $x_i$  and some “new” values; the new values are those  $x_i$  for which  $i < j$ .

Again this takes less than  $2n^2$  operations. Or less than  $2nk$  if  $\mathbf{A}$  is sufficiently sparse.

An alteration of the Gauss Seidel Iteration is to make successive “sweeps” of this redefinition, one for  $j = 1, 2, \dots, n$ , the next for  $j = n, n-1, \dots, 2, 1$ . This amounts to running Gauss Seidel once with  $\mathbf{Q}$  the lower triangular part of  $\mathbf{A}$ , then running it with  $\mathbf{Q}$  the upper triangular part. This iterative method is known as “red-black Gauss Seidel.”

### 3.4.7 Error Analysis

Suppose that  $\mathbf{x}$  is the solution to equation 3.4. Define the error vector:

$$\mathbf{e}^{(k)} = \mathbf{x}^{(k)} - \mathbf{x}.$$

Now notice that

$$\begin{aligned}\mathbf{x}^{(k+1)} &= \mathbf{Q}^{-1}(\mathbf{Q} - \omega\mathbf{A})\mathbf{x}^{(k)} + \mathbf{Q}^{-1}\omega\mathbf{b}, \\ \mathbf{x}^{(k+1)} &= \mathbf{Q}^{-1}\mathbf{Q}\mathbf{x}^{(k)} - \omega\mathbf{Q}^{-1}\mathbf{A}\mathbf{x}^{(k)} + \omega\mathbf{Q}^{-1}\mathbf{A}\mathbf{x}, \\ \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} - \omega\mathbf{Q}^{-1}\mathbf{A}(\mathbf{x}^{(k)} - \mathbf{x}), \\ \mathbf{x}^{(k+1)} - \mathbf{x} &= \mathbf{x}^{(k)} - \mathbf{x} - \omega\mathbf{Q}^{-1}\mathbf{A}(\mathbf{x}^{(k)} - \mathbf{x}), \\ \mathbf{e}^{(k+1)} &= \mathbf{e}^{(k)} - \omega\mathbf{Q}^{-1}\mathbf{A}\mathbf{e}^{(k)}, \\ \mathbf{e}^{(k+1)} &= (\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A})\mathbf{e}^{(k)}.\end{aligned}$$

Reusing this relation we find that

$$\begin{aligned}\mathbf{e}^{(k)} &= (\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A})\mathbf{e}^{(k-1)}, \\ &= (\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A})^2\mathbf{e}^{(k-2)}, \\ &= (\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A})^k\mathbf{e}^{(0)}.\end{aligned}$$

We want to ensure that  $\mathbf{e}^{(k+1)}$  is “smaller” than  $\mathbf{e}^{(k)}$ . To do this we recall matrix and vector norms from Subsection 1.4.1.

$$\|\mathbf{e}^{(k)}\|_2 = \|(\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A})^k\mathbf{e}^{(0)}\|_2 \leq \|\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A}\|_2^k \|\mathbf{e}^{(0)}\|_2.$$

(See Example Problem 1.29.)

Thus our iteration converges ( $\mathbf{e}^{(k)}$  goes to the zero vector, *i.e.*,  $\mathbf{x}^{(k)} \rightarrow \mathbf{x}$ ) if

$$\|\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A}\|_2 < 1.$$

This gives the theorem:

**Theorem 3.8.** An iterative solution scheme converges for any starting  $\mathbf{x}^{(0)}$  if and only if all eigenvalues of  $\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A}$  are less than 1 in absolute value, *i.e.*, if and only if

$$\|\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A}\|_2 < 1$$

Another way of saying this is “the spectral radius of  $\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A}$  is less than 1.”

In fact, the *speed* of convergence is decided by the spectral radius of the matrix—convergence is faster for smaller values. Recall our introduction to iterative methods in the scalar case, where the result relied on  $\omega$  being chosen such that  $|1 - \omega A| < 1$ . You should now think about how eigenvalues generalize the absolute value of a scalar, and how this relates to the norm of matrices.

Let  $\mathbf{y}$  be an eigenvector for  $\mathbf{Q}^{-1}\mathbf{A}$ , with corresponding eigenvalue  $\lambda$ . Then

$$(\mathbf{I} - \omega\mathbf{Q}^{-1}\mathbf{A})\mathbf{y} = \mathbf{y} - \omega\mathbf{Q}^{-1}\mathbf{A}\mathbf{y} = \mathbf{y} - \omega\lambda\mathbf{y} = (1 - \omega\lambda)\mathbf{y}.$$

This relation may allow us to pick the optimal  $\omega$  for given  $\mathbf{A}, \mathbf{Q}$ . It can also show us that sometimes no choice of  $\omega$  will give convergence of the method. There are a number of different related results that show when various methods will work for certain choices of  $\omega$ . We leave these to the exercises.

**Example Problem 3.9.** Find conditions on  $\omega$  which guarantee convergence of Richardson's Iteration for finding approximate iterative solutions to the system  $\mathbf{Ax} = \mathbf{b}$ , where

$$\mathbf{A} = \begin{bmatrix} 6 & 1 & 1 \\ 2 & 4 & 0 \\ 1 & 2 & 6 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 12 \\ 0 \\ 6 \end{bmatrix}.$$

*Solution:* By Theorem 3.8, with  $\mathbf{Q}$  the identity matrix, we have convergence if and only if

$$\|I - \omega\mathbf{A}\|_2 < 1$$

We now use the fact that “eigenvalues commute with polynomials;” that is if  $f(x)$  is a polynomial and  $\lambda$  is an eigenvalue of a matrix  $\mathbf{A}$ , then  $f(\lambda)$  is an eigenvalue of the matrix  $f(\mathbf{A})$ . In this case the polynomial we consider is  $f(x) = x^0 - \omega x^1$ . Using octave or Matlab you will find that the eigenvalues of  $\mathbf{A}$  are approximately 7.7321, 4.2679, and 4. Thus the eigenvalues of  $I - \omega\mathbf{A}$  are approximately

$$1 - 7.7321\omega, 1 - 4.2679\omega, 1 - 4\omega.$$

With some work it can be shown that all three of these values will be less than one in absolute value if and only if

$$0 < \omega < \frac{3}{7.7321} \approx 0.388$$

(See also Exercise (3.10).)

Compare this to the results of Example Problem 3.4, where for this system,  $\omega = 1$  apparently did not lead to convergence, while for Example Problem 3.5, with  $\omega = 1/6$ , convergence was observed.

–

### 3.4.8 A Free Lunch?

The analysis leading to Theorem 3.8 leads to an interesting possible variant of the iterative scheme. For simplicity we will only consider an alteration of Richardson's Iteration. In the altered algorithm we presuppose the existence, via some oracle, of a sequence of weightings,  $\omega_i$ , which we use in each iterative update. Thus our algorithm becomes:

1. Select some initial iterate  $\mathbf{x}^{(0)}$ .
2. Given iterate  $\mathbf{x}^{(k-1)}$ , define

$$\mathbf{x}^{(k)} = (I - \omega_k\mathbf{A})\mathbf{x}^{(k-1)} + \omega_k\mathbf{b}.$$

Following the analysis for Theorem 3.8, it can be shown that

$$\mathbf{e}^{(k)} = (I - \omega_k\mathbf{A})\mathbf{e}^{(k-1)}$$

where, again,  $\mathbf{e}^{(k)} = \mathbf{x}^{(k)} - \mathbf{x}$ , with  $\mathbf{x}$  the actual solution to the linear system. Expanding  $\mathbf{e}^{(k-1)}$  similarly gives

$$\begin{aligned} \mathbf{e}^{(k)} &= (I - \omega_k\mathbf{A})(I - \omega_{k-1}\mathbf{A})\mathbf{e}^{(k-2)} \\ &= \left( \prod_{i=1}^k I - \omega_i\mathbf{A} \right) \mathbf{e}^{(0)}. \end{aligned}$$

Remember that we want  $e^{(k)}$  to be small in magnitude, or, better yet, to be zero. One way to guarantee that  $e^{(k)}$  is zero, regardless of the choice of  $e^{(0)}$  is to somehow ensure that the matrix

$$B = \prod_{i=1}^k I - \omega_i A$$

has all zero eigenvalues.

We again make use of the fact that eigenvalues “commute” with polynomials to claim that if  $\lambda_j$  is an eigenvalue of  $A$ , then

$$\prod_{i=1}^k 1 - \omega_i \lambda_j$$

is an eigenvalue of  $B$ . This eigenvalue is zero if one of the  $\omega_i$  for  $1 \leq i \leq k$  is  $1/\lambda_j$ . This suggests how we are to pick the weightings: let them be the inverses of the eigenvalues of  $A$ .

In fact, if  $A$  has a small number of distinct eigenvalues, say  $m$  eigenvalues, then convergence to the exact solution could be guaranteed after only  $m$  iterations, regardless of the *size* of the matrix.

As you may have guessed from the title of this subsection, this is not exactly a practical algorithm. The problem is that it is not simple to find, for a given arbitrary matrix  $A$ , one, some, or all its eigenvalues. This problem is of sufficient complexity to outweigh any savings to be gotten from our “free lunch” algorithm.

However, in some limited situations this algorithm might be practical if the eigenvalues of  $A$  are known *a priori*.

## EXERCISES

(3.1) Find the LU decomposition of the following matrices, using naïve Gaussian Elimination

$$(a) \begin{bmatrix} 3 & -1 & -2 \\ 9 & -1 & -4 \\ -6 & 10 & 13 \end{bmatrix} \quad (b) \begin{bmatrix} 8 & 24 & 16 \\ 1 & 12 & 11 \\ 4 & 13 & 19 \end{bmatrix} \quad (c) \begin{bmatrix} -3 & 6 & 0 \\ 1 & -2 & 0 \\ -4 & 5 & -8 \end{bmatrix}$$

(3.2) Perform back substitution to solve the equation

$$\begin{bmatrix} 1 & 3 & 5 & 3 \\ 0 & 2 & 4 & 3 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 0 & 2 \end{bmatrix} \mathbf{x} = \begin{bmatrix} -1 \\ -1 \\ 1 \\ 2 \end{bmatrix}$$

(3.3) Perform Naïve Gaussian Elimination to prove Cramer's rule for the 2D case. That is, prove that the solution to

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

is given by

$$y = \frac{\det \begin{bmatrix} a & f \\ c & g \end{bmatrix}}{\det \begin{bmatrix} a & b \\ c & d \end{bmatrix}} \quad \text{and} \quad x = \frac{\det \begin{bmatrix} f & b \\ g & d \end{bmatrix}}{\det \begin{bmatrix} a & b \\ c & d \end{bmatrix}}$$

(3.4) Implement Cramer's rule to solve a pair of linear equations in 2 variables. Your m-file should have header line like:

```
function x = cramer2(A,b)
```

where  $\mathbf{A}$  is a  $2 \times 2$  matrix, and  $\mathbf{b}$  and  $\mathbf{x}$  are  $2 \times 1$  vectors. Your code should find the  $\mathbf{x}$  such that  $\mathbf{Ax} = \mathbf{b}$ . (See Exercise (3.3))

Test your code on the following (augmented) systems:

$$(a) \left( \begin{array}{cc|c} 3 & -2 & 1 \\ 4 & -3 & -1 \end{array} \right) \quad (b) \left( \begin{array}{cc|c} 1.24 & -3.48 & 1 \\ -0.744 & 2.088 & 2 \end{array} \right) \quad (c) \left( \begin{array}{cc|c} 1.24 & -3.48 & 1 \\ -0.744 & 2.088 & -0.6 \end{array} \right)$$

$$(d) \left( \begin{array}{cc|c} -0.0590 & 0.2372 & -0.3528 \\ 0.1080 & -0.4348 & 0.6452 \end{array} \right)$$

(3.5) Given two lines parametrized by  $\mathbf{f}(t) = \mathbf{at} + \mathbf{b}$ , and  $\mathbf{g}(s) = \mathbf{cs} + \mathbf{d}$ , set up a linear  $2 \times 2$  system of equations to find the  $t, s$  at the point of intersection of the two lines. If you were going to write a program to detect the intersection of two lines, how would you detect whether they are parallel? How is this related to the form of the solution to a system of two linear equations? (See Exercise (3.3))

(3.6) Prove that the inverse of the matrix

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ a_2 & 1 & 0 & \cdots & 0 \\ a_3 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_n & 0 & 0 & \cdots & 1 \end{bmatrix}$$

is the matrix

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -a_2 & 1 & 0 & \cdots & 0 \\ -a_3 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -a_n & 0 & 0 & \cdots & 1 \end{bmatrix}$$

(Hint: Multiply them together.)

- (3.7) Under the strategy of scaled partial pivoting, which row of the following matrix will be the first pivot row?

$$\begin{bmatrix} 10 & 17 & -10 & 0.1 & 0.9 \\ -3 & 3 & -3 & 0.3 & -4 \\ 0.3 & 0.1 & 0.01 & -1 & 0.5 \\ 2 & 3 & 4 & -3 & 5 \\ 10 & 100 & 1 & 0.1 & 0 \end{bmatrix}$$

- (3.8) Let  $\mathbf{A}$  be a symmetric positive definite  $n \times n$  matrix with  $n$  distinct eigenvalues. Letting  $\mathbf{y}^{(0)} = \mathbf{b} / \|\mathbf{b}\|_2$ , consider the iteration

$$\mathbf{y}^{(k+1)} = \frac{\mathbf{A}\mathbf{y}^{(k)}}{\|\mathbf{A}\mathbf{y}^{(k)}\|_2}.$$

- (a) What is  $\|\mathbf{y}^{(k)}\|_2$ ?  
 (b) Show that  $\mathbf{y}^{(k)} = \mathbf{A}^k \mathbf{b} / \|\mathbf{A}^k \mathbf{b}\|_2$ .  
 (c) Show that as  $k \rightarrow \infty$ ,  $\mathbf{y}^{(k)}$  converges to the (normalized) eigenvector associated with the largest eigenvalue of  $\mathbf{A}$ .
- (3.9) Consider the equation

$$\begin{bmatrix} 1 & 3 & 5 \\ -2 & 2 & 4 \\ 4 & -3 & -4 \end{bmatrix} \mathbf{x} = \begin{bmatrix} -5 \\ -6 \\ 10 \end{bmatrix}$$

Letting  $\mathbf{x}^{(0)} = [1 \ 1 \ 0]^T$ , find the iterate  $\mathbf{x}^{(1)}$  by one step of Richardson's Method. And by one step of Jacobi Iteration. And by Gauss Seidel.

- (3.10) Let  $\mathbf{A}$  be a symmetric  $n \times n$  matrix with eigenvalues in the interval  $[\alpha, \beta]$ , with  $0 < \alpha \leq \beta$ , and  $\alpha + \beta \neq 0$ . Consider Richardson's Iteration

$$\mathbf{x}^{(k+1)} = (\mathbf{I} - \omega \mathbf{A}) \mathbf{x}^{(k)} + \omega \mathbf{b}.$$

Recall that  $\mathbf{e}^{(k+1)} = (\mathbf{I} - \omega \mathbf{A}) \mathbf{e}^{(k)}$ .

- (a) Show that the eigenvalues of  $\mathbf{I} - \omega \mathbf{A}$  are in the interval  $[1 - \omega\beta, 1 - \omega\alpha]$ .  
 (b) Prove that

$$\max \{ |\lambda| : 1 - \omega\beta \leq \lambda \leq 1 - \omega\alpha \}$$

is minimized when we choose  $\omega$  such that  $1 - \omega\beta = -(1 - \omega\alpha)$ . (Hint: It may help to look at the graph of something versus  $\omega$ .)

- (c) Show that this relationship is satisfied by  $\omega = 2 / (\alpha + \beta)$ .  
 (d) For this choice of  $\omega$  show that the spectral radius of  $\mathbf{I} - \omega \mathbf{A}$  is

$$\frac{|\alpha - \beta|}{|\alpha + \beta|}.$$

- (e) Show that when  $0 < \alpha$ , this quantity is always smaller than 1.
- (f) Prove that if  $\mathbf{A}$  is positive definite, then there is an  $\omega$  such that Richardson's Iteration with this  $\omega$  will converge for any choice of  $\mathbf{x}^{(0)}$ .
- (g) For which matrix do you expect faster convergence of Richardson's Iteration:  $\mathbf{A}_1$  with eigenvalues in  $[10, 20]$  or  $\mathbf{A}_2$  with eigenvalues in  $[1010, 1020]$ ? Why?
- (3.11) Implement Richardson's Iteration to solve the system  $\mathbf{Ax} = \mathbf{b}$ . Your m-file should have header line like:

```
function xk = richardsons(A,b,x0,w,k)
```

Your code should return  $\mathbf{x}^{(k)}$  based on the iteration

$$\mathbf{x}^{(j+1)} = \mathbf{x}^{(j)} - \omega (\mathbf{Ax}^{(j)} - \mathbf{b}).$$

Let  $\mathbf{w}$  take the place of  $\omega$ , and let  $\mathbf{x0}$  be the initial iterate  $\mathbf{x}^{(0)}$ . Test your code for  $\mathbf{A}, \mathbf{b}$  for which you know the actual solution to the problem. (*Hint*: Start with  $\mathbf{A}$  and the solution  $\mathbf{x}$  and generate  $\mathbf{b}$ .) Test your code on the following matrices:

- Let  $\mathbf{A}$  be the *Hilbert Matrix*. This is generated by the octave command  $\mathbf{A} = \text{hilb}(10)$ , or whatever (smallish) integer. Try different values of  $\omega$ , including  $\omega = 1$ .
- Let  $\mathbf{A}$  be a *Toeplitz* matrix of the form:

$$\mathbf{A} = \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -2 \end{bmatrix}$$

These can be generated by the octave command  $\mathbf{A} = \text{toeplitz}([-2 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0])$ . Try different values of  $\omega$ , including  $\omega = -1/2$ .

- (3.12) Let  $\mathbf{A}$  be a nonsingular  $n \times n$  matrix. We wish to solve  $\mathbf{Ax} = \mathbf{b}$ . Let  $\mathbf{x}^{(0)}$  be some starting vector, let  $\mathcal{D}_k$  be  $\text{span}\{\mathbf{r}^{(0)}, \mathbf{Ar}^{(0)}, \dots, \mathbf{A}^k \mathbf{r}^{(0)}\}$ , and let  $\mathcal{P}_k$  be the set of polynomials,  $p(x)$  of degree  $k$  with  $p(0) = 1$ . Consider the following iterative method: Let  $\mathbf{x}^{(k+1)}$  be the  $\mathbf{x}$  that solves

$$\min_{\mathbf{x} \in \mathbf{x}^{(0)} + \mathcal{D}_k} \|\mathbf{b} - \mathbf{Ax}\|_2.$$

Let  $\mathbf{r}^{(k)} = \mathbf{b} - \mathbf{Ax}^{(k)}$ .

- (a) Show that if  $\mathbf{x} \in \mathbf{x}^{(0)} + \mathcal{D}_k$ , then  $\mathbf{b} - \mathbf{Ax} = p(\mathbf{A})\mathbf{r}^{(0)}$  for some  $p \in \mathcal{P}_k$ .
- (b) Prove that, conversely, for any  $p \in \mathcal{P}_k$  there is some  $\mathbf{x} \in \mathbf{x}^{(0)} + \mathcal{D}_k$ , such that  $\mathbf{b} - \mathbf{Ax} = p(\mathbf{A})\mathbf{r}^{(0)}$ .
- (c) Argue that

$$\|\mathbf{r}^{(k+1)}\|_2 = \min_{p \in \mathcal{P}_k} \|p(\mathbf{A})\mathbf{r}^{(0)}\|_2.$$

- (d) Prove that this iteration converges in at most  $n$  steps. (*Hint*: Argue for the existence of a polynomial in  $\mathcal{P}_n$  that vanishes at all the eigenvalues of  $\mathbf{A}$ . Use this polynomial to show that  $\|\mathbf{r}^{(n)}\|_2 \leq 0$ .)



# Chapter 4

## Finding Roots

### 4.1 Bisection

We are now concerned with the problem of finding a zero for the function  $f(x)$ , *i.e.*, some  $c$  such that  $f(c) = 0$ .

The simplest method is that of bisection. The following theorem, from calculus class, insures the success of the method

**Theorem 4.1 (Intermediate Value Theorem).** If  $f(x)$  is continuous on  $[a, b]$  then for any  $y$  such that  $y$  is between  $f(a)$  and  $f(b)$  there is a  $c \in [a, b]$  such that  $f(c) = y$ .

The IVT is best illustrated graphically. Note that continuity is really a requirement here—a single point of discontinuity could ruin your whole day, as the following example illustrates.

**Example 4.2.** The function  $f(x) = \frac{1}{x}$  is not continuous at 0. Thus if  $0 \in [a, b]$ , we *cannot* apply the IVT. In particular, if  $0 \in [a, b]$  it happens to be the case that for *every*  $y$  between  $f(a), f(b)$  there is no  $c \in [a, b]$  such that  $f(c) = y$ .

In particular, the IVT tells us that if  $f(x)$  is continuous and we know  $a, b$  such that  $f(a), f(b)$  have different sign, then there is some root in  $[a, b]$ . A decent estimate of the root is  $c = \frac{a+b}{2}$ . We can check whether  $f(c) = 0$ . If this does not hold then one and only one of the two following options holds:

1.  $f(a), f(c)$  have different signs.
2.  $f(c), f(b)$  have different signs.

We now choose to recursively apply bisection to either  $[a, c]$  or  $[c, b]$ , respectively, depending on which of these two options hold.

#### 4.1.1 Modifications

Unfortunately, it is impossible for a computer to test whether a given black box function is continuous. Thus malicious or incompetent users could cause a naïvely implemented bisection algorithm to fail. There are a number of easily conceivable problems:

1. The user might give  $f, a, b$  such that  $f(a), f(b)$  have the same sign. In this case the function  $f$  might be legitimately continuous, and might have a root in the interval  $[a, b]$ . If, taking  $c = \frac{a+b}{2}$ ,  $f(a), f(b), f(c)$  all have the same sign, the algorithm would be at an impasse. We should perform a “sanity check” on the input to make sure  $f(a), f(b)$  have different signs.

2. The user might give  $f, a, b$  such that  $f$  is not continuous on  $[a, b]$ , moreover has no root in the interval  $[a, b]$ . For a poorly implemented algorithm, this might lead to an infinite search on smaller and smaller intervals about some discontinuity of  $f$ . In fact, the algorithm might descend to intervals as small as machine precision, in which case the midpoint of the interval will, due to rounding, be the same as one of the endpoints, resulting in an infinite recursion.
3. The user might give  $f$  such that  $f$  has no root  $c$  that is representable in the computer's memory. Recall that we think of computers as storing numbers in the form  $\pm r \times 10^k$ ; given a finite number of bits to represent a number, only a finite number of such numbers can be represented. It may legitimately be the case that none of them is a root to  $f$ . In this case, the behaviour of the algorithm may be like that of the previous case. A well implemented version of bisection should check the length of its input interval, and give up if the length is too small, compared to machine precision.

Another common error occurs in the testing of the signs of  $f(a), f(b)$ . A slick programmer might try to implement this test in the pseudocode:

```
if (f(a)f(b) > 0) then ...
```

Note however, that  $|f(a)|, |f(b)|$  might be very small, and that  $f(a)f(b)$  might be too small to be representable in the computer; this calculation would be rounded to zero, and unpredictable behaviour would ensue. A wiser choice is

```
if (sign(f(a)) * sign(f(b)) > 0) then ...
```

where the function  $\text{sign}(x)$  returns  $-1, 0, 1$  depending on whether  $x$  is negative, zero, or positive, respectively.

The pseudocode bisection algorithm is given as Algorithm 1.

### 4.1.2 Convergence

We can see that each time `recursive_bisection`( $f, a, b, \dots$ ) is called that  $|b - a|$  is half the length of the interval in the previous call. Formally call the first interval  $[a_0, b_0]$ , and the first midpoint  $c_0$ . Let the second interval be  $[a_1, b_1]$ , etc. Note that one of  $a_1, b_1$  will be  $c_0$ , and the other will be either  $a_0$  or  $b_0$ . We are claiming that

$$\begin{aligned} b_n - a_n &= \frac{b_{n-1} - a_{n-1}}{2} \\ &= \frac{b_0 - a_0}{2^n} \end{aligned}$$

**Theorem 4.3 (Bisection Method Theorem).** If  $f(x)$  is a continuous function on  $[a, b]$  such that  $f(a)f(b) < 0$ , then after  $n$  steps, the algorithm `run_bisection` will return  $c$  such that  $|c - c'| \leq \frac{|b-a|}{2^n}$ , where  $c'$  is some root of  $f$ .

## 4.2 Newton's Method

Newton's method is an *iterative* method for root finding. That is, starting from some guess at the root,  $x_0$ , one iteration of the algorithm produces a number  $x_1$ , which is supposed to be closer to a root; guesses  $x_2, x_3, \dots, x_n$  follow identically.

Newton's method uses "linearization" to find an approximate root. Recalling Taylor's Theorem, we know that

$$f(x+h) \approx f(x) + f'(x)h.$$

**Algorithm 1:** Algorithm for finding root by bisection.

**Input:** a function, two endpoints, a  $x$ -tolerance, and a  $y$ -tolerance

**Output:** a  $c$  such that  $|f(c)|$  is smaller than the  $y$ -tolerance.

```

RUN_BISECTION( $f, a, b, \delta, \epsilon$ )
(1)  Let  $fa \leftarrow \text{sign}(f(a))$ .
(2)  Let  $fb \leftarrow \text{sign}(f(b))$ .
(3)  if  $fab > 0$ 
(4)    throw an error.
(5)  else if  $fab = 0$ 
(6)    if  $fa = 0$ 
(7)      return  $a$ 
(8)    else
(9)      return  $b$ 
(10) Let  $c \leftarrow \frac{a+b}{2}$ 
(11) while  $b - a > 2\delta$ 
(12)   Let  $fc \leftarrow f(c)$ .
(13)   if  $|fc| < \epsilon$ 
(14)     return  $c$ 
(15)   if  $\text{sign}(fa)\text{sign}(fc) < 0$ 
(16)     Let  $b \leftarrow c, fb \leftarrow fc, c \leftarrow \frac{a+c}{2}$ .
(17)   else
(18)     Let  $a \leftarrow c, fa \leftarrow fc, c \leftarrow \frac{c+b}{2}$ .
(19) return  $c$ 

```

This approximation is better when  $f''(\cdot)$  is “well-behaved” between  $x$  and  $x + h$ . Newton’s method attempts to find some  $h$  such that

$$0 = f(x + h) = f(x) + f'(x)h.$$

This is easily solved as

$$h = \frac{-f(x)}{f'(x)}.$$

An iteration of Newton’s method, then, takes some guess  $x_k$  and returns  $x_{k+1}$  defined by

$$\boxed{x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}}. \quad (4.1)$$

An iteration of Newton’s method is shown in Figure 4.1, along with the linearization of  $f(x)$  at  $x_k$ .

### 4.2.1 Implementation

Use of Newton’s method requires that the function  $f(x)$  be differentiable. Moreover, the derivative of the function must be known. This may preclude Newton’s method from being used when  $f(x)$  is a black box. As is the case for the bisection method, our algorithm cannot explicitly check for continuity of  $f(x)$ . Moreover, the success of Newton’s method is dependent on the initial guess  $x_0$ . This was also the case with bisection, but for bisection there was an easy test of the initial interval—*i.e.*, test if  $f(a_0)f(b_0) < 0$ .

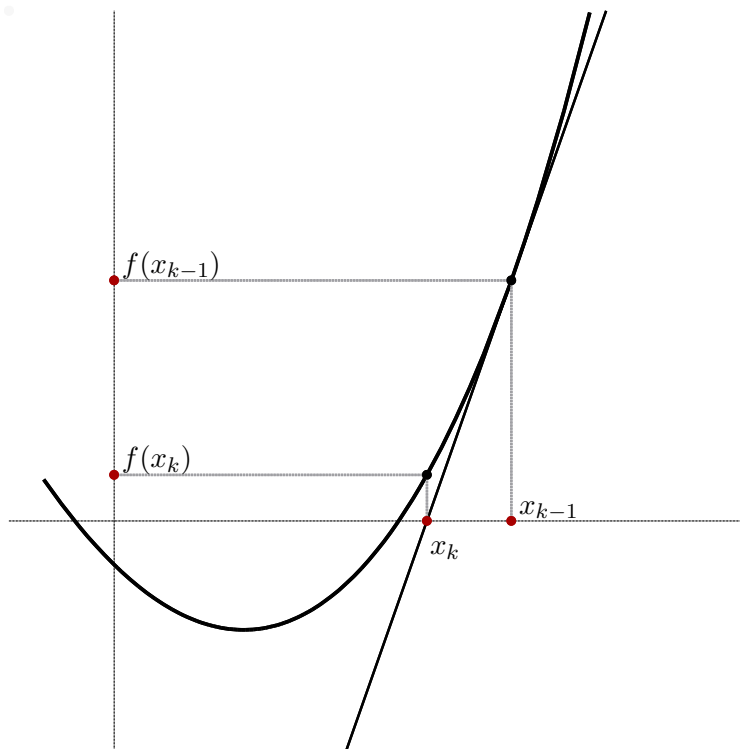


Figure 4.1: One iteration of Newton's method is shown for a quadratic function  $f(x)$ . The linearization of  $f(x)$  at  $x_k$  is shown. It is clear that  $x_{k+1}$  is a root of the linearization. It happens to be the case that  $|f(x_{k+1})|$  is smaller than  $|f(x_k)|$ , *i.e.*,  $x_{k+1}$  is a better guess than  $x_k$ .

Our algorithm will test for goodness of the estimate by looking at  $|f(x_k)|$ . The algorithm will also test for near-zero derivative. Note that if it were the case that  $f'(x_k) = 0$  then  $h$  would be ill defined.

**Algorithm 2:** Algorithm for finding root by Newton's Method.

**Input:** a function, its derivative, an initial guess, an iteration limit, and a tolerance

**Output:** a point for which the function has small value.

RUN\_NEWTON( $f, f', x_0, N, tol$ )

- (1) Let  $x \leftarrow x_0, n \leftarrow 0$ .
- (2) **while**  $n \leq N$
- (3)     Let  $fx \leftarrow f(x)$ .
- (4)     **if**  $|fx| < tol$
- (5)         **return**  $x$ .
- (6)     Let  $fp_x \leftarrow f'(x)$ .
- (7)     **if**  $|fp_x| < tol$
- (8)         Warn " $f'(x)$  is small; giving up."
- (9)     **return**  $x$ .
- (10)    Let  $x \leftarrow x - fx/fp_x$ .
- (11)    Let  $n \leftarrow n + 1$ .

### 4.2.2 Problems

As mentioned above, convergence is dependent on  $f(x)$ , and the initial estimate  $x_0$ . A number of conceivable problems might come up. We illustrate them here.

**Example 4.4.** Consider Newton's method applied to the function  $f(x) = x^j$  with  $j > 1$ , and with initial estimate  $x_0 \neq 0$ .

Note that  $f(x) = 0$  has the single root  $x = 0$ . Now note that

$$x_{k+1} = x_k - \frac{x_k^j}{jx_k^{j-1}} = \left(1 - \frac{1}{j}\right)x_k.$$

Since the equation has the single root  $x = 0$ , we find that  $x_k$  is converging to the root. However, it is converging at a rate slower than we expect from Newton's method: at each step we have a constant decrease of  $1 - (1/j)$ , which is a larger number (and thus worse decrease) when  $j$  is larger.

**Example 4.5.** Consider Newton's method applied to the function  $f(x) = \frac{\ln x}{x}$ , with initial estimate  $x_0 = 3$ .

Note that  $f(x)$  is continuous on  $\mathbb{R}^+$ . It has a single root at  $x = 1$ . Our initial guess is not too far from this root. However, consider the derivative:

$$f'(x) = \frac{x^{\frac{1}{x}} - \ln x}{x^2} = \frac{1 - \ln x}{x^2}$$

If  $x > e^1$ , then  $1 - \ln x < 0$ , and so  $f'(x) < 0$ . However, for  $x > 1$ , we know  $f(x) > 0$ . Thus taking

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} > x_k.$$

The estimates will "run away" from the root  $x = 1$ .

**Example 4.6.** Consider Newton's method applied to the function  $f(x) = \sin(x)$  for the initial estimate  $x_0 \neq 0$ , where  $x_0$  has the odious property  $2x_0 = \tan x_0$ .

You should verify that there are an infinite number of such  $x_0$ . Consider the identity of  $x_1$ :

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = x_0 - \frac{\sin(x_0)}{\cos(x_0)} = x_0 - \tan x_0 = x_0 - 2x_0 = -x_0.$$

Now consider  $x_2$ :

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = -x_0 - \frac{\sin(-x_0)}{\cos(-x_0)} - x_0 + \frac{\sin(x_0)}{\cos(x_0)} = -x_0 + \tan x_0 = -x_0 + 2x_0 = x_0.$$

Thus Newton's method "cycles" between the two values  $x_0, -x_0$ .

Of course, Newton's method may find some iterate  $x_k$  for which  $f'(x_k) = 0$ , in which case, there is no well-defined  $x_{k+1}$ .

### 4.2.3 Convergence

When Newton's Method converges, it actually displays *quadratic convergence*. That is, if  $e_k = x_k - r$ , where  $r$  is the root that the  $x_k$  are converging to, that  $|e_{k+1}| \leq C|e_k|^2$ . If, for example, it were the case that  $C = 1$ , then we would double the accuracy of our root estimate with each iterate. That is, if  $e_0$  were 0.001, we would expect  $e_1$  to be on the order of 0.000001. The following theorem formalizes our claim:

**Theorem 4.7 (Newton’s Method Convergence).** If  $f(x)$  has two continuous derivatives, and  $r$  is a simple root of  $f(x)$ , then there is some  $D$  such that if  $|x_0 - r| < D$ , Newton’s method will converge quadratically to  $r$ .

The proof is based on arguments from real analysis, and is omitted; see Cheney & Kincaid for the proof [7]. Take note of the following, though:

1. The proof requires that  $r$  be a simple root, that is that  $f'(r) \neq 0$ . When this does not hold we may get only linear convergence, as in Example 4.4.
2. The key to the proof is using Taylor’s theorem, and the definition of Newton’s method to show that

$$e_{k+1} = \frac{-f''(\xi_k)e_k^2}{2f'(x_k)},$$

where  $\xi_k$  is between  $x_k$  and  $r = x_k + e_k$ .

The proof then proceeds by showing that there is some region about  $r$  such that

- (a) in this region  $|f''(x)|$  is not too large and  $|f'(x)|$  is not too small, and
- (b) if  $x_k$  is in the region, then  $x_{k+1}$  is in the region.

In particular the region is chosen to be so small that if  $x_k$  is in the region, then the factor  $e_k^2$  will outweigh the factor  $|f''(\xi_k)|/2|f'(x_k)|$ . You can roughly think of this region as an “attractor” region for the root.

3. The theorem never guarantees that some  $x_k$  will fall into the “attractor” region of a root  $r$  of the function, as in Example 4.5 and Example 4.6. The theorem that follows gives sufficient conditions for convergence to a particular root.

**Theorem 4.8 (Newton’s Method Convergence II [2]).** If  $f(x)$  has two continuous derivatives on  $[a, b]$ , and

1.  $f(a)f(b) < 0$ ,
2.  $f'(x) \neq 0$  on  $[a, b]$ ,
3.  $f''(x)$  does not change sign on  $[a, b]$ ,
4. Both  $|f(a)| \leq (b - a)|f'(a)|$  and  $|f(b)| \leq (b - a)|f'(b)|$  hold,

then Newton’s method converges to the unique root of  $f(x) = 0$  for any choice of  $x_0 \in [a, b]$ .

#### 4.2.4 Using Newton’s Method

Newton’s Method can be used to program more complex functions using only simple functions. Suppose you had a computer which could perform addition, subtraction, multiplication, division, and storing and retrieving numbers, and it was your task to write a subroutine to compute some complex function  $g(\cdot)$ . One way of solving this problem is to have your subroutine use Newton’s Method to solve some equation equivalent to  $g(z) - x = 0$ , where  $z$  is the input to the subroutine. Note that it is assumed the subroutine cannot evaluate  $g(z)$  directly, so this equation needs to be modified to satisfy the computer’s constraints.

Quite often when dealing with problems of this type, students make the mistake of using Newton’s Method to try to solve a linear equation. This should be an indication that a mistake was made, since Newton’s Method can solve a linear equation in a single step:

**Example 4.9.** Consider Newton’s method applied to the function  $f(x) = ax + b$ . The iteration is given as

$$x_{k+1} \leftarrow x_k - \frac{ax_k + b}{a}.$$

This can be rewritten simply as  $x_{k+1} \leftarrow -b/a$ .

The following example problems should illustrate this process of “bootstrapping” via Newton’s Method.

**Example Problem 4.10.** Devise a subroutine using only subtraction and multiplication that can find the multiplicative inverse of an input number  $z$ , *i.e.*, can find  $(1/z)$ .

*Solution:* We are tempted to use the linear function  $f(x) = (1/z) - x$ . But this is a linear equation for which Newton’s Method would reduce to  $x_{k+1} \leftarrow (1/z)$ . Since the subroutine can only use subtraction and multiplication, this will not work.

Instead apply Newton’s Method to  $f(x) = z - (1/x)$ . The Newton step is

$$x_{k+1} \leftarrow x_k - \frac{z - (1/x_k)}{(1/x_k^2)} = x_k - zx_k^2 + x_k = x_k(2 - zx_k).$$

Note this step uses only multiplication and subtraction. The subroutine is given in Algorithm 3. +

**Algorithm 3:** Algorithm for finding a multiplicative inverse using simple operations.

**Input:** a number

**Output:** its multiplicative inverse

INVS( $z$ )

- (1) if  $z = 0$  throw an error.
- (2) Let  $x \leftarrow \text{sign}(z)$ ,  $n \leftarrow 0$ .
- (3) **while**  $n \leq 50$
- (4)     Let  $x \leftarrow x(2 - zx)$ .
- (5)     Let  $n \leftarrow n + 1$ .

**Example Problem 4.11.** Devise a subroutine using only simple operations which computes the square root of an input number  $z$ .

*Solution:* The temptation is to find a zero for  $f(x) = \sqrt{z} - x$ . However, this equation is linear in  $x$ . Instead let  $f(x) = z - x^2$ . You can easily see that if  $x$  is a positive root of  $f(x) = 0$ , then  $x = \sqrt{z}$ . The Newton step becomes

$$x_{k+1} \leftarrow x_k - \frac{z - x_k^2}{-2x_k}.$$

after some simplification this becomes

$$x_{k+1} \leftarrow \frac{x_k}{2} + \frac{z}{2x_k}.$$

Note this relies only on addition, multiplication and division.

The final subroutine is given in Algorithm 4. +

### 4.3 Secant Method

The secant method for root finding is roughly based on Newton’s method; however, it is not assumed that the derivative of the function is known, rather the derivative is approximated by the value of the function at some of the iterates,  $x_k$ . More specifically, the slope of the *tangent*

**Algorithm 4:** Algorithm for finding a square root using simple operations.

**Input:** a number

**Output:** its square root

SQRT( $z$ )

- (1) if  $z < 0$  throw an error.
- (2) Let  $x \leftarrow 1, n \leftarrow 0$ .
- (3) **while**  $n \leq 50$
- (4)     Let  $x \leftarrow (x + z/x) / 2$ .
- (5)     Let  $n \leftarrow n + 1$ .

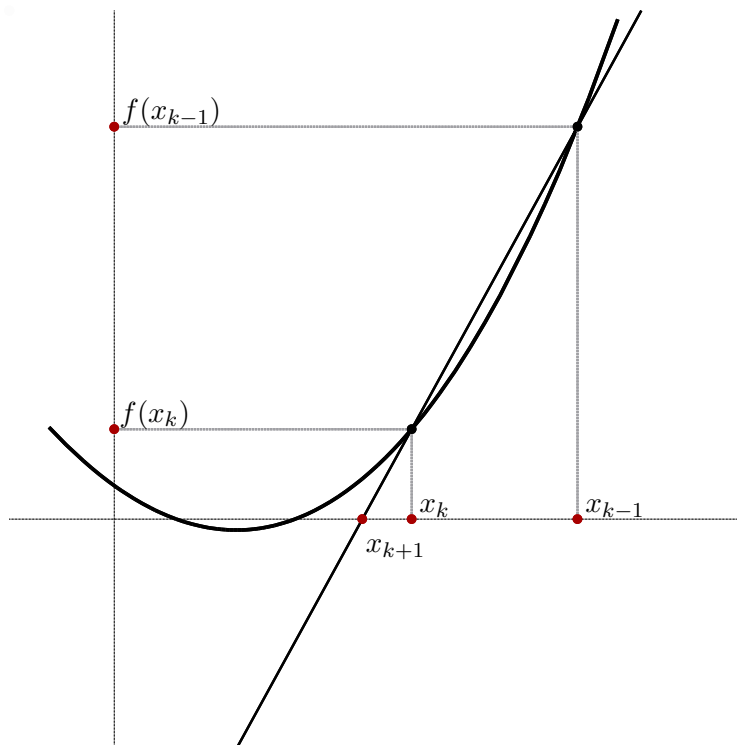


Figure 4.2: One iteration of the Secant method is shown for some quadratic function  $f(x)$ . The secant line through  $(x_{k-1}, f(x_{k-1}))$  and  $(x_k, f(x_k))$  is shown. It happens to be the case that  $|f(x_{k+1})|$  is smaller than  $|f(x_k)|$ , *i.e.*,  $x_{k+1}$  is a better guess than  $x_k$ .

line at  $(x_k, f(x_k))$ , which is  $f'(x_k)$  is approximated by the slope of the *secant* line passing through  $(x_{k-1}, f(x_{k-1}))$  and  $(x_k, f(x_k))$ , which is

$$\frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$

Thus the iterate  $x_{k+1}$  is the root of this secant line. That is, it is a root to the equation

$$\frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} (x - x_k) = y - f(x_k).$$



Since the root has a  $y$  value of 0, we have

$$\begin{aligned} \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} (x_{k+1} - x_k) &= -f(x_k), \\ x_{k+1} - x_k &= - \left( \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} \right) f(x_k), \\ x_{k+1} &= x_k - \left( \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} \right) f(x_k). \end{aligned} \quad (4.2)$$

You will note this is the recurrence of Newton's method, but with the slope  $f'(x_k)$  substituted by the slope of the secant line. Note also that the secant method requires two initial guesses,  $x_0, x_1$ , but can be used on a black box function. The secant method can suffer from some of the same problems that Newton's method does, as we will see.

An iteration of the secant method is shown in Figure 4.2, along with the secant line.

**Example 4.12.** Consider the secant method used on  $x^3 + x^2 - x - 1$ , with  $x_0 = 2, x_1 = \frac{1}{2}$ . Note that this function is continuous and has roots  $\pm 1$ . We give the iterates here:

$k$	$x_k$	$f(x_k)$
0	2	9
1	0.5	-1.125
2	0.666666666666667	-0.925925925925926
3	1.44186046511628	2.63467367653163
4	0.868254072087394	-0.459842466254495
5	0.953491494113659	-0.177482458876898
6	1.00706900811804	0.0284762692197613
7	0.999661272951803	-0.0013544492875992
8	0.999997617569723	$-9.52969840528617 \times 10^{-06}$
9	1.0000000008072	$3.22880033820638 \times 10^{-09}$
10	0.999999999999998	$-7.43849426498855 \times 10^{-15}$

### 4.3.1 Problems

As with Newton's method, convergence is dependent on  $f(x)$ , and the initial estimates  $x_0, x_1$ . We illustrate a few possible problems:

**Example 4.13.** Consider the secant method for the function  $f(x) = \frac{\ln x}{x}$ , with  $x_0 = 3, x_1 = 4$ . As with Newton's method, the iterates diverge towards infinity, looking for a nonexistent root. We

give some iterates here:

$k$	$x_k$	$f(x_k)$
0	3	0.366204096222703
1	4	0.346573590279973
2	21.6548475770851	0.142011128224341
3	33.9111765137635	0.103911011441661
4	67.3380435135758	0.0625163004418104
5	117.820919458675	0.0404780904944712
6	210.543986613847	0.0254089165873003
7	366.889164762149	0.0160949419231219
8	637.060241341843	0.010135406045582
9	1096.54125113444	0.00638363233543847
10	1878.34688714646	0.00401318169994875
11	3201.94672271613	0.0025208146648422
12	5437.69020766155	0.00158175793894727
13	9203.60222260594	0.000991714984152597
14	15533.1606791089	0.000621298692241343
15	26149.7196085218	0.000388975250950428
16	43924.8466075548	0.000243375589137882
17	73636.673898472	0.000152191807070607

**Example 4.14.** Consider Newton's method applied to the function  $f(x) = \frac{1}{1+x^2} - \frac{1}{17}$ , with initial estimates  $x_0 = -1, x_1 = 1$ .

You can easily verify that  $f(x_0) = f(x_1)$ , and thus the secant line is horizontal. And thus  $x_2$  is not defined.

**Algorithm 5:** Algorithm for finding root by secant method.

**Input:** a function, initial guesses, an iteration limit, and a tolerance

**Output:** a point for which the function has small value.

RUN\_SECANT( $f, x_0, x_1, N, tol$ )

- (1) Let  $x \leftarrow x_1, xp \leftarrow x_0, fh \leftarrow f(x_1), fp \leftarrow f(x_0), n \leftarrow 0$ .
- (2) **while**  $n \leq N$
- (3)     **if**  $|fh| < tol$
- (4)         **return**  $x$ .
- (5)     Let  $fp_x \leftarrow (fh - fp)/(x - xp)$ .
- (6)     **if**  $|fp_x| < tol$
- (7)         Warn "secant slope is too small; giving up."
- (8)         **return**  $x$ .
- (9)     Let  $xp \leftarrow x, fp \leftarrow fh$ .
- (10)     Let  $x \leftarrow x - fh/fp_x$ .
- (11)     Let  $fh \leftarrow f(x)$ .
- (12)     Let  $n \leftarrow n + 1$ .

### 4.3.2 Convergence

We consider convergence analysis as in Newton's method. We assume that  $r$  is a root of  $f(x)$ , and let  $e_n = r - x_n$ . Because the secant method involves two iterates, we assume that we will find some

relation between  $e_{k+1}$  and the previous two errors,  $e_k, e_{k-1}$ .

Indeed, this is the case. Omitting all the nasty details (see Cheney & Kincaid [7]), we arrive at the imprecise equation:

$$e_{k+1} \approx -\frac{f''(r)}{2f'(r)}e_k e_{k-1} = C e_k e_{k-1}.$$

Again, the proof relies on finding some “attractor” region and using continuity.

We now postulate that the error terms for the secant method follow some power law of the following type:

$$|e_{k+1}| \sim A |e_k|^\alpha.$$

Recall that this held true for Newton’s method, with  $\alpha = 2$ . We try to find the  $\alpha$  for the secant method. Note that

$$|e_k| = A |e_{k-1}|^\alpha,$$

so

$$|e_{k-1}| = A^{-\frac{1}{\alpha}} |e_k|^{\frac{1}{\alpha}}.$$

Then we have

$$A |e_k|^\alpha = |e_{k+1}| = C |e_k| |e_{k-1}| = C A^{-\frac{1}{\alpha}} |e_k|^{1+\frac{1}{\alpha}},$$

Since this equation is to hold for all  $e_k$ , we must have

$$\alpha = 1 + \frac{1}{\alpha}.$$

This is solved by  $\alpha = \frac{1}{2} (1 + \sqrt{5}) \approx 1.62$ . Thus we say that the secant method enjoys *superlinear* convergence; This is somewhere between the convergence rates for bisection and Newton’s method.

## EXERCISES

- (4.1) Consider the bisection method applied to find the zero of the function  $f(x) = x^2 - 5x + 3$ , with  $a_0 = 0, b_0 = 1$ . What are  $a_1, b_1$ ? What are  $a_2, b_2$  ?
- (4.2) Approximate  $\sqrt{10}$  by using two steps of Newton's method, with an initial estimate of  $x_0 = 3$ . (cf. Example Problem 4.11) Your answer should be correct to 5 decimal places.
- (4.3) Consider bisection for finding the root to  $\cos x = 0$ . Let the initial interval  $I_0$  be  $[0, 2]$ . What is the next interval considered, call it  $I_1$ ? What is  $I_2$ ?  $I_6$ ?
- (4.4) What does the sequence defined by

$$x_0 = 1, \quad x_{k+1} = \frac{1}{2}x_k + \frac{1}{x_k}$$

converge to?

- (4.5) Devise a subroutine using only simple operations that finds, via Newton's Method, the cubed root of some input number  $z$ .
- (4.6) Use Newton's Method to approximate  $\sqrt[3]{9}$ . Start with  $x_0 = 2$ . Find  $x_2$ .
- (4.7) Use Newton's Method to devise a sequence  $x_0, x_1, \dots$  such that  $x_k \rightarrow \ln 10$ . Is this a reasonable way to write a subroutine that, given  $z$ , computes  $\ln z$ ? (*Hint*: such a subroutine would require computation of  $e^{x_k}$ . Is this possible for rational  $x_k$  without using a logarithm? Is it practical?)
- (4.8) Give an example (graphical or analytic) of a function,  $f(x)$  for which Newton's Method:
- Does not find a root for some choices of  $x_0$ .
  - Finds a root for every choice of  $x_0$ .
  - Falls into a cycle for some choice of  $x_0$ .
  - Converges slowly to the zero of  $f(x)$ .
- (4.9) How will Newton's Method perform for finding the root to  $f(x) = \sqrt{|x|} = 0$ ?
- (4.10) Implement the inverse finder described in Example Problem 4.10. Your m-file should have header line like:
- ```
function c = invs(z)
```
- where  $z$  is the number to be inverted. You may wish to use the builtin function `sign`. As an extra termination condition, you should have the subroutine return the current iterate if  $zx$  is sufficiently close to 1, say within the interval  $(0.9999, 0.0001)$ . Can you find some  $z$  for which the algorithm performs poorly?
- (4.11) Implement the bisection method in octave/Matlab. Your m-file should have header line like:
- ```
function c = run_bisection(f, a, b, tol)
```
- where  $f$  is the name of the function. Recall that `feval(f,x)` when  $f$  is a string with the name of some function evaluates that function at  $x$ . This works for builtin functions and m-files.
- Run your code on the function  $f(x) = \cos x$ , with  $a_0 = 0, b_0 = 2$ . In this case you can set  $f = \text{"cos"}$ .
  - Run your code on the function  $f(x) = x^2 - 5x + 3$ , with  $a_0 = 0, b_0 = 1$ . In this case you will have to set  $f$  to the name of an m-file (without the ".m") which will evaluate the given  $f(x)$ .
  - Run your code on the function  $f(x) = x - \cos x$ , with  $a_0 = 0, b_0 = 1$ .
- (4.12) Implement Newton's Method. Your m-file should have header line like:
- ```
function x = run_newton(f, fp, x0, N, tol)
```
- where  $f$  is the name of the function, and  $fp$  is its derivative. Run your code to find zeroes of the following functions:

- $f(x) = \tan x - x$ .

- (b)  $f(x) = x^2 - (2 + \epsilon)x + 1 + \epsilon$ , for  $\epsilon$  small.
- (c)  $f(x) = x^7 - 7x^6 + 21x^5 - 35x^4 + 35x^3 - 21x^2 + 7x - 1$ .
- (d)  $f(x) = (x - 1)^7$ .

(4.13) Implement the secant method Your m-file should have header line like:

```
function x = run_secant(f, x0, x1, N, tol)
```

where **f** is the name of the function. Run your code to find zeroes of the following functions:

- (a)  $f(x) = \tan x - x$ .
- (b)  $f(x) = x^2 + 1$ . (*Note:* This function has no zeroes.)
- (c)  $f(x) = 2 + \sin x$ . (*Note:* This function also has no zeroes.)



# Chapter 5

## Interpolation

### 5.1 Polynomial Interpolation

We consider the problem of finding a polynomial that interpolates a given set of values:

$$\begin{array}{c|c|c|c|c} x & x_0 & x_1 & \dots & x_n \\ \hline y & y_0 & y_1 & \dots & y_n \end{array}$$

where the  $x_i$  are all distinct. A polynomial  $p(x)$  is said to interpolate these data if  $p(x_i) = y_i$  for  $i = 0, 1, \dots, n$ . The  $x_i$  values are called “nodes.”

Sometimes, we will consider a variant of this problem: we have some black box function,  $f(x)$ , which we want to approximate with a polynomial  $p(x)$ . We do this by finding the polynomial interpolant to the data

$$\begin{array}{c|c|c|c|c} x & x_0 & x_1 & \dots & x_n \\ \hline f(x) & f(x_0) & f(x_1) & \dots & f(x_n) \end{array}$$

for some choice of distinct nodes  $x_i$ .

#### 5.1.1 Lagrange's Method

As you might have guessed, for any such set of data, there is an  $n$ -degree polynomial that interpolates it. We present a constructive proof of this fact by use of Lagrange Polynomials.

**Definition 5.1 (Lagrange Polynomials).** For a given set of  $n + 1$  nodes  $x_i$ , the Lagrange polynomials are the  $n + 1$  polynomials  $\ell_i$  defined by

$$\ell_i(x_j) = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

Then we define the interpolating polynomial as

$$p_n(x) = \sum_{i=0}^n y_i \ell_i(x).$$

If each Lagrange Polynomial is of degree at most  $n$ , then  $p_n$  also has this property. The Lagrange Polynomials can be characterized as follows:

$$\boxed{\ell_i(x) = \prod_{j=0, j \neq i}^n \frac{x - x_j}{x_i - x_j}.} \tag{5.1}$$

By evaluating this product for each  $x_j$ , we see that this is indeed a characterization of the Lagrange Polynomials. Moreover, each polynomial is clearly the product of  $n$  monomials, and thus has degree no greater than  $n$ .

This gives the theorem

**Theorem 5.2 (Interpolant Existence and Uniqueness).** Let  $\{x_i\}_{i=0}^n$  be distinct nodes. Then for any values at the nodes,  $\{y_i\}_{i=0}^n$ , there is exactly one polynomial,  $p(x)$  of degree no greater than  $n$  such that  $p(x_i) = y_i$  for  $i = 0, 1, \dots, n$ .

*Proof.* The Lagrange Polynomial construction gives existence of such a polynomial  $p(x)$  of degree no greater than  $n$ .

Suppose there were two such polynomials, call them  $p(x), q(x)$ , each of degree no greater than  $n$ , both interpolating the data. Let  $r(x) = p(x) - q(x)$ . Note that  $r(x)$  can have degree no greater than  $n$ , yet it has roots at  $x_0, x_1, \dots, x_n$ . The only polynomial of degree  $\leq n$  that has  $n + 1$  distinct roots is the zero polynomial, *i.e.*,  $0 \equiv r(x) = p(x) - q(x)$ . Thus  $p(x), q(x)$  are equal everywhere, *i.e.*, they are the same polynomial.  $\square$

**Example Problem 5.3.** Construct the polynomial interpolating the data

$$\begin{array}{c|c|c|c} x & 1 & \frac{1}{2} & 3 \\ \hline y & 3 & -10 & 2 \end{array}$$

by using Lagrange Polynomials.

*Solution:* We construct the Lagrange Polynomials:

$$\begin{aligned} \ell_0(x) &= \frac{(x - \frac{1}{2})(x - 3)}{(1 - \frac{1}{2})(1 - 3)} = -(x - \frac{1}{2})(x - 3) \\ \ell_1(x) &= \frac{(x - 1)(x - 3)}{(\frac{1}{2} - 1)(\frac{1}{2} - 3)} = \frac{4}{5}(x - 1)(x - 3) \\ \ell_2(x) &= \frac{(x - 1)(x - \frac{1}{2})}{(3 - 1)(3 - \frac{1}{2})} = \frac{1}{5}(x - 1)(x - \frac{1}{2}) \end{aligned}$$

Then the interpolating polynomial, in ‘‘Lagrange Form’’ is

$$p_2(x) = -3(x - \frac{1}{2})(x - 3) - 8(x - 1)(x - 3) + \frac{2}{5}(x - 1)(x - \frac{1}{2})$$

+

### 5.1.2 Newton’s Method

There is another way to prove existence. This method is also constructive, and leads to a different algorithm for constructing the interpolant. One way to view this construction is to imagine how one would update the Lagrangian form of an interpolant. That is, suppose some data were given, and the interpolating polynomial calculated using Lagrange Polynomials; then a new point was given  $(x_{n+1}, y_{n+1})$ , and an interpolant for the augmented set of data is to be found. Each Lagrange Polynomial would have to be updated. This could take a lot of calculation (especially if  $n$  is large).

So the alternative method constructs the polynomials iteratively. Thus we create polynomials  $p_k(x)$  such that  $p_k(x_i) = y_i$  for  $0 \leq i \leq k$ . This is simple for  $k = 0$ , we simply let

$$p_0(x) = y_0,$$



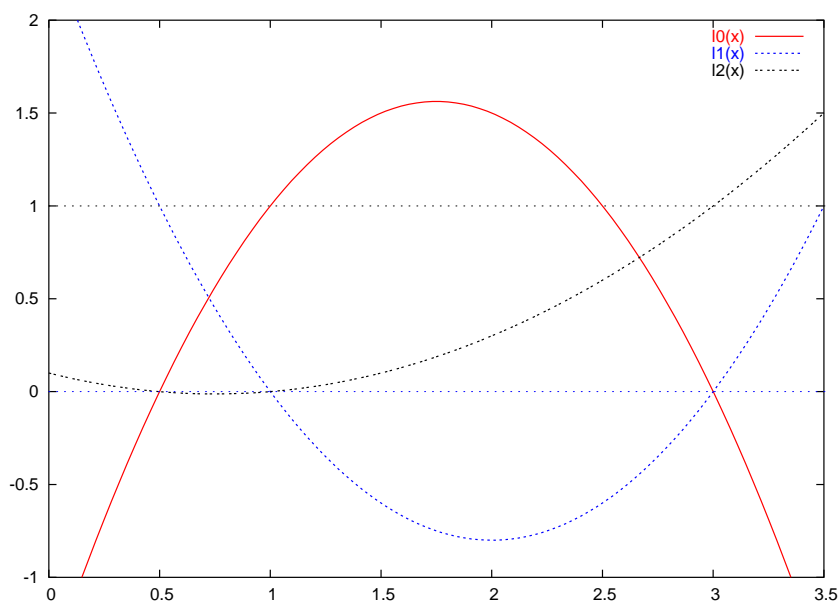


Figure 5.1: The 3 Lagrange polynomials for the example are shown. Verify, graphically, that these polynomials have the property  $l_i(x_j) = \delta_{ij}$  for the nodes  $1, \frac{1}{2}, 3$ .

the constant polynomial with value  $y_0$ . Then assume we have a proper  $p_k(x)$  and want to construct  $p_{k+1}(x)$ . The following construction works:

$$p_{k+1}(x) = p_k(x) + c(x - x_0)(x - x_1) \cdots (x - x_k),$$

for some constant  $c$ . Note that the second term will be zero for any  $x_i$  for  $0 \leq i \leq k$ , so  $p_{k+1}(x)$  will interpolate the data at  $x_0, x_1, \dots, x_k$ . To get the value of the constant we calculate  $c$  such that

$$y_{k+1} = p_{k+1}(x_{k+1}) = p_k(x_{k+1}) + c(x_{k+1} - x_0)(x_{k+1} - x_1) \cdots (x_{k+1} - x_k).$$

This construction is known as Newton's Algorithm, and the resultant form is Newton's form of the interpolant

**Example Problem 5.4.** Construct the polynomial interpolating the data

$$\begin{array}{c|c|c|c} x & 1 & \frac{1}{2} & 3 \\ \hline y & 3 & -10 & 2 \end{array}$$

by using Newton's Algorithm.

*Solution:* We construct the polynomial iteratively:

$$\begin{aligned} p_0(x) &= 3 \\ p_1(x) &= 3 + c(x - 1) \end{aligned}$$

We want  $-10 = p_1(\frac{1}{2}) = 3 + c(-\frac{1}{2})$ , and thus  $c = 26$ . Then

$$p_2(x) = 3 + 26(x - 1) + c(x - 1)(x - \frac{1}{2})$$

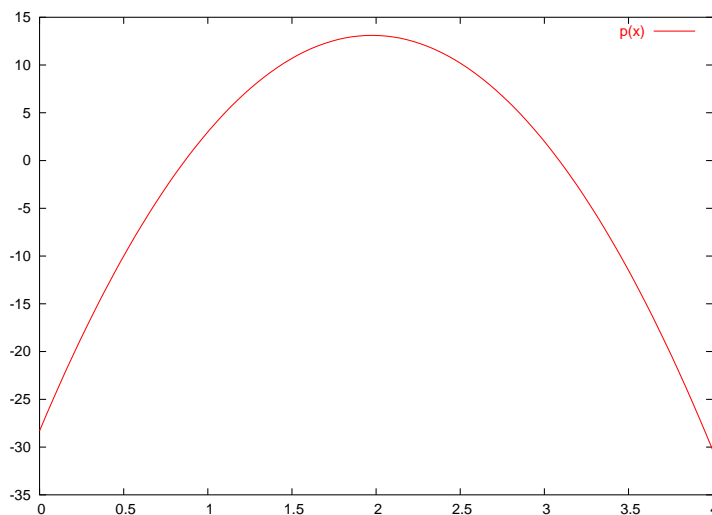


Figure 5.2: The interpolating polynomial for the example is shown.

We want  $2 = p_2(3) = 3 + 26(2) + c(2)(\frac{5}{2})$ , and thus  $c = \frac{-53}{5}$ . Then we get

$$p_2(x) = 3 + 26(x - 1) + \frac{-53}{5}(x - 1)(x - \frac{1}{2}).$$

—

Does Newton’s Algorithm give a different polynomial? It is easy to show, by induction, that the degree of  $p_n(x)$  is no greater than  $n$ . Then, by Theorem 5.2, it must be the same polynomial as the Lagrange interpolant.

The two methods give the same interpolant, we may wonder “Which should we use?” Newton’s Algorithm seems more flexible—it can deal with adding new data. There also happens to be a way of storing Newton’s form of the interpolant that makes the polynomial simple to evaluate (in the sense of number of calculations required).

### 5.1.3 Newton’s Nested Form

Recall the iterative construction of Newton’s Form:

$$p_{k+1}(x) = p_k(x) + c_k(x - x_0)(x - x_1) \cdots (x - x_k).$$

The previous iterate  $p_k(x)$  was constructed similarly, so we can write:

$$p_{k+1}(x) = [p_{k-1}(x) + c_{k-1}(x - x_0)(x - x_1) \cdots (x - x_{k-1})] + c_k(x - x_0)(x - x_1) \cdots (x - x_k).$$

Continuing in this way we see that we can write

$$\boxed{p_n(x) = \sum_{k=0}^n c_k \left[ \prod_{0 \leq j < k} (x - x_j) \right]}, \quad (5.2)$$

where an empty product has value 1 by convention. This can be rewritten in a funny form, where a monomial is factored out of each successive summand:

$$p_n(x) = c_0 + (x - x_0)[c_1 + (x - x_1)[c_2 + (x - x_2)[\dots]]]$$

Supposing for an instant that the constants  $c_k$  were known, this provides a better way of calculating  $p_n(t)$  at arbitrary  $t$ . By “better” we mean requiring few multiplications and additions. This nested calculation is performed iteratively:

$$\begin{aligned} v_0 &= c_n \\ v_1 &= c_{n-1} + (t - x_{n-1})v_0 \\ v_2 &= c_{n-2} + (t - x_{n-2})v_1 \\ &\vdots \\ v_n &= c_0 + (t - x_0)v_{n-1} \end{aligned}$$

This requires only  $n$  multiplications and  $2n$  additions. Compare this with the number required for using the Lagrange form: at least  $n^2$  additions and multiplications.

#### 5.1.4 Divided Differences

It turns out that the coefficients  $c_k$  for Newton’s nested form can be calculated relatively easily by using *divided differences*. We assume, for the remainder of this section, that we are considering interpolating a function, that is, we have values of  $f(x_i)$  at the nodes  $x_i$ .

**Definition 5.5 (Divided Differences).** For a given collection of nodes  $\{x_i\}_{i=0}^n$  and values  $\{f(x_i)\}_{i=0}^n$ , a  $k^{\text{th}}$  order divided difference is a function of  $k + 1$  (not necessarily distinct) nodes, written as

$$f[x_{i_0}, x_{i_1}, \dots, x_{i_k}]$$

The divided differences are defined recursively as follows:

- The  $0^{\text{th}}$  order divided differences are simply defined:

$$f[x_i] = f(x_i).$$

- Higher order divided differences are the ratio of differences:

$$f[x_{i_0}, x_{i_1}, \dots, x_{i_k}] = \frac{f[x_{i_1}, x_{i_2}, \dots, x_{i_k}] - f[x_{i_0}, x_{i_1}, \dots, x_{i_{k-1}}]}{x_{i_k} - x_{i_0}}$$

We care about divided differences because coefficients for the Newton nested form are divided differences:

$$\boxed{c_k = f[x_0, x_1, \dots, x_k]}. \quad (5.3)$$

Because we are only interested in the Newton method coefficients, we will only consider divided differences with successive nodes, *i.e.*, those of the form  $f[x_j, x_{j+1}, \dots, x_{j+k}]$ . In this case the higher order differences can more simply be written as

$$f[x_j, x_{j+1}, \dots, x_{j+k}] = \frac{f[x_{j+1}, x_{j+2}, \dots, x_{j+k}] - f[x_j, x_{j+1}, \dots, x_{j+k-1}]}{x_{j+k} - x_j}$$

The graphical way to calculate these things is a “pyramid scheme”<sup>1</sup>, where you compute the following table columnwise, from left to right:

| $x$   | $f[ ]$   | $f[ , ]$      | $f[ , , ]$         | $f[ , , , ]$            |
|-------|----------|---------------|--------------------|-------------------------|
| $x_0$ | $f[x_0]$ |               |                    |                         |
|       |          | $f[x_0, x_1]$ |                    |                         |
| $x_1$ | $f[x_1]$ |               | $f[x_0, x_1, x_2]$ |                         |
|       |          | $f[x_1, x_2]$ |                    | $f[x_0, x_1, x_2, x_3]$ |
| $x_2$ | $f[x_2]$ |               | $f[x_1, x_2, x_3]$ |                         |
|       |          | $f[x_2, x_3]$ |                    |                         |
| $x_3$ | $f[x_3]$ |               |                    |                         |

Note that by definition, the first column just echoes the data:  $f[x_i] = f(x_i)$ .

We drag out our example one last time:

**Example Problem 5.6.** Find the divided differences for the following data

| $x$    | 1 | $\frac{1}{2}$ | 3 |
|--------|---|---------------|---|
| $f(x)$ | 3 | -10           | 2 |

*Solution:* We start by writing in the data:

| $x$           | $f[ ]$ | $f[ , ]$ | $f[ , , ]$ |
|---------------|--------|----------|------------|
| 1             | 3      |          |            |
| $\frac{1}{2}$ | -10    |          |            |
| 3             | 2      |          |            |

Then we calculate:

$$f[x_0, x_1] = \frac{-10 - 3}{(1/2) - 1} = 26, \quad \text{and} \quad f[x_1, x_2] = \frac{2 - -10}{3 - (1/2)} = 24/5.$$

Adding these to the table, we have

| $x$           | $f[ ]$ | $f[ , ]$       | $f[ , , ]$ |
|---------------|--------|----------------|------------|
| 1             | 3      |                |            |
|               |        | 26             |            |
| $\frac{1}{2}$ | -10    |                |            |
|               |        | $\frac{24}{5}$ |            |
| 3             | 2      |                |            |

Then we calculate

$$f[x_0, x_1, x_2] = \frac{24/5 - 26}{3 - 1} = \frac{-53}{5}.$$

So we complete the table:

| $x$           | $f[ ]$ | $f[ , ]$       | $f[ , , ]$      |
|---------------|--------|----------------|-----------------|
| 1             | 3      |                |                 |
|               |        | 26             |                 |
| $\frac{1}{2}$ | -10    |                | $\frac{-53}{5}$ |
|               |        | $\frac{24}{5}$ |                 |
| 3             | 2      |                |                 |

<sup>1</sup>That’s supposed to be a joke.

You should verify that along the top line of this pyramid you can read off the coefficients for Newton's form, as found in Example Problem 5.4.  $\dashv$

## 5.2 Errors in Polynomial Interpolation

We now consider two questions:

1. If we want to interpolate some function  $f(x)$  at  $n + 1$  nodes over some closed interval, how should we pick the nodes?
2. How accurate can we make a polynomial interpolant over a closed interval?

You may be surprised to find that the answer to the first question is *not* that we should make the  $x_i$  equally spaced over the closed interval, as the following example illustrates.

**Example 5.7 (Runge Function).** Let

$$f(x) = (1 + x^2)^{-1},$$

(known as the *Runge Function*), and let  $p_n(x)$  interpolate  $f$  on  $n$  equally spaced nodes, including the endpoints, on  $[-5, 5]$ . Then

$$\lim_{n \rightarrow \infty} \max_{x \in [-5, 5]} |p_n(x) - f(x)| = \infty.$$

This behaviour is shown in Figure 5.3.

It turns out that a much better choice is related to the *Chebyshev Polynomials* (“of the first kind”). If our closed interval is  $[-1, 1]$ , then we want to define our nodes as

$$x_i = \cos \left[ \left( \frac{2i + 1}{2n + 2} \right) \pi \right], \quad 0 \leq i \leq n.$$

Literally interpreted, these *Chebyshev Nodes* are the projections of points uniformly spaced on a semi circle; see Figure 5.4. By using the Chebyshev nodes, a good polynomial interpolant of the Runge function of Example 5.7 can be found, as shown in Figure 5.5.

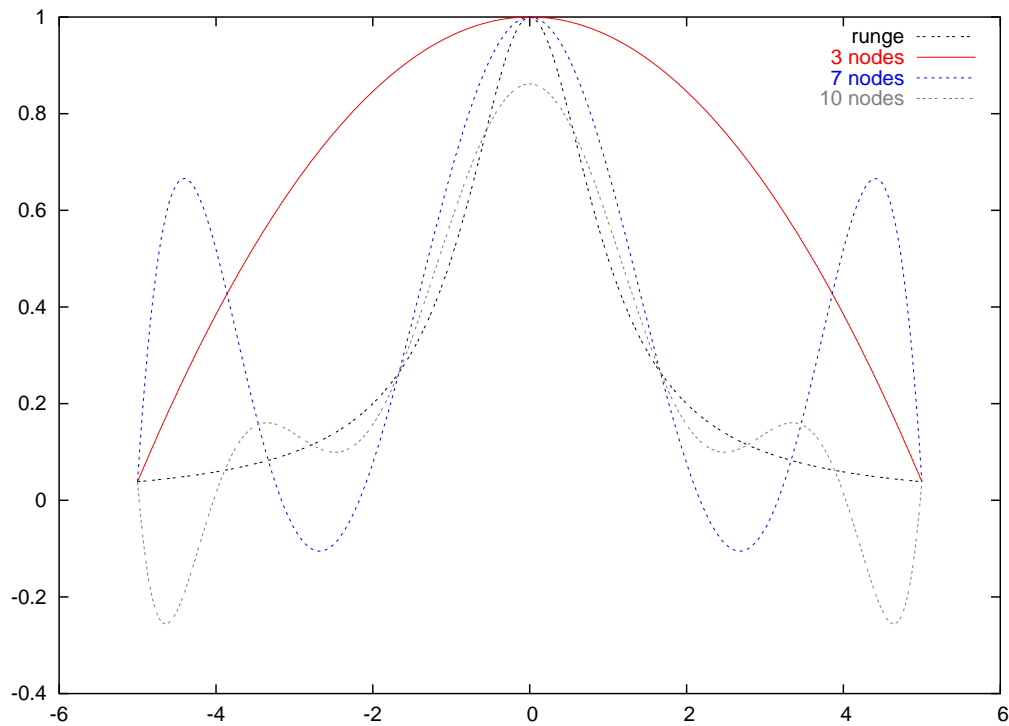
### 5.2.1 Interpolation Error Theorem

We did not just invent the Chebyshev nodes. The fact that they are “good” for interpolation follows from the following theorem:

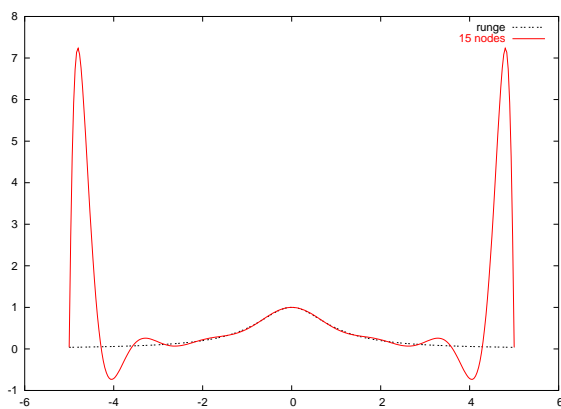
**Theorem 5.8 (Interpolation Error Theorem).** Let  $p$  be the polynomial of degree at most  $n$  interpolating function  $f$  at the  $n + 1$  distinct nodes  $x_0, x_1, \dots, x_n$  on  $[a, b]$ . Let  $f^{(n+1)}$  be continuous. Then for each  $x \in [a, b]$  there is some  $\xi \in [a, b]$  such that

$$f(x) - p(x) = \frac{1}{(n + 1)!} f^{(n+1)}(\xi) \prod_{i=0}^n (x - x_i).$$

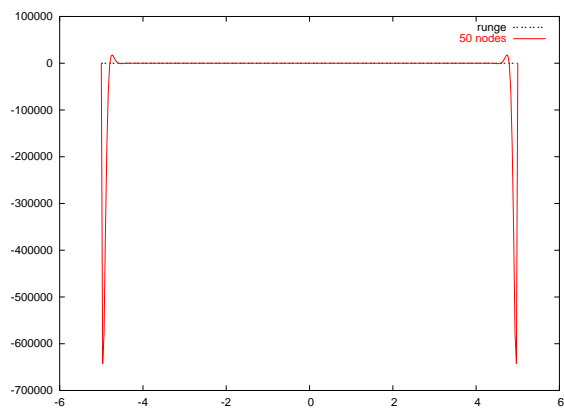
You should be thinking that the term on the right hand side resembles the error term in Taylor's Theorem.



(a) 3,7,10 equally spaced nodes



(b) 15 equally spaced nodes



(c) 50 equally spaced nodes

Figure 5.3: The Runge function is poorly interpolated at  $n$  equally spaced nodes, as  $n$  gets large. At first, the interpolations appear to improve with larger  $n$ , as in (a). In (b) it becomes apparent that the interpolant is good in center of the interval, but bad at the edges. As shown in (c), this gets worse as  $n$  gets larger.

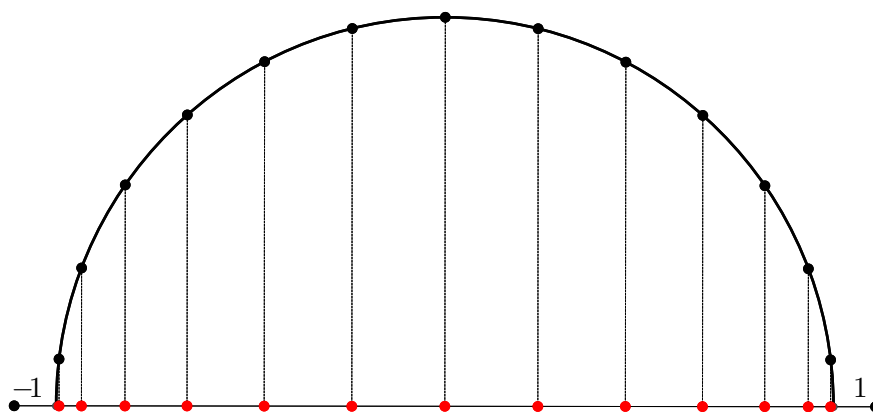
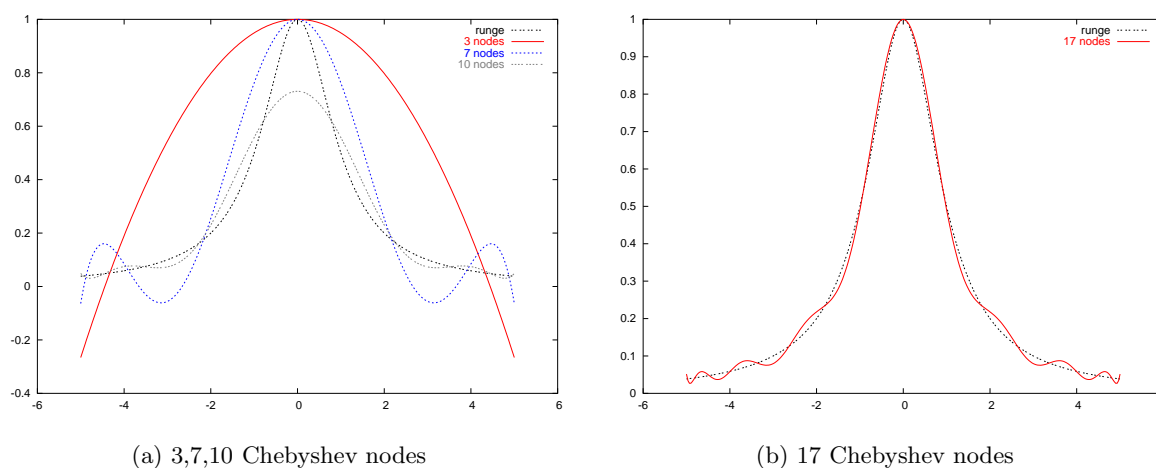


Figure 5.4: The Chebyshev nodes are the projections of nodes equally spaced on a semi circle.



(a) 3,7,10 Chebyshev nodes

(b) 17 Chebyshev nodes

Figure 5.5: The Chebyshev nodes yield good polynomial interpolants of the Runge function. Compare these figures to those of Figure 5.3. For more than about 25 nodes, the interpolant is indistinguishable from the Runge function by eye.

*Proof.* First consider when  $x$  is one of the nodes  $x_i$ ; in this case both the LHS and RHS are zero. So assume  $x$  is not a node. Make the following definitions

$$w(t) = \prod_{i=0}^n (t - x_i),$$

$$c = \frac{f(x) - p(x)}{w(x)},$$

$$\phi(t) = f(t) - p(t) - cw(t).$$

Since  $x$  is not a node,  $w(x)$  is nonzero. Now note that  $\phi(x_i)$  is zero for each node  $x_i$ , and that by definition of  $c$ , that  $\phi(x) = 0$  for our  $x$ . That is  $\phi(t)$  has  $n + 2$  roots.

Some other facts:  $f, p, w$  have  $n + 1$  continuous derivatives, by assumption and definition; thus  $\phi$  has this many continuous derivatives. Apply Rolle's Theorem to  $\phi(t)$  to find that  $\phi'(t)$  has  $n + 1$

roots. Then apply Rolle's Theorem again to find  $\phi''(t)$  has  $n$  roots. In this way we see that  $\phi^{(n+1)}(t)$  has a root, call it  $\xi$ . That is

$$0 = \phi^{(n+1)}(\xi) = f^{(n+1)}(\xi) - p^{(n+1)}(\xi) - cw^{(n+1)}(\xi).$$

But  $p(t)$  is a polynomial of degree  $\leq n$ , so  $p^{(n+1)}$  is identically zero. And  $w(t)$  is a polynomial of degree  $n + 1$  in  $t$ , so its  $n + 1^{\text{th}}$  derivative is easily seen to be  $(n + 1)!$ . Thus

$$\begin{aligned} 0 &= f^{(n+1)}(\xi) - c(n + 1)! \\ c(n + 1)! &= f^{(n+1)}(\xi) \\ \frac{f(x) - p(x)}{w(x)} &= \frac{1}{(n + 1)!} f^{(n+1)}(\xi) \\ f(x) - p(x) &= \frac{1}{(n + 1)!} f^{(n+1)}(\xi) w(x), \end{aligned}$$

which is what was to be proven.  $\square$

Thus the error in a polynomial interpolation is given as

$$f(x) - p(x) = \frac{1}{(n + 1)!} f^{(n+1)}(\xi) \prod_{i=0}^n (x - x_i).$$

We have no control over the function  $f(x)$  or its derivatives, and once the nodes and  $f$  are fixed,  $p$  is determined; thus the only way we can make the error  $|f(x) - p(x)|$  small is by judicious choice of the nodes  $x_i$ .

The Chebyshev nodes on  $[-1, 1]$  have the remarkable property that

$$\left| \prod_{i=0}^n (t - x_i) \right| \leq 2^{-n}$$

for any  $t \in [-1, 1]$ . Moreover, it can be shown that for *any* choice of nodes  $x_i$  that

$$\max_{t \in [-1, 1]} \left| \prod_{i=0}^n (t - x_i) \right| \geq 2^{-n}.$$

Thus the Chebyshev nodes are considered the best for polynomial interpolation.

Merging this result with Theorem 5.8, the error for polynomial interpolants defined on Chebyshev nodes can be bounded as

$$|f(x) - p(x)| \leq \frac{1}{2^n (n + 1)!} \max_{\xi \in [-1, 1]} |f^{(n+1)}(\xi)|.$$

The Chebyshev nodes can be rescaled and shifted for use on the general interval  $[\alpha, \beta]$ . In this case they take the form

$$x_i = \frac{\beta - \alpha}{2} \cos \left[ \left( \frac{2i + 1}{2n + 2} \right) \pi \right] + \frac{\alpha + \beta}{2}, \quad 0 \leq i \leq n.$$

In this case, the rescaling of the nodes changes the bound on  $\prod (t - x_i)$  so the overall error bound becomes

$$|f(x) - p(x)| \leq \frac{(\beta - \alpha)^{n+1}}{2^{2n+1} (n + 1)!} \max_{\xi \in [\alpha, \beta]} |f^{(n+1)}(\xi)|,$$

for  $x \in [\alpha, \beta]$ .



**Example Problem 5.9.** How many Chebyshev nodes are required to interpolate the function  $f(x) = \sin(x) + \cos(x)$  to within  $10^{-8}$  on the interval  $[0, \pi]$ ?

*Solution:* We first find the derivatives of  $f$

$$\begin{aligned} f'(x) &= \cos(x) - \sin(x) \\ f''(x) &= -\sin(x) - \cos(x) \\ f'''(x) &= -\cos(x) + \sin(x) \\ &\vdots \end{aligned}$$

As a crude approximation we can assert that

$$\left| f^{(k)}(x) \right| \leq |\cos x| + |\sin x| \leq 2.$$

Thus it suffices to take  $n$  large enough such that

$$\frac{\pi^{n+1}}{2^{2n+1} (n+1)!} 2 \leq 10^{-8}$$

By trial and error we see that  $n = 10$  suffices. +

### 5.2.2 Interpolation Error for Equally Spaced Nodes

Despite the proven superiority of Chebyshev Nodes, and the problems with the Runge Function, equally spaced nodes are frequently used for interpolation, since they are easy to calculate<sup>2</sup>. We now consider bounding

$$\max_{x \in [a,b]} \prod_{i=0}^n |x - x_i|,$$

where

$$x_i = a + hi = a + \frac{(b-a)}{n}i, \quad i = 0, 1, \dots, n.$$

Start by picking an  $x$ . We can assume  $x$  is not one of the nodes, otherwise the product in question is zero. Then  $x$  is between some  $x_j, x_{j+1}$ . We can show that

$$|x - x_j| |x - x_{j+1}| \leq \frac{h^2}{4}.$$

by simple calculus.

Now we claim that  $|x - x_i| \leq (j - i + 1)h$  for  $i < j$ , and  $|x - x_i| \leq (i - j)h$  for  $j + 1 < i$ . Then

$$\prod_{i=0}^n |x - x_i| \leq \frac{h^2}{4} [(j+1)!h^j] [(n-j)!h^{n-j-1}].$$

It can be shown that  $(j+1)!(n-j)! \leq n!$ , and so we get an overall bound

$$\prod_{i=0}^n |x - x_i| \leq \frac{h^{n+1}n!}{4}.$$

---

<sup>2</sup>Never underestimate the power of laziness.

The interpolation theorem then gives us

$$|f(x) - p(x)| \leq \frac{h^{n+1}}{4(n+1)} \max_{\xi \in [a,b]} |f^{(n+1)}(\xi)|,$$

where  $h = (b - a)/n$ .

The reason this result does not seem to apply to Runge's Function is that  $f^{(n)}$  for Runge's Function becomes unbounded as  $n \rightarrow \infty$ .

**Example Problem 5.10.** How many equally spaced nodes are required to interpolate the function  $f(x) = \sin(x) + \cos(x)$  to within  $10^{-8}$  on the interval  $[0, \pi]$ ?

*Solution:* As in Example Problem 5.9, we make the crude approximation

$$|f^{(k)}(x)| \leq |\cos x| + |\sin x| \leq 2.$$

Thus we want to make  $n$  sufficiently large such that

$$\frac{h^{n+1}}{4(n+1)} 2 \leq 10^{-8},$$

where  $h = (\pi - 0)/n$ . That is we want to find  $n$  large enough such that

$$\frac{\pi^{n+1}}{2n^{n+1}(n+1)} \leq 10^{-8},$$

By simply trying small numbers, we can see this is satisfied if  $n = 12$ . +

## EXERCISES

- (5.1) Find the Lagrange Polynomials for the nodes  $\{-1, 1\}$ .  
 (5.2) Find the Lagrange Polynomials for the nodes  $\{-1, 1, 5\}$ .  
 (5.3) Find the polynomial of degree no greater than 2 that interpolates

|     |    |   |    |
|-----|----|---|----|
| $x$ | -1 | 1 | 5  |
| $y$ | 3  | 3 | -2 |

- (5.4) Complete the divided differences table:

|     |        |          |            |
|-----|--------|----------|------------|
| $x$ | $f[ ]$ | $f[ , ]$ | $f[ , , ]$ |
| -1  | 3      |          |            |
| 1   | 3      |          |            |
| 5   | -2     |          |            |

Find the Newton form of the polynomial interpolant.

- (5.5) Find the polynomial of degree no greater than 3 that interpolates

|     |    |   |    |    |
|-----|----|---|----|----|
| $x$ | -1 | 1 | 5  | -3 |
| $y$ | 3  | 3 | -2 | 4  |

(*Hint:* reuse the Newton form of the polynomial from the previous question.)

- (5.6) Find the nested form of the polynomial interpolant of the data

|     |    |    |    |   |
|-----|----|----|----|---|
| $x$ | 1  | 3  | 4  | 6 |
| $y$ | -3 | 13 | 21 | 1 |

by completing the following divided differences table:

|     |        |          |            |              |
|-----|--------|----------|------------|--------------|
| $x$ | $f[ ]$ | $f[ , ]$ | $f[ , , ]$ | $f[ , , , ]$ |
| 1   | -3     |          |            |              |
| 3   | 13     |          |            |              |
| 4   | 21     |          |            |              |
| 6   | 1      |          |            |              |

- (5.7) Find the polynomial of degree no greater than 3 that interpolates

|     |   |   |        |   |
|-----|---|---|--------|---|
| $x$ | 1 | 0 | $3/2$  | 2 |
| $y$ | 3 | 2 | $37/8$ | 8 |

- (5.8) Complete the divided differences table:

|     |        |          |            |              |
|-----|--------|----------|------------|--------------|
| $x$ | $f[ ]$ | $f[ , ]$ | $f[ , , ]$ | $f[ , , , ]$ |
| -1  | 6      |          |            |              |
| 0   | 3      |          |            |              |
| 1   | 2      |          |            |              |
| 2   | 3      |          |            |              |

(Something a little odd should have happened in the last column.) Find the Newton form of the polynomial interpolant. Of what degree is the polynomial interpolant?

- (5.9) Let  $p(x)$  interpolate the function  $\cos(x)$  at  $n$  equally spaced nodes on the interval  $[0, 2]$ . Bound the error

$$\max_{0 \leq x \leq 2} |p(x) - \cos(x)|$$

as a function of  $n$ . How small is the error when  $n = 10$ ? How small would the error be if Chebyshev nodes were used instead? How about when  $n = 10$ ?

- (5.10) Let  $p(x)$  interpolate the function  $x^{-2}$  at  $n$  equally spaced nodes on the interval  $[0.5, 1]$ . Bound the error

$$\max_{0.5 \leq x \leq 1} |p(x) - x^{-2}|$$

as a function of  $n$ . How small is the error when  $n = 10$ ?

- (5.11) How many Chebyshev nodes are required to interpolate the function  $\frac{1}{x}$  to within  $10^{-6}$  on the interval  $[1, 2]$ ?

- (5.12) Write code to calculate the Newton form coefficients, by divided differences, for the nodes  $x_i$  and values  $f(x_i)$ . Your m-file should have header line like:

```
function coefs = newtonCoef(xs,fxs)
```

where **xs** is the vector of  $n + 1$  nodes, and **fxs** the vector of  $n + 1$  values. Test your code on the following input:

```
octave:1> xs = [1 -1 2 -2 3 -3 4 -4];
```

```
octave:2> fxs = [1 1 2 3 5 8 13 21];
```

```
octave:3> newtonCoef(xs,fxs)
```

```
ans =
```

```
1.00000 -0.00000 0.33333 -0.08333 0.05000 0.00417 -0.00020 -0.00040
```

- (a) What do you get when you try the following?

```
octave:4> xs = [1 4 5 9 14 23 37 60];
```

```
octave:5> fxs = [3 1 4 1 5 9 2 6];
```

```
octave:6> newtonCoef(xs,fxs)
```

- (b) Try the following:

```
octave:7> xs = [1 3 4 2 8 -2 0 14 23 15];
```

```
octave:8> fxs = xs.*xs + xs .+ 4;
```

```
octave:9> newtonCoef(xs,fxs)
```

- (5.13) Write code to calculate a polynomial interpolant from its Newton form coefficients and the node values. Your m-file should have header line like:

```
function y = calcNewton(t,coefs,xs)
```

where **coefs** is a vector of the Newton coefficients, **xs** is a vector of the nodes  $x_i$ , and **y** is the value of the interpolating polynomial at **t**. Check your code against the following values:

```
octave:1> xs = [1 3 4];
```

```
octave:2> coefs = [6 5 1];
```

```
octave:3> calcNewton (5,coefs,xs)
```

```
ans = 34
```

```
octave:4> calcNewton (-3,coefs,xs)
```

```
ans = 10
```

- (a) What do you get when you try the following?

```
octave:5> xs = [3 1 4 5 9 2 6 8 7 0];
```

```
octave:6> coefs = [1 -1 2 -2 3 -3 4 -4 5 -5];  
octave:7> calcNewton(0.5,coefs,xs)
```

(b) Try the following

```
octave:8> xs = [3 1 4 5 9 2 6 8 7 0];  
octave:9> coefs = [1 -1 2 -2 3 -3 4 -4 5 -5];  
octave:10> calcNewton(1,coefs,xs)
```



# Chapter 6

## Spline Interpolation

Splines are used to approximate complex functions and shapes. A spline is a function consisting of simple functions glued together. In this way a spline is different from a polynomial interpolation, which consists of a single well defined function that approximates a given shape; splines are normally piecewise polynomial.

### 6.1 First and Second Degree Splines

Splines make use of partitions, which are a way of cutting an interval into a number of subintervals.

**Definition 6.1 (Partition).** A *partition* of the interval  $[a, b]$  is an ordered sequence  $\{t_i\}_{i=0}^n$  such that

$$a = t_0 < t_1 < \dots < t_{n-1} < t_n = b$$

The numbers  $t_i$  are known as *knots*.

A spline of degree 1, also known as a *linear spline*, is a function which is linear on each subinterval defined by a partition:

**Definition 6.2 (Linear Splines).** A function  $S$  is a spline of degree 1 on  $[a, b]$  if

1. The domain of  $S$  is  $[a, b]$ .
2.  $S$  is continuous on  $[a, b]$ .
3. There is a partition  $\{t_i\}_{i=0}^n$  of  $[a, b]$  such that on each  $[t_i, t_{i+1}]$ ,  $S$  is a linear polynomial.

A linear spline is defined entirely by its value at the knots. That is, given

$$\begin{array}{c|c|c|c|c} t & t_0 & t_1 & \dots & t_n \\ \hline y & y_0 & y_1 & \dots & y_n \end{array}$$

there is only one linear spline with these values at the knots and linear on each given subinterval.

For a spline with this data, the linear polynomial on each subinterval is defined as

$$S_i(x) = y_i + \frac{y_{i+1} - y_i}{t_{i+1} - t_i} (x - t_i).$$

Note that if  $x \in [t_i, t_{i+1}]$ , then  $x - t_i > 0$ , but  $x - t_{i-1} \leq 0$ . Thus if we wish to evaluate  $S(x)$ , we search for the largest  $i$  such that  $x - t_i > 0$ , then evaluate  $S_i(x)$ .

**Example 6.3.** The linear spline for the following data

$$\begin{array}{c|c|c|c|c|c|c} t & 0.0 & 0.1 & 0.4 & 0.5 & 0.75 & 1.0 \\ \hline y & 1.3 & 4.5 & 2.0 & 2.1 & 5.0 & 3 \end{array}$$

is shown in Figure 6.1.

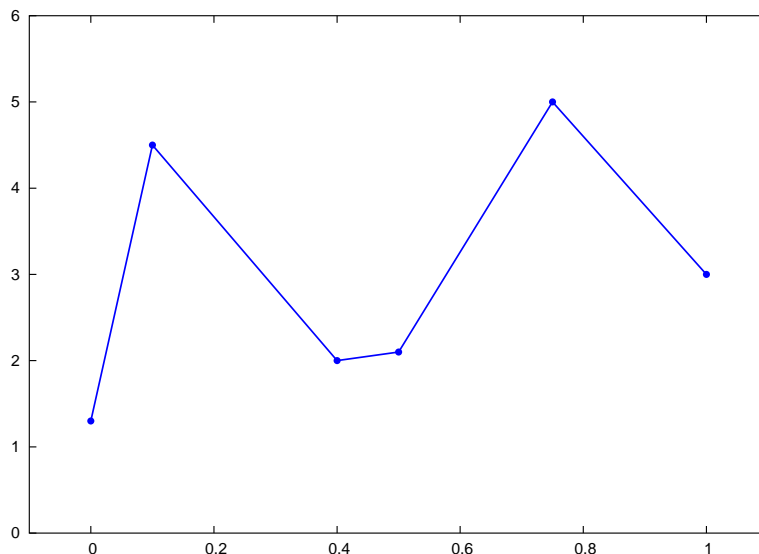


Figure 6.1: A linear spline. The spline is piecewise linear, and is linear between each knot.

### 6.1.1 First Degree Spline Accuracy

As with polynomial functions, splines are used to interpolate tabulated data as well as functions. In the latter case, if the spline is being used to interpolate the function  $f$ , say, then this is equivalent to interpolating the data

$$\begin{array}{c|c|c|c|c} t & t_0 & t_1 & \dots & t_n \\ \hline y & f(t_0) & f(t_1) & \dots & f(t_n) \end{array}$$

A function and its linear spline interpolant are shown in Figure 6.2. The spline interpolant in that figure is fairly close to the function over some of the interval in question, but it also deviates greatly from the function at other points of the interval. We are interested in finding bounds on the possible error between a function and its spline interpolant.

To find the error bound, we will consider the error on a single interval of the partition, and use a little calculus.<sup>1</sup> Suppose  $p(t)$  is the linear polynomial interpolating  $f(t)$  at the endpoints of the subinterval  $[t_i, t_{i+1}]$ , then for  $t \in [t_i, t_{i+1}]$ ,

$$|f(t) - p(t)| \leq \max\{|f(t) - f(t_i)|, |f(t) - f(t_{i+1})|\}.$$

That is,  $|f(t) - p(t)|$  is no larger than the “maximum variation” of  $f(t)$  on this interval.

In particular, if  $f'(t)$  exists and is bounded by  $M_1$  on  $[t_i, t_{i+1}]$ , then

$$|f(t) - p(t)| \leq \frac{M_1}{2} (t_{i+1} - t_i).$$

Similarly, if  $f''(t)$  exists and is bounded by  $M_2$  on  $[t_i, t_{i+1}]$ , then

$$|f(t) - p(t)| \leq \frac{M_2}{8} (t_{i+1} - t_i)^2.$$

Over a given partition, these become, respectively

<sup>1</sup>Although we could directly claim Theorem 5.8, it is a bit of overkill.



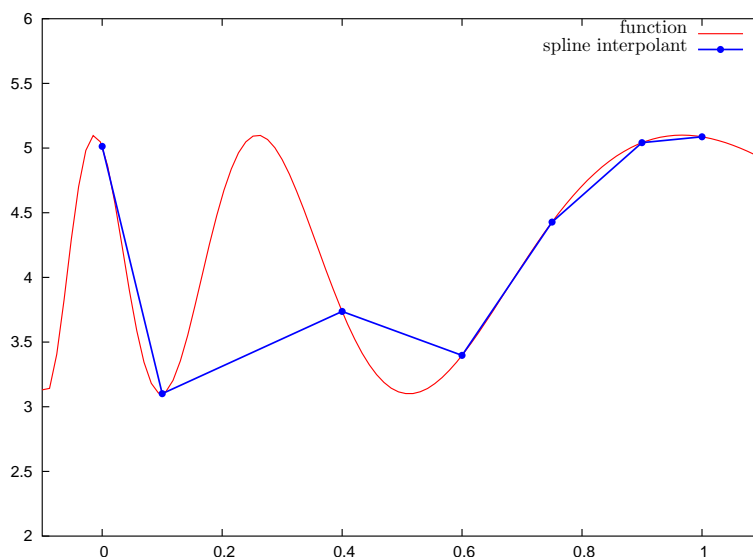


Figure 6.2: The function  $f(t) = 4.1 + \sin(1/(0.08t + 0.5))$  is shown, along with the linear spline interpolant, for the knots  $0, 0.1, 0.4, 0.6, 0.75, 0.9, 1.0$ . For some values of  $t$ , the function and its interpolant are very close, while they vary greatly in the middle of the interval.

$$\begin{aligned} |f(t) - p(t)| &\leq \frac{M_1}{2} \max_{0 \leq i < n} (t_{i+1} - t_i), \\ |f(t) - p(t)| &\leq \frac{M_2}{8} \max_{0 \leq i < n} (t_{i+1} - t_i)^2. \end{aligned} \quad (6.1)$$

If equally spaced nodes are used, these bounds guarantee that spline interpolants become better as the number of nodes is increased. This contrasts with polynomial interpolants, which may get worse as the number of nodes is increased, *cf.* Example 5.7.

### 6.1.2 Second Degree Splines

Piecewise quadratic splines, or splines of degree 2, are defined similarly:

**Definition 6.4 (Quadratic Splines).** A function  $Q$  is a quadratic spline on  $[a, b]$  if

1. The domain of  $Q$  is  $[a, b]$ .
2.  $Q$  is continuous on  $[a, b]$ .
3.  $Q'$  is continuous on  $(a, b)$ .
4. There is a partition  $\{t_i\}_{i=0}^n$  of  $[a, b]$  such that on  $[t_i, t_{i+1}]$ ,  $Q$  is a polynomial of degree at most 2.

**Example 6.5.** The following is a quadratic spline:

$$Q(x) = \begin{cases} -x & x \leq 0, \\ x^2 - x & 0 \leq x \leq 2, \\ -x^2 + 7x - 8 & 2 \leq x. \end{cases}$$

Unlike linear splines, quadratic splines are *not* defined entirely by their values at the knots. We consider why that is. The spline  $Q(x)$  is defined by its piecewise polynomials,

$$Q_i(x) = a_i x^2 + b_i x + c_i.$$

Thus there are  $3n$  parameters to define  $Q(x)$ .

For each of the  $n$  subintervals, the data

$$\begin{array}{c|c|c|c|c} t & t_0 & t_1 & \dots & t_n \\ \hline y & y_0 & y_1 & \dots & y_n \end{array}$$

give two equations regarding  $Q_i(x)$ , namely that  $Q_i(t_i)$  must equal  $y_i$  and  $Q_i(t_{i+1})$  must equal  $y_{i+1}$ . This is  $2n$  equations. The condition on continuity of  $Q'$  gives a single equation for each of the  $n-1$  internal nodes. This totals  $3n-1$  equations, but  $3n$  unknowns. This system is underdetermined.

Thus some additional user-chosen condition is required to determine the quadratic spline. One might choose, for example,  $Q'(a) = 0$ , or  $Q''(a) = 0$ , or some other condition.

### 6.1.3 Computing Second Degree Splines

Suppose the data

$$\begin{array}{c|c|c|c|c} t & t_0 & t_1 & \dots & t_n \\ \hline y & y_0 & y_1 & \dots & y_n \end{array}$$

are given. Let  $z_i = Q'_i(t_i)$ , and suppose that the additional condition to define the quadratic spline is given by specifying  $z_0$ . We want to be able to compute the form of  $Q_i(x)$ .

Because  $Q_i(t_i) = y_i$ ,  $Q'_i(t_i) = z_i$ ,  $Q'_i(t_{i+1}) = z_{i+1}$ , we see that we can define

$$Q_i(x) = \frac{z_{i+1} - z_i}{2(t_{i+1} - t_i)} (x - t_i)^2 + z_i(x - t_i) + y_i.$$

Use this at  $t_{i+1}$ :

$$\begin{aligned} y_{i+1} &= Q_i(t_{i+1}) = \frac{z_{i+1} - z_i}{2(t_{i+1} - t_i)} (t_{i+1} - t_i)^2 + z_i(t_{i+1} - t_i) + y_i, \\ y_{i+1} - y_i &= \frac{z_{i+1} - z_i}{2} (t_{i+1} - t_i) + z_i(t_{i+1} - t_i), \\ y_{i+1} - y_i &= \frac{z_{i+1} + z_i}{2} (t_{i+1} - t_i). \end{aligned}$$

Thus we can determine, from the data alone,  $z_{i+1}$  from  $z_i$ :

$$z_{i+1} = 2 \frac{y_{i+1} - y_i}{t_{i+1} - t_i} - z_i.$$

## 6.2 (Natural) Cubic Splines

If you recall the definition of the linear and quadratic splines, probably you can guess the definition of the spline of degree  $k$ :

**Definition 6.6 (Splines of Degree  $k$ ).** A function  $S$  is a spline of degree  $k$  on  $[a, b]$  if

1. The domain of  $S$  is  $[a, b]$ .
2.  $S, S', S'', \dots, S^{(k-1)}$  are continuous on  $(a, b)$ .
3. There is a partition  $\{t_i\}_{i=0}^n$  of  $[a, b]$  such that on  $[t_i, t_{i+1}]$ ,  $S$  is a polynomial of degree  $\leq k$ .

You would also expect that a spline of degree  $k$  has  $k-1$  “degrees of freedom,” as we show here. If the partition has  $n+1$  knots, the spline of degree  $k$  is defined by  $n(k+1)$  parameters. The given data

$$\begin{array}{c|c|c|c|c} t & t_0 & t_1 & \dots & t_n \\ \hline y & y_0 & y_1 & \dots & y_n \end{array}$$

provide  $2n$  equations. The continuity of  $S', S'', \dots, S^{(k-1)}$  at the  $n - 1$  internal knots gives  $(k - 1)(n - 1)$  equations. This is a total of  $n(k + 1) - (k - 1)$  equations. Thus we have  $k - 1$  more unknowns than equations. Thus, barring some singularity, we can (and must) add  $k - 1$  constraints to uniquely define the spline. These are the degrees of freedom.

Often  $k$  is chosen as 3. This yields cubic splines. We must add 2 extra constraints to define the spline. The usual choice is to make

$$S''(t_0) = S''(t_n) = 0.$$

This yields the *natural cubic spline*.

### 6.2.1 Why Natural Cubic Splines?

It turns out that natural cubic splines are a good choice in the sense that they are the “interpolant of minimal  $H^2$  seminorm.” The corollary following this theorem states this in more easily understandable terms:

**Theorem 6.7.** Suppose  $f$  has two continuous derivatives, and  $S$  is the natural cubic spline interpolating  $f$  at knots  $a = t_0 < t_1 < \dots < t_n = b$ . Then

$$\int_a^b [S''(x)]^2 dx \leq \int_a^b [f''(x)]^2 dx$$

*Proof.* We let  $g(x) = f(x) - S(x)$ . Then  $g(x)$  is zero on the  $(n + 1)$  knots  $t_i$ . Derivatives are linear, meaning that

$$f''(x) = S''(x) + g''(x).$$

Then

$$\int_a^b [f''(x)]^2 dx = \int_a^b [S''(x)]^2 dx + \int_a^b [g''(x)]^2 dx + \int_a^b 2S''(x)g''(x) dx.$$

We show that the last integral is zero. Integrating by parts we get

$$\int_a^b S''(x)g''(x) dx = S''g' \Big|_a^b - \int_a^b S'''g' dx = - \int_a^b S'''g' dx,$$

because  $S''(a) = S''(b) = 0$ . Then notice that  $S$  is a polynomial of degree  $\leq 3$  on each interval, thus  $S'''(x)$  is a piecewise constant function, taking value  $c_i$  on each interval  $[t_i, t_{i+1}]$ . Thus

$$\int_a^b S'''g' dx = \sum_{i=0}^{n-1} \int_a^b c_i g' dx = \sum_{i=0}^{n-1} c_i g \Big|_{t_i}^{t_{i+1}} = 0,$$

with the last equality holding because  $g(x)$  is zero at the knots. □

**Corollary 6.8.** The natural cubic spline is best twice-continuously differentiable interpolant for a twice-continuously differentiable function, under the measure given by the theorem.

*Proof.* Let  $f$  be twice-continuously differentiable, and let  $S$  be the natural cubic spline interpolating  $f(x)$  at some given nodes  $\{t_i\}_{i=0}^n$ . Let  $R(x)$  be some twice-continuously differentiable function which also interpolates  $f(x)$  at these nodes. Then  $S(x)$  interpolates  $R(x)$  at these nodes. Apply the theorem to get

$$\int_a^b [S''(x)]^2 dx \leq \int_a^b [R''(x)]^2 dx$$

□

### 6.2.2 Computing Cubic Splines

First we present an example of computing the natural cubic spline by hand:

**Example Problem 6.9.** Construct the natural cubic spline for the following data:

$$\frac{t}{y} \left\| \begin{array}{c|c|c} -1 & 0 & 2 \\ \hline 3 & -1 & 3 \end{array} \right.$$

*Solution:* The natural cubic spline is defined by eight parameters:

$$S(x) = \begin{cases} ax^3 + bx^2 + cx + d & x \in [-1, 0] \\ ex^3 + fx^2 + gx + h & x \in [0, 2] \end{cases}$$

We interpolate to find that  $d = h = -1$  and

$$\begin{aligned} -a + b - c - 1 &= 3 \\ 8e + 4f + 2g - 1 &= 3 \end{aligned}$$

We take the derivative of  $S$ :

$$S'(x) = \begin{cases} 3ax^2 + 2bx + c & x \in [-1, 0] \\ 3ex^2 + 2fx + g & x \in [0, 2] \end{cases}$$

Continuity at the middle node gives  $c = g$ . Now take the second derivative of  $S$ :

$$S''(x) = \begin{cases} 6ax + 2b & x \in [-1, 0] \\ 6ex + 2f & x \in [0, 2] \end{cases}$$

Continuity at the middle node gives  $b = f$ . The natural cubic spline condition gives  $-6a + 2b = 0$  and  $12e + 2f = 0$ . Solving this by “divide and conquer” gives

$$S(x) = \begin{cases} x^3 + 3x^2 - 2x - 1 & x \in [-1, 0] \\ -\frac{1}{2}x^3 + 3x^2 - 2x - 1 & x \in [0, 2] \end{cases}$$

+

Finding the constants for the previous example was fairly tedious. And this is for the case of only three nodes. We would like a method easier than setting up the  $4n$  equations and unknowns, something akin to the description in Subsection 6.1.3. The method is rather tedious, so we leave it to the exercises.

## 6.3 B Splines

The B splines form a *basis* for spline functions, whence the name. We presuppose the existence of an *infinite* number of knots:

$$\dots < t_2 < t_1 < t_0 < t_1 < t_2 < \dots,$$

with  $\lim_{k \rightarrow -\infty} t_k = -\infty$  and  $\lim_{k \rightarrow \infty} t_k = \infty$ .

The B splines of degree 0 are defined as single “blocks”:

$$B_i^0(x) = \begin{cases} 1 & t_i \leq x < t_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

The zero degree B splines are continuous from the right, are nonzero only on one subinterval  $[t_i, t_{i+1})$ , sum to 1 everywhere.

We justify the description of B splines as basis splines: If  $S$  is a spline of degree 0 on the given knots and is continuous from the right then

$$S(x) = \sum_i S(x_i) B_i^0(x).$$

That is, the basis splines work in the same way that Lagrange Polynomials worked for polynomial interpolation.

The B splines of degree  $k$  are defined recursively:

$$B_i^k(x) = \left( \frac{x - t_i}{t_{i+k} - t_i} \right) B_i^{k-1}(x) + \left( \frac{t_{i+k+1} - x}{t_{i+k+1} - t_{i+1}} \right) B_{i+1}^{k-1}(x).$$

Some B splines are shown in Figure 6.3.

The B splines quickly become unwieldy. We focus on the case  $k = 1$ . The B spline  $B_i^1(x)$  is

- Piecewise linear.
- Continuous.
- Nonzero only on  $(t_i, t_{i+2})$ .
- 1 at  $t_{i+1}$ .

These B splines are sometimes called *hat functions*. Imagine wearing a hat shaped like this! Whatever.

The nice thing about the hat functions is they allow us to use analogy. Harken back to polynomial interpolation and the Lagrange Functions. The hat functions play a similar role because

$$B_i^1(t_j) = \delta_{(i+1)j} = \begin{cases} 1 & (i+1) = j \\ 0 & (i+1) \neq j \end{cases}$$

Then if we want to interpolate the following data with splines of degree 1:

$$\begin{array}{c|c|c|c|c} t & t_0 & t_1 & \dots & t_n \\ \hline y & y_0 & y_1 & \dots & y_n \end{array}$$

We can immediately set

$$S(x) = \sum_{i=0}^n y_i B_{i-1}^1(x).$$

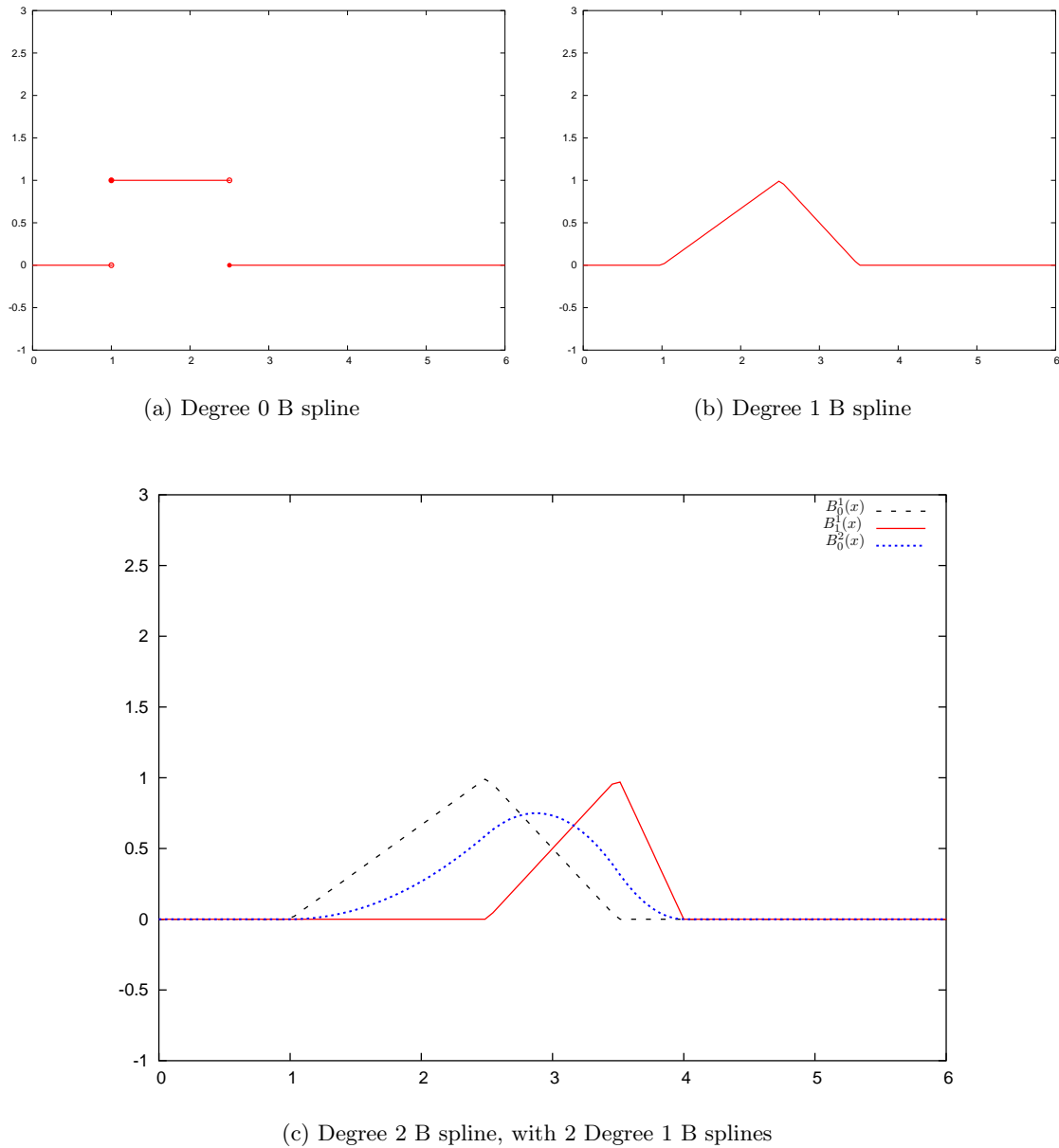


Figure 6.3: Some B splines for the knots  $t_0 = 1, t_1 = 2.5, t_2 = 3.5, t_3 = 4$  are shown. In (a), one of the degree 0 B splines; in (b), a degree 1 B spline; in (c), two of the degree 1 B splines and a degree 2 B spline are shown. The two hat functions “merge” together to give the quadratic B spline.

## EXERCISES

(6.1) Is the following function a linear spline on  $[0, 4]$ ? Why or why not?

$$S(x) = \begin{cases} 3x + 2 & : 0 \leq x < 1 \\ -2x + 4 & : 1 \leq x \leq 4 \end{cases}$$

(6.2) Is the following function a linear spline on  $[0, 2]$ ? Why or why not?

$$S(x) = \begin{cases} x + 3 & : 0 \leq x < 1 \\ 3 & : 1 \leq x \leq 2 \end{cases}$$

(6.3) Is the following function a linear spline on  $[0, 4]$ ? Why or why not?

$$S(x) = \begin{cases} x^2 + 3 & : 0 \leq x < 3 \\ 5x - 6 & : 3 \leq x \leq 4 \end{cases}$$

(6.4) Find constants,  $\alpha, \beta$  such that the following is a linear spline on  $[0, 5]$ .

$$S(x) = \begin{cases} 4x - 2 & : 0 \leq x < 1 \\ \alpha x + \beta & : 1 \leq x < 3 \\ -2x + 10 & : 3 \leq x \leq 5 \end{cases}$$

(6.5) Is the following function a quadratic spline on  $[0, 4]$ ? Why or why not?

$$Q(x) = \begin{cases} x^2 + 3 & : 0 \leq x < 3 \\ 5x - 6 & : 3 \leq x \leq 4 \end{cases}$$

(6.6) Is the following function a quadratic spline on  $[0, 2]$ ? Why or why not?

$$Q(x) = \begin{cases} x^2 + 3x + 2 & : 0 \leq x < 1 \\ 2x^2 + x + 3 & : 1 \leq x \leq 2 \end{cases}$$

(6.7) Find constants,  $\alpha, \beta, \gamma$  such that the following is a quadratic spline on  $[0, 5]$ .

$$Q(x) = \begin{cases} \frac{1}{2}x^2 + 2x + \frac{3}{2} & : 0 \leq x < 1 \\ \alpha x^2 + \beta x + \gamma & : 1 \leq x < 3 \\ 3x^2 - 7x + 12 & : 3 \leq x \leq 5 \end{cases}$$

(6.8) Find the quadratic spline that interpolates the following data:

$$\begin{array}{c|c|c|c} t & 0 & 1 & 4 \\ \hline y & 1 & -2 & 1 \end{array}$$

To resolve the single degree of freedom, assume that  $Q'(0) = -Q'(4)$ . Assume your solution takes the form

$$Q(x) = \begin{cases} \alpha_1 (x - 1)^2 + \beta_1 (x - 1) - 2 & : 0 \leq x < 1 \\ \alpha_2 (x - 1)^2 + \beta_2 (x - 1) - 2 & : 1 \leq x \leq 4 \end{cases}$$

Find the constants  $\alpha_1, \beta_1, \alpha_2, \beta_2$ .

(6.9) Find the natural cubic spline that interpolates the data

$$\begin{array}{c|c|c|c} x & 0 & 1 & 3 \\ \hline y & 4 & 2 & 7 \end{array}$$

It may help to assume your answer has the form

$$S(x) = \begin{cases} Ax^3 + Bx^2 + Cx + 4 & : 0 \leq x < 1 \\ D(x-1)^3 + E(x-1)^2 + F(x-1) + 2 & : 1 \leq x \leq 3 \end{cases}$$



## Chapter 7

# Approximating Derivatives

### 7.1 Finite Differences

Suppose we have some blackbox function  $f(x)$  and we wish to calculate  $f'(x)$  at some given  $x$ . Not surprisingly, we start with Taylor's theorem:

$$f(x+h) = f(x) + f'(x)h + \frac{f''(\xi)h^2}{2}.$$

Rearranging we get

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{f''(\xi)h}{2}.$$

Remember that  $\xi$  is between  $x$  and  $x+h$ , but its exact value is not known. If we wish to calculate  $f'(x)$ , we cannot evaluate  $f''(\xi)$ , so we approximate the derivative by dropping the last term. That is, we calculate  $[f(x+h) - f(x)]/h$  as an approximation<sup>1</sup> to  $f'(x)$ . In so doing, we have dropped the last term. If there is a finite bound on  $f''(z)$  on the interval in question then the dropped term is bounded by a constant times  $h$ . That is,

$$\boxed{f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)} \quad (7.1)$$

The error that we incur when we approximate  $f'(x)$  by calculating  $[f(x+h) - f(x)]/h$  is called *truncation error*. It has nothing to do with the kind of error that you get when you do calculations with a computer with limited precision; even if you worked in infinite precision, you would still have truncation error.

The truncation error can be made small by making  $h$  small. However, as  $h$  gets smaller, precision will be lost in equation 7.1 due to subtractive cancellation. The error in calculation for small  $h$  is called *roundoff error*. Generally the roundoff error will increase as  $h$  decreases. Thus there is a nonzero  $h$  for which the sum of these two errors is minimized. See Example Problem 7.5 for an example of this.

The truncation error for this approximation is  $\mathcal{O}(h)$ . We may want a more precise approximation. By now, you should know that any calculation starts with Taylor's Theorem:

$$\begin{aligned} f(x+h) &= f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(\xi_1)}{3!}h^3 \\ f(x-h) &= f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(\xi_2)}{3!}h^3 \end{aligned}$$

---

<sup>1</sup>This approximation for  $f'(x)$  should remind you of the definition of  $f'(x)$  as a limit.

By subtracting these two lines, we get

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{f'''(\xi_1) + f'''(\xi_2)}{3!}h^3.$$

Thus

$$\begin{aligned} 2f'(x)h &= f(x+h) - f(x-h) - \frac{f'''(\xi_1) + f'''(\xi_2)}{3!}h^3 \\ f'(x) &= \frac{f(x+h) - f(x-h)}{2h} - \left[ \frac{f'''(\xi_1) + f'''(\xi_2)}{2} \right] \frac{h^2}{6} \end{aligned}$$

If  $f'''(x)$  is continuous, then there is some  $\xi$  between  $\xi_1, \xi_2$  such that  $f'''(\xi) = \frac{f'''(\xi_1) + f'''(\xi_2)}{2}$ . (This is the MVT at work.) Assuming some uniform bound on  $f'''(\cdot)$ , we get

$$\boxed{f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2)} \quad (7.2)$$

In some situations it may be necessary to use evaluations of a function at “odd” places to approximate a derivative. These are usually straightforward to derive, involving the use of Taylor’s Theorem. The following examples illustrate:

**Example Problem 7.1.** Use evaluations of  $f$  at  $x+h$  and  $x+2h$  to approximate  $f'(x)$ , assuming  $f(x)$  is an *analytic* function, *i.e.*, one with infinitely many derivatives.

*Solution:* First use Taylor’s Theorem to expand  $f(x+h)$  and  $f(x+2h)$ , then subtract to get some factor of  $f'(x)$ :

$$\begin{aligned} f(x+2h) &= f(x) + 2hf'(x) + \frac{4h^2}{2!}f''(x) + \frac{8h^3}{3!}f'''(x) + \frac{16h^4}{4!}f^{(4)}(x) + \dots \\ f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \dots \\ \hline f(x+2h) - f(x+h) &= hf'(x) + \frac{3h^2}{2!}f''(x) + \frac{7h^3}{3!}f'''(x) + \frac{15h^4}{4!}f^{(4)}(x) + \dots \\ (f(x+2h) - f(x+h))/h &= f'(x) + \frac{3h}{2!}f''(x) + \frac{7h^2}{3!}f'''(x) + \frac{15h^3}{4!}f^{(4)}(x) + \dots \end{aligned}$$

Thus  $(f(x+2h) - f(x+h))/h = f'(x) + \mathcal{O}(h)$  ←

**Example Problem 7.2.** Show that

$$\frac{4f(x+h) - f(x+2h) - 3f(x)}{2h} = f'(x) + \mathcal{O}(h^2),$$

for  $f$  with sufficient number of derivatives

*Solution:* In this case we do not have to find the approximation scheme, it is given to us. We only have to expand the appropriate terms with Taylor’s Theorem. As before:

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \dots \\ 4f(x+h) &= 4f(x) + 4hf'(x) + \frac{4h^2}{2!}f''(x) + \frac{4h^3}{3!}f'''(x) + \dots \\ f(x+2h) &= f(x) + 2hf'(x) + \frac{4h^2}{2!}f''(x) + \frac{8h^3}{3!}f'''(x) + \dots \\ \hline 4f(x+h) - f(x+2h) &= 3f(x) + 2hf'(x) + 0f''(x) + \frac{-4h^3}{3!}f'''(x) + \dots \\ 4f(x+h) - f(x+2h) - 3f(x) &= 2hf'(x) + \frac{-4h^3}{3!}f'''(x) + \dots \\ (4f(x+h) - f(x+2h) - 3f(x))/2h &= f'(x) + \frac{-2h^2}{3!}f'''(x) + \dots \end{aligned}$$

←

### 7.1.1 Approximating the Second Derivative

Suppose we want to approximate the second derivative of some blackbox function  $f(x)$ . Again, start with Taylor's Theorem:

$$\begin{aligned} f(x+h) &= f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}(x)}{4!}h^4 + \dots \\ f(x-h) &= f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}(x)}{4!}h^4 - \dots \end{aligned}$$

Now *add* the two series to get

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + 2\frac{f^{(4)}(x)}{4!}h^4 + 2\frac{f^{(6)}(x)}{6!}h^6 + \dots$$

Then let

$$\begin{aligned} \psi(h) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} &= f''(x) + 2\frac{f^{(4)}(x)}{4!}h^2 + 2\frac{f^{(6)}(x)}{6!}h^4 + \dots, \\ &= f''(x) + \sum_{k=1}^{\infty} b_{2k}h^{2k}. \end{aligned}$$

Thus we can use Richardson Extrapolation on  $\psi(h)$  to get higher order approximations.

This derivation also gives us the *centered difference* approximation to the second derivative:

$$\boxed{f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2)}. \quad (7.3)$$

## 7.2 Richardson Extrapolation

The centered difference approximation gives a truncation error of  $\mathcal{O}(h^2)$ , which is better than  $\mathcal{O}(h)$ . Can we do better? Let's define

$$\phi(h) = \frac{1}{2h} [f(x+h) - f(x-h)].$$

Had we expanded the Taylor's Series for  $f(x+h)$ ,  $f(x-h)$  to more terms we would have seen that

$$\phi(h) = f'(x) + a_2 h^2 + a_4 h^4 + a_6 h^6 + a_8 h^8 + \dots$$

The constants  $a_i$  are a function of  $f^{(i+1)}(x)$  only. (In fact, they should take the value of  $\frac{f^{(i+1)}(x)}{(i+1)!}$ .) What happens if we now calculate  $\phi(h/2)$ ?

$$\phi(h/2) = f'(x) + \frac{1}{4}a_2 h^2 + \frac{1}{16}a_4 h^4 + \frac{1}{64}a_6 h^6 + \frac{1}{256}a_8 h^8 + \dots$$

But we can combine this with  $\phi(h)$  to get better accuracy. We have to be a little tricky, but we can get the  $\mathcal{O}(h^2)$  terms to cancel by taking the right multiples of these two approximations:

$$\begin{aligned} \phi(h) - 4\phi(h/2) &= -3f'(x) + \frac{3}{4}4h^4 + \frac{15}{16}a_6 h^6 + \frac{63}{64}a_8 h^8 + \dots \\ \frac{4\phi(h/2) - \phi(h)}{3} &= f'(x) - \frac{1}{4}4h^4 - \frac{5}{16}a_6 h^6 - \frac{21}{64}a_8 h^8 + \dots \end{aligned}$$



### 7.2.2 Using Richardson Extrapolation

We now try out the technique on an example or two.

**Example Problem 7.4.** Approximate the derivative of  $f(x) = \log x$  at  $x = 1$ .

*Solution:* The real answer is  $f'(1) = 1/1 = 1$ , but our computer doesn't know that. Define

$$\phi(h) = \frac{1}{2h} [f(1+h) - f(1-h)] = \frac{\log \frac{1+h}{1-h}}{2h}.$$

Let's use  $h = 0.1$ . We now try to find  $D(2, 2)$ , which is supposed to be a  $\mathcal{O}(h^6)$  approximation to  $f'(1) = 1$ :

| $n \setminus m$ | 0                                                           | 1                     | 2                     |
|-----------------|-------------------------------------------------------------|-----------------------|-----------------------|
| 0               | $\frac{\log \frac{1.1}{0.9}}{0.2} \approx 1.003353477$      |                       |                       |
| 1               | $\frac{\log \frac{1.05}{0.95}}{0.1} \approx 1.000834586$    | $\approx 0.999994954$ |                       |
| 2               | $\frac{\log \frac{1.025}{0.975}}{0.05} \approx 1.000208411$ | $\approx 0.999999686$ | $\approx 1.000000002$ |

This shows that the Richardson method is pretty good. However, notice that for this simple example, we have, already, that  $\phi(0.00001) \approx 0.999999999$ . +

**Example Problem 7.5.** Consider the ugly function:

$$f(x) = \arctan(x).$$

Attempt to find  $f'(\sqrt{2})$ . Recall that  $f'(x) = \frac{1}{1+x^2}$ , so the value that we are seeking is  $\frac{1}{3}$ .

*Solution:* Let's use  $h = 0.01$ . We now try to find  $D(2, 2)$ , which is supposed to be a  $\mathcal{O}(h^6)$  approximation to  $\frac{1}{3}$ :

| $n \setminus m$ | 0                 | 1                 | 2                |
|-----------------|-------------------|-------------------|------------------|
| 0               | 0.333339506181068 |                   |                  |
| 1               | 0.333334876543723 | 0.333333333331274 |                  |
| 2               | 0.33333371913582  | 0.333333333333186 | 0.33333333333313 |

Note that we have some motivation to use Richardson's method in this case: If we let

$$\phi(h) = \frac{1}{2h} [f(\sqrt{2} + h) - f(\sqrt{2} - h)],$$

then making  $h$  small gives a good approximation to  $f'(\sqrt{2})$  until subtractive cancelling takes over. The following table illustrates this:

| $h$                 | $\phi(h)$           |
|---------------------|---------------------|
| 1.0                 | 0.39269908169872408 |
| 0.1                 | 0.33395069677431943 |
| 0.01                | 0.33333950618106845 |
| 0.001               | 0.33333339506169679 |
| 0.0001              | 0.33333333395058062 |
| $1 \times 10^{-5}$  | 0.33333333334106813 |
| $1 \times 10^{-6}$  | 0.33333333332441484 |
| $1 \times 10^{-7}$  | 0.33333333315788138 |
| $1 \times 10^{-8}$  | 0.33333332760676626 |
| $1 \times 10^{-9}$  | 0.33333336091345694 |
| $1 \times 10^{-10}$ | 0.333333360913457   |
| $1 \times 10^{-11}$ | 0.333333360913457   |
| $1 \times 10^{-12}$ | 0.33339997429493451 |
| $1 \times 10^{-13}$ | 0.33306690738754696 |
| $1 \times 10^{-14}$ | 0.33306690738754696 |
| $1 \times 10^{-15}$ | 0.33306690738754691 |
| $1 \times 10^{-16}$ | 0                   |

The data are illustrated in Figure 7.1. Notice that  $\phi(h)$  gives at most 10 decimal places of accuracy, then begins to deteriorate; Note however, we get 13 decimal places from  $D(2, 2)$ .  $\dashv$

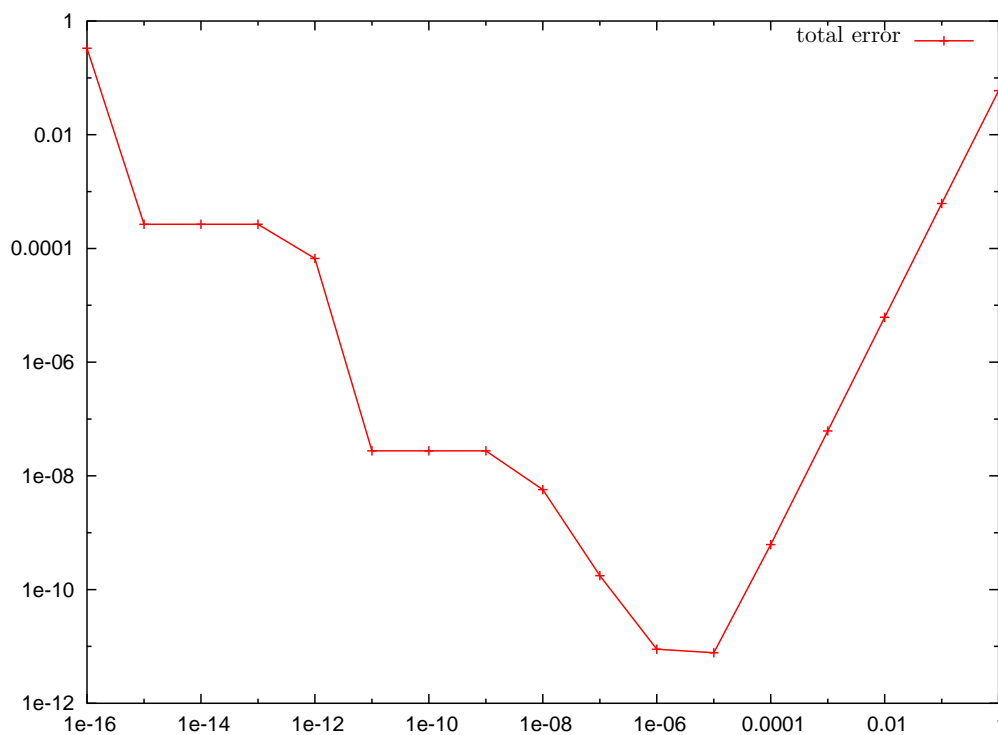


Figure 7.1: The total error for the centered difference approximation to  $f'(\sqrt{2})$  is shown versus  $h$ . The total error is the sum of a truncation term which decreases as  $h$  decreases, and a roundoff term which increases. The optimal  $h$  value is around  $1 \times 10^{-5}$ . Note that Richardson's  $D(2, 2)$  approximation with  $h = 0.01$  gives much better results than this optimal  $h$ .

## EXERCISES

(7.1) Derive the approximation

$$f'(x) \approx \frac{4f(x+h) - 3f(x) - f(x-2h)}{6h}$$

using Taylor's Theorem.

- (a) Assuming that  $f(x)$  has bounded derivatives, give the accuracy of the above approximation. Your answer should be something like  $\mathcal{O}(h^?)$ .
- (b) Let  $f(x) = x^3$ . Approximate  $f'(0)$  with this approximation, using  $h = \frac{1}{4}$ .
- (7.2) Let  $f(x)$  be an *analytic* function, *i.e.*, one which is infinitely differentiable. Let  $\psi(h)$  be the centered difference approximation to the first derivative:

$$\psi(h) = \frac{f(x+h) - f(x-h)}{2h}$$

- (a) Show that  $\psi(h) = f'(x) + \frac{h^2}{3!}f'''(x) + \frac{h^4}{5!}f^{(5)}(x) + \frac{h^6}{7!}f^{(7)}(x) + \dots$
- (b) Show that

$$\frac{8(\psi(h) - \psi(h/2))}{h^2} = f'''(x) + \mathcal{O}(h^2).$$

(7.3) Derive the approximation

$$f'(x) \approx \frac{4f(x+3h) + 5f(x) - 9f(x-2h)}{30h}$$

using Taylor's Theorem.

- (a) What order approximation is this? (Assume  $f(x)$  has bounded derivatives of arbitrary order.)
- (b) Use this formula to approximate  $f'(0)$ , where  $f(x) = x^4$ , and  $h = 0.1$
- (7.4) Suppose you want to know quantity  $Q$ , and can approximate it with some formula, say  $\phi(h)$ , which depends on parameter  $h$ , and such that  $\phi(h) = Q + a_1h + a_2h^2 + a_3h^3 + a_4h^4 + \dots$ . Find some linear combination of  $\phi(h)$  and  $\phi(-h)$  which is a  $\mathcal{O}(h^2)$  approximation to  $Q$ .
- (7.5) Assuming that  $\phi(h) = Q + a_2h^2 + a_4h^4 + a_6h^6 \dots$ , find some combination of  $\phi(h), \phi(h/3)$  which is a  $\mathcal{O}(h^4)$  approximation to  $Q$ .
- (7.6) Let  $\lambda$  be some number in  $(0, 1)$ . Assuming that  $\phi(h) = Q + a_2h^2 + a_4h^4 + a_6h^6 \dots$ , find some combination of  $\phi(h), \phi(\lambda h)$  which is a  $\mathcal{O}(h^4)$  approximation to  $Q$ . To make the constant associated with the  $h^4$  term small in magnitude, what should you do with  $\lambda$ ? Is this practical? Note that the method of Richardson Extrapolation that we considered used the value  $\lambda = 1/2$ .
- (7.7) Assuming that  $\phi(h) = Q + a_2h^2 + a_4h^4 + a_6h^6 \dots$ , find some combination of  $\phi(h), \phi(h/4)$  which is a  $\mathcal{O}(h^4)$  approximation to  $Q$ .
- (7.8) Suppose you have some great computational approximation to the quantity  $Q$  such that  $\psi(h) = Q + a_3h^3 + a_6h^6 + a_9h^9 \dots$ . Can you find some combination of  $\psi(h), \psi(h/2)$  which is a  $\mathcal{O}(h^6)$  approximation to  $Q$ ?
- (7.9) Complete the following Richardson's Extrapolation Table, assuming the first column consists of values  $D(n, 0)$  for  $n = 0, 1, 2$ :

| $n \backslash m$ | 0    | 1 | 2 |
|------------------|------|---|---|
| 0                | 2    |   |   |
| 1                | 1.5  | ? |   |
| 2                | 1.25 | ? | ? |

(See equation 7.4 if you've forgotten the definitions.)

(7.10) Write code to complete a Richardson's Method table, given the first column. Your m-file should have header line like:

```
function Dnn = richardsons(col0)
```

where  $D_{nn}$  is the value at the lower left corner of the table,  $D(n, n)$  while  $col0$  is the column of  $n + 1$  values  $D(i, 0)$ , for  $i = 0, 1, \dots, n$ . Test your code on the following input:

```
octave:1> col0 = [1 0.5 0.25 0.125 0.0625 0.03125];
```

```
octave:2> richardsons(col0)
```

```
ans = 0.019042
```

(a) What do you get when you try the following?

```
octave:5> col0 = [1.5 0.5 1.5 0.5 1.5 0.5 1.5];
```

```
octave:6> richardsons(col0)
```

(b) What do you get when you try the following?

```
octave:7> col0 = [0.9 0.99 0.999 0.9999 0.99999];
```

```
octave:8> richardsons(col0)
```



## Chapter 8

# Integrals and Quadrature

### 8.1 The Definite Integral

Often enough the numerical analyst is presented with the challenge of finding the definite integral of some function:

$$\int_a^b f(x) dx.$$

In your golden years of Calculus, you learned the Fundamental Theorem of Calculus, which claims that if  $f(x)$  is continuous, and  $F(x)$  is an antiderivative of  $f(x)$ , then

$$\int_a^b f(x) dx = F(b) - F(a).$$

What you might not have been told in Calculus is there are some functions for which a closed form antiderivative does not exist or at least is not known to humankind. Nevertheless, you may find yourself in a situation where you have to evaluate an integral for just such an integrand. An approximation will have to do.

#### 8.1.1 Upper and Lower Sums

We will review the definition of the Riemann integral of a function. A *partition* of an interval  $[a, b]$  is a finite, ordered collection of nodes  $x_i$ :

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b.$$

Given such a partition,  $P$ , define the upper and lower bounds on each subinterval  $[x_j, x_{j+1}]$  as follows:

$$m_i = \inf \{f(x) \mid x_i \leq x \leq x_{i+1}\}$$
$$M_i = \sup \{f(x) \mid x_i \leq x \leq x_{i+1}\}$$

Then for this function  $f$  and partition  $P$ , define the upper and lower sums:

$$L(f, P) = \sum_{i=0}^{n-1} m_i (x_{i+1} - x_i)$$
$$U(f, P) = \sum_{i=0}^{n-1} M_i (x_{i+1} - x_i)$$

We can interpret the upper and lower sums graphically as the sums of areas of rectangles defined by the function  $f$  and the partition  $P$ , as in Figure 8.1.

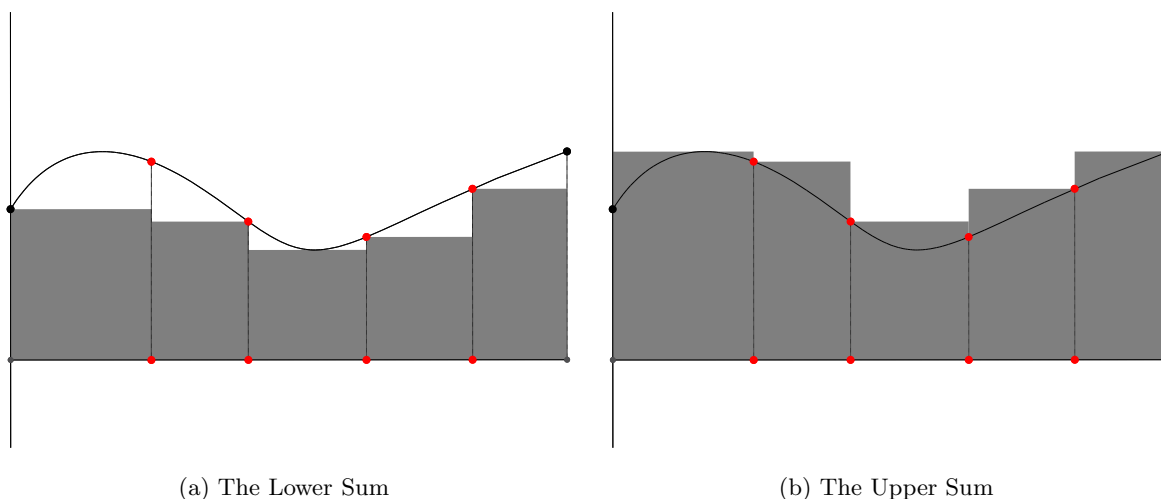


Figure 8.1: The (a) lower, and (b) upper sums of a function on a given interval are shown. These approximations to the integral are the sums of areas of rectangles. Note that the lower sums are an underestimate, and the upper sums an overestimate of the integral.

Notice a few things about the upper, lower sums:

- (i)  $L(f, P) \leq U(f, P)$ .
- (ii) If we switch to a “better” partition (*i.e.*, a finer one), we expect that  $L(f, \cdot)$  increases and  $U(f, \cdot)$  decreases.

The notion of integrability familiar from Calculus class (that is Riemann Integrability) is defined in terms of the upper and lower sums.

**Definition 8.1.** A function  $f$  is Riemann Integrable over interval  $[a, b]$  if

$$\sup_P L(f, P) = \inf_P U(f, P),$$

where the supremum and infimum are over all partitions of the interval  $[a, b]$ . Moreover, in case  $f(x)$  is integrable, we define the integral

$$\int_a^b f(x) dx = \inf_P U(f, P),$$

You may recall the following

**Theorem 8.2.** Every continuous function on a closed bounded interval of the real line is Riemann Integrable (on that interval).

Continuity is sufficient, but not necessary.

**Example 8.3.** Consider the *Heaviside function*:

$$f(x) = \begin{cases} 0 & x < 0 \\ 1 & 0 \leq x \end{cases}$$

This function is not continuous on any interval containing 0, but is Riemann Integrable on every closed bounded interval.

**Example 8.4.** Consider the *Dirichlet function*:

$$f(x) = \begin{cases} 0 & x \text{ rational} \\ 1 & x \text{ irrational} \end{cases}$$

For any partition  $P$  of any interval  $[a, b]$ , we have  $L(f, P) = 0$ , while  $U(f, P) = 1$ , so

$$\sup_P L(f, P) = 0 \neq 1 = \inf_P U(f, P),$$

so this function is *not* Riemann Integrable.

### 8.1.2 Approximating the Integral

The definition of the integral gives a simple method of approximating an integral  $\int_a^b f(x) dx$ . The method cuts the interval  $[a, b]$  into a partition of  $n$  equal subintervals  $x_i = a + \frac{b-a}{n}i$ , for  $i = 0, 1, \dots, n$ . The algorithm then has to somehow find the supremum and infimum of  $f(x)$  on each interval  $[x_i, x_{i+1}]$ . The integral is then approximated by the mean of the lower and upper sums:

$$\int_a^b f(x) dx \approx \frac{1}{2} (L(f, P) + U(f, P)).$$

Because the value of the integral is between  $L(f, P)$  and  $U(f, P)$ , this approximation has error at most

$$\frac{1}{2} (U(f, P) - L(f, P)).$$

Note that in general, or for a black box function, it is usually not feasible to find the suprema and infima of  $f(x)$  on the subintervals, and thus the lower and upper sums cannot be calculated. However, if some information is known about the function, it becomes easier:

**Example 8.5.** Consider for example, using this method on some function  $f(x)$  which is *monotone increasing*, that is  $x \leq y$  implies  $f(x) \leq f(y)$ . In this case, the infimum of  $f(x)$  on each interval occurs at the leftmost endpoint, while the supremum occurs at the right hand endpoint. Thus for this partition,  $P$ , we have

$$\begin{aligned} L(f, P) &= \sum_{k=0}^{n-1} m_k |x_{k+1} - x_k| = \frac{|b-a|}{n} \sum_{k=0}^{n-1} f(x_k) \\ U(f, P) &= \sum_{k=0}^{n-1} M_k |x_{k+1} - x_k| = \frac{|b-a|}{n} \sum_{k=0}^{n-1} f(x_{k+1}) = \frac{|b-a|}{n} \sum_{k=1}^n f(x_k) \end{aligned}$$

Then the error of the approximation is

$$\frac{1}{2} (U(f, P) - L(f, P)) = \frac{1}{2} \frac{|b-a|}{n} [f(x_n) - f(x_0)] = \frac{|b-a| [f(b) - f(a)]}{2n}.$$

### 8.1.3 Simple and Composite Rules

For the remainder of this chapter we will study “simple” quadrature rules, *i.e.*, rules which approximate the integral of a function,  $f(x)$  over an interval  $[a, b]$  by means of a number of evaluations of  $f$  at points in this interval. The error of a simple quadrature rule usually depends on the function

$f$ , and the width of the interval  $[a, b]$  to some power which is determined by the rule. That is we usually think of a simple rule as being applied to a small interval.

To use a simple rule on a larger interval, we usually cast it into a “composite” rule. Thus the trapezoidal rule, which we will study next becomes the composite trapezoidal rule. The means of extending a simple rule to a composite rule is straightforward: Partition the given interval into subintervals, apply the simple rule to each subinterval, and sum the results. Thus, for example if the interval in question is  $[\alpha, \beta]$ , and the partition is  $\alpha = x_0 < x_1 < x_2 < \dots < x_n = \beta$ , we have

$$\text{composite rule on } [\alpha, \beta] = \sum_{i=0}^{n-1} \text{simple rule applied to } [x_i, x_{i+1}].$$

## 8.2 Trapezoidal Rule

Suppose we are trying to approximate the integral

$$\int_a^b f(x) dx,$$

for some unpleasant or black box function  $f(x)$ .

The trapezoidal rule approximates the integral

$$\int_a^b f(x) dx$$

by the (signed) area of the trapezoid through the points  $(a, f(a))$ ,  $(b, f(b))$ , and with one side the segment from  $a$  to  $b$ . See Figure 8.2.

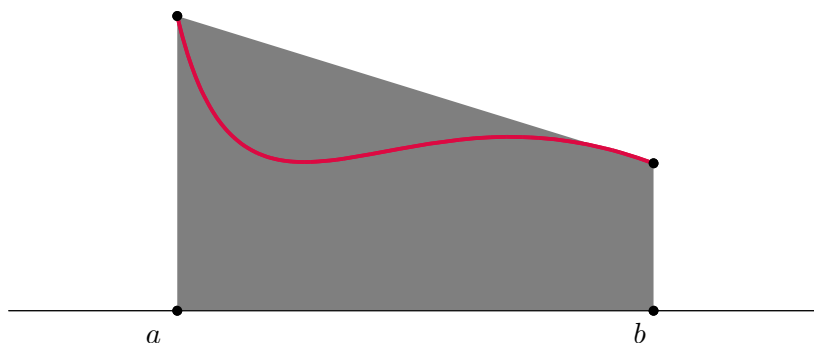


Figure 8.2: The trapezoidal rule for approximating the integral of a function over  $[a, b]$  is shown.

By old school math, we can find this signed area easily. This gives the (simple) trapezoidal rule:

$$\int_a^b f(x) dx \approx (b - a) \frac{f(a) + f(b)}{2}.$$

The composite trapezoidal rule can be written in a simplified form, one which you saw in your calculus class, if the interval in question is partitioned into equal width subintervals. That is if you let  $[\alpha, \beta]$  be partitioned by

$$\alpha = x_0 < x_1 < x_2 < x_3 < \dots < x_n = \beta,$$

with  $x_i = \alpha + ih$ , where  $h = (\beta - \alpha)/n$ , then the composite trapezoidal rule is

$$\int_{\alpha}^{\beta} f(x) dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x) dx \approx \frac{1}{2} \sum_{i=0}^{n-1} (x_{i+1} - x_i) [f(x_i) + f(x_{i+1})]. \quad (8.1)$$

Since each subinterval has equal width,  $x_{i+1} - x_i = h$ , and we have

$$\boxed{\int_a^b f(x) dx \approx \frac{h}{2} \sum_{i=0}^{n-1} [f(x_i) + f(x_{i+1})]}. \quad (8.2)$$

In your calculus class, you saw this in the less comprehensible form:

$$\int_a^b f(x) dx \approx h \left[ \frac{f(a) + f(b)}{2} + \sum_{i=1}^{n-1} f(x_i) \right].$$

Note that the composite trapezoidal rule for equal subintervals is the same as the approximation we found for increasing functions in Example 8.5.

**Example Problem 8.6.** Approximate the integral

$$\int_0^2 \frac{1}{1+x^2} dx$$

by the composite trapezoidal rule with a partition of equally spaced points, for  $n = 2$ .

*Solution:* We have  $h = \frac{2-0}{2} = 1$ , and  $f(x_0) = 1, f(x_1) = \frac{1}{2}, f(x_2) = \frac{1}{5}$ . Then the composite trapezoidal rule gives the value

$$\frac{1}{2} [f(x_0) + f(x_1) + f(x_1) + f(x_2)] = \frac{1}{2} \left[ 1 + 1 + \frac{1}{5} \right] = \frac{11}{10}.$$

The actual value is  $\arctan 2 \approx 1.107149$ , and our approximation is correct to two decimal places.  $\dashv$

### 8.2.1 How Good is the Composite Trapezoidal Rule?

We consider the composite trapezoidal rule for partitions of equal subintervals. Let  $p_i(x)$  be the polynomial of degree  $\leq 1$  that interpolates  $f(x)$  at  $x_i, x_{i+1}$ . Let

$$I_i = \int_{x_i}^{x_{i+1}} f(x) dx, \quad T_i = \int_{x_i}^{x_{i+1}} p_i(x) dx = (x_{i+1} - x_i) \frac{p_i(x_i) + p_i(x_{i+1})}{2} = \frac{h}{2} (f(x_i) + f(x_{i+1})).$$

That's right: the composite trapezoidal rule approximates the integral of  $f(x)$  over  $[x_i, x_{i+1}]$  by the integral of  $p_i(x)$  over the same interval.

Now recall our theorem on polynomial interpolation error. For  $x \in [x_i, x_{i+1}]$ , we have

$$f(x) - p_i(x) = \frac{1}{(2)!} f^{(2)}(\xi_x) (x - x_i) (x - x_{i+1}),$$

for some  $\xi_x \in [x_i, x_{i+1}]$ . Recall that  $\xi_x$  depends on  $x$ . To make things simpler, call it  $\xi(x)$ .

Now integrate:

$$I_i - T_i = \int_{x_i}^{x_{i+1}} f(x) - p_i(x) dx = \frac{1}{2} \int_{x_i}^{x_{i+1}} f''(\xi(x)) (x - x_i)(x - x_{i+1}) dx.$$

We will now attack the integral on the right hand side. Recall the following theorem:

**Theorem 8.7 (Mean Value Theorem for Integrals).** Suppose  $f$  is continuous,  $g$  is Riemann Integrable and does not change sign on  $[\alpha, \beta]$ . Then there is some  $\zeta \in [\alpha, \beta]$  such that

$$\int_{\alpha}^{\beta} f(x)g(x) dx = f(\zeta) \int_{\alpha}^{\beta} g(x) dx.$$

We use this theorem on our integral. Note that  $(x - x_i)(x - x_{i+1})$  is nonpositive on the interval of question,  $[x_i, x_{i+1}]$ . We assume continuity of  $f''(x)$ , and wave our hands to get continuity of  $f''(\xi(x))$ . Then we have

$$I_i - T_i = \frac{1}{2} f''(\xi) \int_{x_i}^{x_{i+1}} (x - x_i)(x - x_{i+1}) dx,$$

for some  $\xi_i \in [x_i, x_{i+1}]$ . By boring calculus and algebra, we find that

$$\int_{x_i}^{x_{i+1}} (x - x_i)(x - x_{i+1}) dx = -\frac{h^3}{6}.$$

This gives

$$I_i - T_i = -\frac{h^3}{12} f''(\xi_i),$$

for some  $\xi_i \in [x_i, x_{i+1}]$ .

We now sum over all subintervals to find the total error of the composite trapezoidal rule

$$E = \sum_{i=0}^{n-1} I_i - T_i = -\frac{h^3}{12} \sum_{i=0}^{n-1} f''(\xi_i) = -\frac{(b-a)h^2}{12} \left[ \frac{1}{n} \sum_{i=0}^{n-1} f''(\xi_i) \right].$$

On the far right we have an average value,  $\frac{1}{n} \sum_{i=0}^{n-1} f''(\xi_i)$ , which lies between the least and greatest values of  $f''$  on the interval  $[a, b]$ , and thus by the IVT, there is some  $\xi$  which takes this value. So

$$E = -\frac{(b-a)h^2}{12} f''(\xi)$$

This gives us the theorem:

**Theorem 8.8 (Error of the Composite Trapezoidal Rule).** Let  $f''(x)$  be continuous on  $[a, b]$ . Let  $T$  be the value of the trapezoidal rule applied to  $f(x)$  on this interval with a partition of uniform spacing,  $h$ , and let  $I = \int_a^b f(x) dx$ . Then there is some  $\xi \in [a, b]$  such that

$$I - T = -\frac{(b-a)h^2}{12} f''(\xi).$$

Note that this theorem tells us not only the magnitude of the error, but the sign as well. Thus if, for example,  $f(x)$  is concave up and thus  $f''$  is positive, then  $I - T$  will be negative, *i.e.*, the trapezoidal rule gives an *overestimate* of the integral  $I$ . See Figure 8.3.

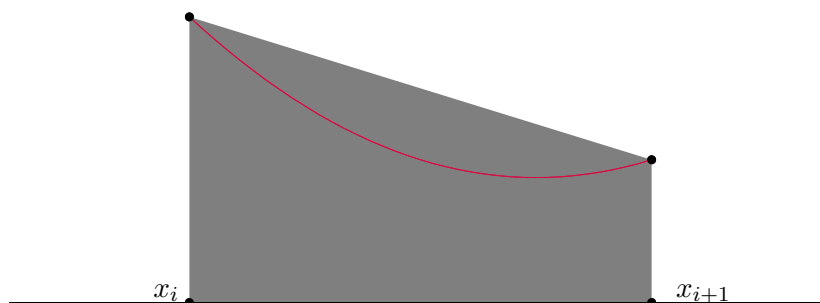


Figure 8.3: The trapezoidal rule is an overestimate for a function which is concave up, *i.e.*, has positive second derivative.

### 8.2.2 Using the Error Bound

**Example Problem 8.9.** How many intervals are required to approximate the integral

$$\ln 2 = I = \int_0^1 \frac{1}{1+x} dx$$

to within  $1 \times 10^{-10}$ ?

*Solution:* We have  $f(x) = \frac{1}{1+x}$ , thus  $f'(x) = -\frac{1}{(1+x)^2}$ . And  $f''(x) = \frac{2}{(1+x)^3}$ . Thus  $f''(\xi)$  is continuous and bounded by 2 on  $[0, 1]$ . If we use  $n$  equal subintervals then Theorem 8.8 tells us the error will be

$$-\frac{1-0}{12} \left( \frac{1-0}{n} \right)^2 f''(\xi) = -\frac{f''(\xi)}{12n^2}.$$

To make this smaller than  $1 \times 10^{-10}$ , in absolute value, we need only take

$$\frac{1}{6n^2} \leq 1 \times 10^{-10},$$

and so  $n \geq \sqrt{\frac{1}{6}} \times 10^5$  suffices. Because  $f''(x)$  is positive on this interval, the trapezoidal rule will be an overestimate.  $\dashv$

**Example Problem 8.10.** How many intervals are required to approximate the integral

$$\int_0^2 x^3 - 1 dx$$

to within  $1 \times 10^{-6}$ ?

*Solution:* We have  $f(x) = x^3 - 1$ , thus  $f'(x) = 3x^2$ , and  $f''(x) = 6x$ . Thus  $f''(\xi)$  is continuous and bounded by 12 on  $[0, 2]$ . If we use  $n$  equal subintervals then by Theorem 8.8 the error will be

$$-\frac{2-0}{12} \left( \frac{2-0}{n} \right)^2 f''(\xi) = -\frac{2f''(\xi)}{3n^2}.$$

To make this smaller than  $1 \times 10^{-6}$ , in absolute value, it suffices to take

$$\frac{24}{3n^2} \leq 1 \times 10^{-6},$$

and so  $n \geq \sqrt{8} \times 10^3$  suffices. Because  $f''(x)$  is positive on this interval, the trapezoidal rule will be an overestimate.  $\dashv$

### 8.3 Romberg Algorithm

Theorem 8.8 tells us, approximately, that the error of the composite trapezoidal rule approximation is  $\mathcal{O}(h^2)$ . If we halve  $h$ , the error is quartered. Sometimes we want to do better than this. We'll use the same trick that we did from Richardson extrapolation. In fact, the forms are exactly the same.

Towards this end, suppose that  $f, a, b$  are given. For a given  $n$ , we are going to use the trapezoidal rule on a partition of  $2^n$  equal subintervals of  $[a, b]$ . That is  $h = \frac{b-a}{2^n}$ . Then define

$$\begin{aligned} \phi(n) &= \frac{1}{2} \frac{b-a}{2^n} \sum_{i=0}^{2^n-1} f(x_i) + f(x_{i+1}) \\ &= \frac{b-a}{2^n} \left[ \frac{f(a)}{2} + \frac{f(b)}{2} + \sum_{i=1}^{2^n-1} f\left(a + i \frac{b-a}{2^n}\right) \right]. \end{aligned}$$

The intervals used to calculate  $\phi(n+1)$  are half the size of those for  $\phi(n)$ . As mentioned above, this means the error is one quarter.

It turns out that if we had proved the error theorem differently, we would have proved the relation:

$$\phi(n) = \int_a^b f(x) dx + a_2 h_n^2 + a_4 h_n^4 + a_6 h_n^6 + a_8 h_n^8 + \dots,$$

where  $h_n = \frac{b-a}{2^n}$ . The constants  $a_i$  are a function of  $f^{(i)}(x)$  only. This should look just like something from Chapter 7. What happens if we now calculate  $\phi(n+1)$ ? We have

$$\begin{aligned} \phi(n+1) &= \int_a^b f(x) dx + a_2 h_{n+1}^2 + a_4 h_{n+1}^4 + a_6 h_{n+1}^6 + a_8 h_{n+1}^8 + \dots, \\ &= \int_a^b f(x) dx + \frac{1}{4} a_2 h_n^2 + \frac{1}{16} a_4 h_n^4 + \frac{1}{64} a_6 h_n^6 + \frac{1}{256} a_8 h_n^8 + \dots \end{aligned}$$

This happens because  $h_{n+1} = \frac{b-a}{2^{n+1}} = \frac{1}{2} \frac{b-a}{2^n} = \frac{h_n}{2}$ . As with Richardson's method for approximating derivatives, we now combine the right multiples of these:

$$\begin{aligned} \phi(n) - 4\phi(n+1) &= -3 \int_a^b f(x) dx + \frac{3}{4} a_2 h_n^2 + \frac{15}{16} a_4 h_n^4 + \frac{63}{64} a_6 h_n^6 + \dots \\ \frac{4\phi(n) - \phi(n+1)}{3} &= \int_a^b f(x) dx - \frac{1}{4} a_2 h_n^2 - \frac{5}{16} a_4 h_n^4 - \frac{21}{64} a_6 h_n^6 + \dots \end{aligned}$$

This approximation has a truncation error of  $\mathcal{O}(h_n^4)$ .

Like in Richardson's method, we can use this to get better and better approximations to the integral. We do this by constructing a triangular array of approximations, each entry depending on two others. Towards this end, we let

$$R(n, 0) = \phi(n),$$



then define, for  $m > 0$

$$R(n, m) = \frac{4^m R(n, m-1) - R(n-1, m-1)}{4^m - 1}. \quad (8.3)$$

The familiar pyramid table then is:

$$\begin{array}{ccccccc} R(0, 0) & & & & & & \\ R(1, 0) & R(1, 1) & & & & & \\ R(2, 0) & R(2, 1) & R(2, 2) & & & & \\ \vdots & \vdots & \vdots & \ddots & & & \\ R(n, 0) & R(n, 1) & R(n, 2) & \cdots & R(n, n) & & \end{array}$$

Even though this is *exactly* the same as Richardson's method, it has another name: this is called the Romberg Algorithm.

**Example Problem 8.11.** Approximating the integral

$$\int_0^2 \frac{1}{1+x^2} dx$$

by Romberg's Algorithm; find  $R(1, 1)$ .

*Solution:* The first column is calculated by the trapezoidal rule. Successive columns are found by combining members of previous columns. So we first calculate  $R(0, 0)$  and  $R(1, 0)$ . These are fairly simple, the first is the trapezoidal rule on a single subinterval, the second is the trapezoidal rule on two subintervals. Then

$$\begin{aligned} R(0, 0) &= \frac{2-0}{1} \frac{1}{2} [f(0) + f(2)] = \frac{6}{5}, \\ R(1, 0) &= \frac{2-0}{2} \frac{1}{2} [f(0) + f(1) + f(1) + f(2)] = \frac{11}{10}. \end{aligned}$$

Then, using Romberg's Algorithm we have

$$R(1, 1) = \frac{4R(1, 0) - R(0, 0)}{4 - 1} = \frac{\frac{44}{10} - \frac{12}{10}}{3} = \frac{32}{30} = 1.0\bar{6}.$$

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At this point we are tempted to use Richardson's analysis. This would claim that  $R(n, n)$  is a  $\mathcal{O}(h_0^{2(n+1)})$  approximation to the integral. However,  $h_0 = b - a$ , and need not be smaller than 1. This is a bit different from Richardson's method, where the original  $h$  is independently set before starting the triangular array; for Romberg's algorithm,  $h_0$  is determined by  $a$  and  $b$ .

We can easily deal with this problem by picking some  $k$  such that  $\frac{b-a}{2^k}$  is small enough, say smaller than 1. Then calculating the following array:

$$\begin{array}{ccccccc} R(k, 0) & & & & & & \\ R(k+1, 0) & R(k+1, 1) & & & & & \\ R(k+2, 0) & R(k+2, 1) & R(k+2, 2) & & & & \\ \vdots & \vdots & \vdots & \ddots & & & \\ R(k+n, 0) & R(k+n, 1) & R(k+n, 2) & \cdots & R(k+n, n) & & \end{array}$$

Quite often Romberg's Algorithm is used to compute columns of this array. Subtractive cancelling or unbounded higher derivatives of  $f(x)$  can make successive approximations *less* accurate. For this reason, entries in ever rightward columns are usually not calculated, rather lower entries in a single column are calculated instead. That is, the user calculates the array:

$$\begin{array}{ccccccc}
 & R(k, 0) & & & & & \\
 R(k+1, 0) & & R(k+1, 1) & & & & \\
 R(k+2, 0) & & R(k+2, 1) & & R(k+2, 2) & & \\
 \vdots & & \vdots & & \vdots & & \ddots \\
 R(k+n, 0) & & R(k+n, 1) & & R(k+n, 2) & \cdots & R(k+n, n) \\
 R(k+n+1, 0) & & R(k+n+1, 1) & & R(k+n+1, 2) & \cdots & R(k+n+1, n) \\
 R(k+n+2, 0) & & R(k+n+2, 1) & & R(k+n+2, 2) & \cdots & R(k+n+2, n) \\
 R(k+n+3, 0) & & R(k+n+3, 1) & & R(k+n+3, 2) & \cdots & R(k+n+3, n) \\
 \vdots & & \vdots & & \vdots & & \vdots
 \end{array}$$

Then  $R(k+n+l, n)$  makes a fine approximation to the integral as  $l \rightarrow \infty$ . Usually  $n$  is small, like 2 or 3.

### 8.3.1 Recursive Trapezoidal Rule

It turns out there is an efficient way of calculating  $R(n+1, 0)$  given  $R(n, 0)$ ; first notice from the above example that

$$\begin{aligned}
 R(0, 0) &= \frac{b-a}{1} \frac{1}{2} [f(a) + f(b)], \\
 R(1, 0) &= \frac{b-a}{2} \frac{1}{2} \left[ f(a) + f\left(\frac{a+b}{2}\right) + f\left(\frac{a+b}{2}\right) + f(b) \right].
 \end{aligned}$$

It would be best to calculate  $R(1, 0)$  without recalculating  $f(a)$  and  $f(b)$ . It turns out this is possible. Let  $h_n = \frac{b-a}{2^n}$ , and recall that

$$R(n, 0) = \phi(n) = h_n \left[ \frac{f(a) + f(b)}{2} + \sum_{i=1}^{2^n-1} f(a + ih_n) \right].$$

Thus

$$\begin{aligned}
 R(n+1, 0) &= \phi(n+1) = h_{n+1} \left[ \frac{f(a) + f(b)}{2} + \sum_{i=1}^{2^{n+1}-1} f(a + ih_{n+1}) \right], \\
 &= \frac{1}{2} h_n \left[ \frac{f(a) + f(b)}{2} + \sum_{i=1}^{2^n-1} f(a + (2i-1)h_{n+1}) + f\left(a + (2i)\frac{1}{2}h_n\right) \right], \\
 &= \frac{1}{2} h_n \left[ \frac{f(a) + f(b)}{2} + \sum_{i=1}^{2^n-1} f(a + ih_n) + \sum_{i=1}^{2^n-1} f(a + (2i-1)h_{n+1}) \right], \\
 &= \frac{1}{2} R(n, 0) + h_{n+1} \sum_{i=1}^{2^n-1} f(a + (2i-1)h_{n+1}).
 \end{aligned}$$

Then calculating  $R(n+1, 0)$  requires only  $2^n - 1$  additional evaluations of  $f(x)$ , instead of the  $2^{n+1} + 1$  usually required.

## 8.4 Gaussian Quadrature

The word *quadrature* refers to a method of approximating the integral of a function as the linear combination of the function at certain points, *i.e.*,

$$\int_a^b f(x) dx \approx A_0 f(x_0) + A_1 f(x_1) + \dots + A_n f(x_n), \quad (8.4)$$

for some collection of nodes  $\{x_i\}_{i=0}^n$ , and weights  $\{A_i\}_{i=0}^n$ . Normally one finds the nodes and weights in a table somewhere; we expect a quadrature rule with more nodes to be more accurate in some sense—the tradeoff is in the number of evaluations of  $f(\cdot)$ . We will examine how these rules are created.

### 8.4.1 Determining Weights (Lagrange Polynomial Method)

Suppose that the nodes  $\{x_i\}_{i=0}^n$  are given. An easy way to find “good” weights  $\{A_i\}_{i=0}^n$  for these nodes is to rig them so the quadrature rule gives the integral of  $p(x)$ , the polynomial of degree  $\leq n$  which interpolates  $f(x)$  on these nodes. Recall

$$p(x) = \sum_{i=0}^n f(x_i) \ell_i(x),$$

where  $\ell_i(x)$  is the  $i^{\text{th}}$  Lagrange polynomial. Thus our rigged approximation is the one that gives

$$\int_a^b f(x) dx \approx \int_a^b p(x) dx = \sum_{i=0}^n f(x_i) \int_a^b \ell_i(x) dx.$$

If we let

$$A_i = \int_a^b \ell_i(x) dx,$$

then we have a quadrature rule.

If  $f(x)$  is a polynomial of degree  $\leq n$  then  $f(x) = p(x)$ , and the quadrature rule is exact.

**Example Problem 8.12.** Construct a quadrature rule on the interval  $[0, 4]$  using nodes  $0, 1, 2$ .

*Solution:* The nodes are given, we determine the weights by constructing the Lagrange Polynomials, and integrating them.

$$\begin{aligned} \ell_0(x) &= \frac{(x-1)(x-2)}{(0-1)(0-2)} = \frac{1}{2}(x-1)(x-2), \\ \ell_1(x) &= \frac{(x-0)(x-2)}{(1-0)(1-2)} = -(x)(x-2), \\ \ell_2(x) &= \frac{(x-0)(x-1)}{(2-0)(2-1)} = \frac{1}{2}(x)(x-1). \end{aligned}$$

Then the weights are

$$\begin{aligned} A_0 &= \int_0^4 \ell_0(x) dx = \int_0^4 \frac{1}{2}(x-1)(x-2) dx = \frac{8}{3}, \\ A_1 &= \int_0^4 \ell_1(x) dx = \int_0^4 -(x)(x-2) dx = -\frac{16}{3}, \\ A_2 &= \int_0^4 \ell_2(x) dx = \int_0^4 \frac{1}{2}(x)(x-1) dx = \frac{20}{3}. \end{aligned}$$

Thus our quadrature rule is

$$\int_0^4 f(x) dx \approx \frac{8}{3}f(0) - \frac{16}{3}f(1) + \frac{20}{3}f(2).$$

We expect this rule to be exact for a quadratic function  $f(x)$ . To illustrate this, let  $f(x) = x^2 + 1$ . By calculus we have

$$\int_0^4 x^2 + 1 dx = \frac{1}{3}x^3 + x \Big|_0^4 = \frac{64}{3} + 4 = \frac{76}{3}.$$

The approximation is

$$\int_0^4 x^2 + 1 dx \approx \frac{8}{3}[0 + 1] - \frac{16}{3}[1 + 1] + \frac{20}{3}[4 + 1] = \frac{76}{3}.$$

–

### 8.4.2 Determining Weights (Method of Undetermined Coefficients)

Using the Lagrange Polynomial Method to find the weights  $A_i$  is fine for a computer, but can be tedious (and error-prone) if done by hand (say, on an exam). The method of undetermined coefficients is a good alternative for finding the weights by hand, and for small  $n$ .

The idea behind the method is to find  $n + 1$  equations involving the  $n + 1$  weights. The equations are derived by letting the quadrature rule be exact for  $f(x) = x^j$  for  $j = 0, 1, \dots, n$ . That is, setting

$$\int_a^b x^j dx = \sum_{i=0}^n A_i (x_i)^j.$$

For example, we reconsider Example Problem 8.12.

**Example Problem 8.13.** Construct a quadrature rule on the interval  $[0, 4]$  using nodes 0, 1, 2.

*Solution:* The method of undetermined coefficients gives the equations:

$$\begin{aligned} \int_0^4 1 dx &= 4 = A_0 + A_1 + A_2 \\ \int_0^4 x dx &= 8 = A_1 + 2A_2 \\ \int_0^4 x^2 dx &= 64/3 = A_1 + 4A_2. \end{aligned}$$

We perform Naïve Gaussian Elimination on the system:

$$\left( \begin{array}{ccc|c} 1 & 1 & 1 & 4 \\ 0 & 1 & 2 & 8 \\ 0 & 1 & 4 & 64/3 \end{array} \right)$$

We get the same weights as in Example Problem 8.12:  $A_2 = \frac{20}{3}, A_1 = -\frac{16}{3}, A_0 = \frac{8}{3}$ .

–

Notice the difference compared to the Lagrange Polynomial Method: undetermined coefficients requires solution of a linear system, while the former method calculates the weights “directly.” Since we will not consider  $n$  to be very large, solving the linear system may not be too burdensome.

Moreover, the method of undetermined coefficients is useful in more general settings, as illustrated by the next example:

**Example Problem 8.14.** Determine a “quadrature” rule of the form

$$\int_0^1 f(x) dx \approx Af(1) + Bf'(1) + Cf''(1)$$

that is exact for polynomials of highest possible degree. What is the highest degree polynomial for which this rule is exact?

*Solution:* Since there are three unknown coefficients to be determined, we look for three equations. We get these equations by plugging in successive polynomials. That is, we plug in  $f(x) = 1, x, x^2$  and assuming the coefficients give equality:

$$\begin{aligned} \int_0^1 1 dx &= 1 = A \cdot 1 + B \cdot 0 + C \cdot 0 = A \\ \int_0^1 x dx &= 1/2 = A \cdot 1 + B \cdot 1 + C \cdot 0 = A + B \\ \int_0^1 x^2 dx &= 1/3 = A \cdot 1 + B \cdot 2 + C \cdot 2 = A + 2B + 2C \end{aligned}$$

This is solved by  $A = 1, B = -1/2, C = 1/6$ . This rule should be exact for polynomials of degree no greater than 2, but it might be better. We should check:

$$\int_0^1 x^3 dx = 1/4 \neq 1/2 = 1 - 3/2 + 1 = A + B + C,$$

and thus the rule is *not* exact for cubic polynomials, or those of higher degree. +

### 8.4.3 Gaussian Nodes

It would seem this is the best we can do: using  $n + 1$  nodes we can devise a quadrature rule that is exact for polynomials of degree  $\leq n$  by choosing the weights correctly. It turns out that by choosing the *nodes* in the right way, we can do far better. Gauss discovered that the right nodes to choose are the  $n + 1$  roots of the (nontrivial) polynomial,  $q(x)$ , of degree  $n + 1$  which has the property

$$\int_a^b x^k q(x) dx = 0 \quad (0 \leq k \leq n).$$

(If you view the integral as an inner product, you could say that  $q(x)$  is orthogonal to the polynomials  $x^k$  in the resultant inner product space, but that’s just fancy talk.)

Suppose that we have such a  $q(x)$ —we will not prove existence or uniqueness. Let  $f(x)$  be a polynomial of degree  $\leq 2n + 1$ . We write

$$f(x) = p(x)q(x) + r(x).$$

Both  $p(x), r(x)$  are of degree  $\leq n$ . Because of how we picked  $q(x)$  we have

$$\int_a^b p(x)q(x) dx = 0.$$

Thus

$$\int_a^b f(x) dx = \int_a^b p(x)q(x) dx + \int_a^b r(x) dx = \int_a^b r(x) dx.$$

Now suppose that the  $A_i$  are chosen by Lagrange Polynomials so the quadrature rule on the nodes  $x_i$  is exact for polynomials of degree  $\leq n$ . Then

$$\sum_{i=0}^n A_i f(x_i) = \sum_{i=0}^n A_i [p(x_i)q(x_i) + r(x_i)] = \sum_{i=0}^n A_i r(x_i).$$

The last equality holds because the  $x_i$  are the roots of  $q(x)$ . Because of how the  $A_i$  are chosen we then have

$$\sum_{i=0}^n A_i f(x_i) = \sum_{i=0}^n A_i r(x_i) = \int_a^b r(x) dx = \int_a^b f(x) dx.$$

Thus this rule is exact for  $f(x)$ . We have (or rather, Gauss has) made quadrature twice as good.

**Theorem 8.15 (Gaussian Quadrature Theorem).** Let  $x_i$  be the  $n + 1$  roots of a (nontrivial) polynomial,  $q(x)$ , of degree  $n + 1$  which has the property

$$\int_a^b x^k q(x) dx = 0 \quad (0 \leq k \leq n).$$

Let  $A_i$  be the coefficients for these nodes chosen by integrating the Lagrange Polynomials. Then the quadrature rule for this choice of nodes and coefficients is exact for polynomials of degree  $\leq 2n + 1$ .

#### 8.4.4 Determining Gaussian Nodes

We can determine the Gaussian nodes in the same way we determine coefficients. The example is illustrative

**Example Problem 8.16.** Find the two Gaussian nodes for a quadrature rule on the interval  $[0, 2]$ .

*Solution:* We will find the function  $q(x)$  of degree 2, which is “orthogonal” to  $1, x$  under the inner product of integration over  $[0, 2]$ . Thus we let  $q(x) = c_0 + c_1x + c_2x^2$ . The orthogonality condition becomes

$$\begin{aligned} \int_0^2 1q(x) dx &= \int_0^2 xq(x) dx = 0 && \text{that is,} \\ \int_0^2 c_0 + c_1x + c_2x^2 dx &= \int_0^2 c_0x + c_1x^2 + c_2x^3 dx = 0 \end{aligned}$$

Evaluating these integrals gives the following system of linear equations:

$$\begin{aligned} 2c_0 + 2c_1 + \frac{8}{3}c_2 &= 0, \\ 2c_0 + \frac{8}{3}c_1 + 4c_2 &= 0. \end{aligned}$$

This system is “underdetermined,” that is, there are two equations, but three unknowns. Notice, however, that if  $q(x)$  satisfies the orthogonality conditions, then so does  $\hat{q}(x) = \alpha q(x)$ , for any real number  $\alpha$ . That is, we can pick the scaling of  $q(x)$  as we wish.

With great foresight, we “guess” that we want  $c_2 = 3$ . This reduces the equations to

$$\begin{aligned} 2c_0 + 2c_1 &= -8, \\ 2c_0 + \frac{8}{3}c_1 &= -12. \end{aligned}$$

Simple Gaussian Elimination (*cf.* Chapter 3) yields the answer  $c_0 = 2, c_1 = -6, c_2 = 3$ . Then our nodes are the roots of  $q(x) = 2 - 6x + 3x^2$ . That is the roots

$$\frac{6 \pm \sqrt{36 - 24}}{6} = 1 \pm \frac{\sqrt{3}}{3}.$$

These nodes are a bit ugly. Rather than construct the Lagrange Polynomials, we will use the method of undetermined coefficients. Remember, we want to construct  $A_0, A_1$  such that

$$\int_0^2 f(x) dx \approx A_0 f\left(1 - \frac{\sqrt{3}}{3}\right) + A_1 f\left(1 + \frac{\sqrt{3}}{3}\right)$$

is exact for polynomial  $f(x)$  of degree  $\leq 1$ . It suffices to make this approximation exact for the “building blocks” of such polynomials, that is, for the functions 1 and  $x$ . That is, it suffices to find  $A_0, A_1$  such that

$$\begin{aligned} \int_0^2 1 dx &= A_0 + A_1 \\ \int_0^2 x dx &= A_0\left(1 - \frac{\sqrt{3}}{3}\right) + A_1\left(1 + \frac{\sqrt{3}}{3}\right) \end{aligned}$$

This gives the equations

$$\begin{aligned} 2 &= A_0 + A_1 \\ 2 &= A_0\left(1 - \frac{\sqrt{3}}{3}\right) + A_1\left(1 + \frac{\sqrt{3}}{3}\right) \end{aligned}$$

This is solved by  $A_0 = A_1 = 1$ .

Thus our quadrature rule is

$$\boxed{\int_0^2 f(x) dx \approx f\left(1 - \frac{\sqrt{3}}{3}\right) + f\left(1 + \frac{\sqrt{3}}{3}\right)}.$$

We expect this rule to be exact for cubic polynomials. +

**Example Problem 8.17.** Verify the results of the previous example problem for  $f(x) = x^3$ .

*Solution:* We have

$$\int_0^2 f(x) dx = (1/4) x^4 \Big|_0^2 = 4.$$

The quadrature rule gives

$$\begin{aligned} f\left(1 - \frac{\sqrt{3}}{3}\right) + f\left(1 + \frac{\sqrt{3}}{3}\right) &= \left(1 - \frac{\sqrt{3}}{3}\right)^3 + \left(1 + \frac{\sqrt{3}}{3}\right)^3 \\ &= \left(1 - 3\frac{\sqrt{3}}{3} + 3\frac{3}{9} - \frac{3\sqrt{3}}{27}\right) + \left(1 + 3\frac{\sqrt{3}}{3} + 3\frac{3}{9} + \frac{3\sqrt{3}}{27}\right) \\ &= \left(2 - \sqrt{3} - \sqrt{3}/9\right) + \left(2 + \sqrt{3} + \sqrt{3}/9\right) = 4 \end{aligned}$$

Thus the quadrature rule is exact for  $f(x)$ . +

### 8.4.5 Reinventing the Wheel

While it is good to know the theory, it doesn't make sense in practice to recompute these things all the time. There are books full of quadrature rules; any good textbook will list a few. The simplest ones are given in Table 8.1.

See also <http://mathworld.wolfram.com/Legendre-GaussQuadrature.html>

| $n$ | $x_i$               | $A_i$       |
|-----|---------------------|-------------|
| 0   | $x_0 = 0$           | $A_0 = 2$   |
| 1   | $x_0 = -\sqrt{1/3}$ | $A_0 = 1$   |
|     | $x_1 = \sqrt{1/3}$  | $A_1 = 1$   |
| 2   | $x_0 = -\sqrt{3/5}$ | $A_0 = 5/9$ |
|     | $x_1 = 0$           | $A_1 = 8/9$ |
|     | $x_2 = \sqrt{3/5}$  | $A_2 = 5/9$ |

Table 8.1: Gaussian Quadrature rules for the interval  $[-1, 1]$ . Thus  $\int_{-1}^1 f(x) dx \approx \sum_{i=0}^n A_i f(x_i)$ , with this relation holding exactly for all polynomials of degree no greater than  $2n + 1$ .

Quadrature rules are normally given for the interval  $[-1, 1]$ . On first consideration, it would seem you need a different rule for each interval  $[a, b]$ . This is not the case, as the following example problem illustrates:

**Example Problem 8.18.** Given a quadrature rule which is good on the interval  $[-1, 1]$ , derive a version of the rule to apply to the interval  $[a, b]$ .

*Solution:* Consider the substitution:

$$x = \frac{b-a}{2}t + \frac{b+a}{2}, \quad \text{so} \quad dx = \frac{b-a}{2} dt.$$

Then

$$\int_a^b f(x) dx = \int_{-1}^1 f\left(\frac{b-a}{2}t + \frac{b+a}{2}\right) \frac{b-a}{2} dt.$$

Letting

$$g(t) = \frac{b-a}{2} f\left(\frac{b-a}{2}t + \frac{b+a}{2}\right),$$

if  $f(x)$  is a polynomial,  $g(t)$  is a polynomial of the same degree. Thus we can use the quadrature rule for  $[-1, 1]$  on  $g(t)$  to evaluate the integral of  $f(x)$  over  $[a, b]$ .  $\dashv$

**Example Problem 8.19.** Derive the quadrature rules of Example Problem 8.16 by using the technique of Example Problem 8.18 and the quadrature rules of Table 8.1.

*Solution:* We have  $a = 0, b = 2$ . Thus

$$g(t) = \frac{b-a}{2} f\left(\frac{b-a}{2}t + \frac{b+a}{2}\right) = f(t+1).$$

To integrate  $f(x)$  over  $[0, 2]$ , we integrate  $g(t)$  over  $[-1, 1]$ . The standard Gaussian Quadrature rule approximates this as

$$\int_{-1}^1 g(t) dt \approx g(-\sqrt{1/3}) + g(\sqrt{1/3}) = f(1 - \sqrt{1/3}) + f(1 + \sqrt{1/3}).$$

This is the same rule that was derived (with much more work) in Example Problem 8.16.  $\dashv$



## EXERCISES

- (8.1) Use the composite trapezoidal rule, by hand, to approximate

$$\int_0^3 x^2 dx (= 9)$$

Use the partition  $\{x_i\}_{i=0}^2 = \{0, 1, 3\}$ . Why is your approximation an overestimate?

- (8.2) Use the composite trapezoidal rule, by hand, to approximate

$$\int_0^1 \frac{1}{x+1} dx (= \ln 2 \approx 0.693)$$

Use the partition  $\{x_i\}_{i=0}^3 = \{0, \frac{1}{4}, \frac{1}{2}, 1\}$ . Why is your approximation an overestimate? (*Check: I think the answer is 0.7*)

- (8.3) Use the composite trapezoidal rule, by hand to approximate

$$\int_0^1 \frac{4}{1+x^2} dx.$$

Use  $n = 4$  subintervals. How good is your answer?

- (8.4) Use Theorem 8.8 to bound the error of the composite trapezoidal rule approximation of  $\int_0^2 x^3 dx$  with  $n = 10$  intervals. You should find that the approximation is an overestimate.
- (8.5) How many equal subintervals of  $[0, 1]$  are required to approximate  $\int_0^1 \cos x dx$  with error smaller than  $1 \times 10^{-6}$  by the composite trapezoidal rule? (Use Theorem 8.8.)
- (8.6) How many equal subintervals would be required to approximate

$$\int_0^1 \frac{4}{1+x^2} dx.$$

to within 0.0001 by the composite trapezoidal rule? (*Hint: Use the fact that  $|f''(x)| \leq 8$  on  $[0, 1]$  for  $f(x) = 4/(1+x^2)$ )*)

- (8.7) How many equal subintervals of  $[2, 3]$  are required to approximate  $\int_2^3 e^x dx$  with error smaller than  $1 \times 10^{-3}$  by the composite trapezoidal rule?
- (8.8) *Simpson's Rule* for quadrature is given as

$$\int_a^b f(x) dx \approx \frac{\Delta x}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \dots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)],$$

where  $\Delta x = (b - a)/n$ , and  $n$  is assumed to be even. Show that Simpson's Rule for  $n = 2$  is actually given by Romberg's Algorithm as  $R(1, 1)$ . As such we expect Simpson's Rule to be a  $\mathcal{O}(h^4)$  approximation to the integral.

- (8.9) Find a quadrature rule of the form

$$\int_0^1 f(x) dx \approx Af(0) + Bf(1/2) + Cf(1)$$

that is exact for polynomials of highest possible degree. What is the highest degree polynomial for which this rule is exact?

(8.10) Determine a “quadrature” rule of the form

$$\int_{-1}^1 f(x) dx \approx Af(0) + Bf'(-1) + Cf'(1)$$

that is exact for polynomials of highest possible degree. What is the highest degree polynomial for which this rule is exact? (Since this rule uses derivatives of  $f$ , it does not exactly fit our definition of a quadrature rule, but it may be applicable in some situations.)

(8.11) Determine a “quadrature” rule of the form

$$\int_0^1 f(x) dx \approx Af(0) + Bf'(0) + Cf(1)$$

that is exact for polynomials of highest possible degree. What is the highest degree polynomial for which this rule is exact?

(8.12) Consider the so-called order  $n$  *Chebyshev Quadrature* rule:

$$\int_{-1}^1 f(x) dx \approx c_n \sum_{i=0}^n f(x_i)$$

Find the weighting  $c_n$  and nodes  $x_i$  for the case  $n = 2$  and the case  $n = 3$ . For what order polynomials are these rules exact?

(8.13) Find the Gaussian Quadrature rule with 2 nodes for the interval  $[1, 5]$ , *i.e.*, find a rule

$$\int_1^5 f(x) dx \approx Af(x_0) + Bf(x_1)$$

Before you solve the problem, consider the following questions: do you expect the nodes to be the endpoints 1 and 5? do you expect the nodes to be arranged symmetrically around the midpoint of the interval?

(8.14) Find the Gaussian Quadrature rule with 3 nodes for the interval  $[-1, 1]$ , *i.e.*, find a rule

$$\int_{-1}^1 f(x) dx \approx Af(x_0) + Bf(x_1) + Cf(x_2)$$

To find the nodes  $x_0, x_1, x_2$  you will have to find the zeroes of a cubic equation, which could be difficult. However, you may use the simplifying assumption that the nodes are symmetrically placed in the interval  $[-1, 1]$ .

(8.15) Write code to approximate the integral of a  $f$  on  $[a, b]$  by the composite trapezoidal rule on  $n$  equal subintervals. Your m-file should have header line like:

```
function iappx = trapezoidal(f,a,b,n)
```

You may wish to use the code:

```
x = a .+ (b-a) .* (0:n) ./ n;
```

If  $f$  is defined to work on vectors element-wise, you can probably speed up your computation by using

```
bigsum = 0.5 * ( f(x(1)) + f(x(n+1)) ) + sum( f(x(2:(n))) );
```

(8.16) Write code to implement the Gaussian Quadrature rule for  $n = 2$  to integrate  $f$  on the interval  $[a, b]$ . Your m-file should have header line like:

```
function iappx = gauss2(f,a,b)
```

(8.17) Write code to implement composite Gaussian Quadrature based on code from the previous problem. Something like the following probably works:

```
function iappx = gaussComp(f,a,b,n)
% code to approximate integral of f over n equal subintervals of [a,b]
x = a .+ (b-a) .* (0:n) ./ n;
iappx = 0;
for i=1:n
    iappx += gauss2(f,x(i),x(i+1));
end
```

Use your code to approximate the *error function*:

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt.$$

Compare your results with the octave/Matlab builtin function `erf`. (Try `help erf` in octave, or see <http://mathworld.wolfram.com/Erf.html>)

The error function is used in probability. In particular, the probability that a normal random variable is within  $z$  standard deviations from its mean is

$$\operatorname{erf}(z/\sqrt{2})$$

Thus  $\operatorname{erf}(1/\sqrt{2}) \approx 0.683$ , and  $\operatorname{erf}(2/\sqrt{2}) \approx 0.955$ . These numbers should look familiar to you.



# Chapter 9

## Least Squares

### 9.1 Least Squares

Least squares is a general class of methods for fitting observed data to a theoretical model function. In the general setting we are given a set of data

$$\begin{array}{c|c|c|c|c} x & x_0 & x_1 & \dots & x_n \\ \hline y & y_0 & y_1 & \dots & y_n \end{array}$$

and some class of functions,  $\mathcal{F}$ . The goal then is to find the “best”  $f \in \mathcal{F}$  to fit the data to  $y = f(x)$ . Usually the class of functions  $\mathcal{F}$  will be determined by some small number of parameters; the number of parameters will be smaller (usually much smaller) than the number of data points. The theory here will be concerned with defining “best,” and examining methods for finding the “best” function to fit the data.

#### 9.1.1 The Definition of Ordinary Least Squares

First we consider the data to be two vectors of length  $n + 1$ . That is we let

$$\mathbf{x} = [x_0 \ x_1 \ \dots \ x_n]^\top, \quad \text{and} \quad \mathbf{y} = [y_0 \ y_1 \ \dots \ y_n]^\top.$$

The *error*, or *residual*, of a given function with respect to this data is the vector  $\mathbf{r} = \mathbf{y} - f(\mathbf{x})$ . That is

$$\mathbf{r} = [r_0 \ r_1 \ \dots \ r_n]^\top, \quad \text{where } r_i = y_i - f(x_i).$$

Our goal is to find  $f \in \mathcal{F}$  such that  $\mathbf{r}$  is reasonably small. We measure the size of a vector by the use of norms, which were explored in Subsection 1.4.1. The most useful norms are the  $\ell^p$  norms. For a given  $p$  with  $0 < p < \infty$ , the  $\ell^p$  norm of  $\mathbf{r}$  is defined as

$$\|\mathbf{r}\|_p = \left( \sum_{i=0}^n r_i^p \right)^{1/p}$$

For the purposes of approximation, the easiest norm to use is the  $\ell^2$  norm:

**Definition 9.1.1 ((Ordinary) Least Squares Best Approximant).** The *least-squares best approximant* to a set of data,  $\mathbf{x}$ ,  $\mathbf{y}$  from a class of functions,  $\mathcal{F}$ , is the function  $f^* \in \mathcal{F}$  that minimizes the  $\ell^2$  norm of the error. That is, if  $f^*$  is the least squares best approximant, then

$$\|\mathbf{y} - f^*(\mathbf{x})\|_2 = \min_{f \in \mathcal{F}} \|\mathbf{y} - f(\mathbf{x})\|_2$$

We will generally assume uniqueness of the minimum. This method is sometimes called the *ordinary* least squares method. It assumes there is no error in the measurement of the data  $\mathbf{x}$ , and usually admits a relatively straightforward solution.

### 9.1.2 Linear Least Squares

We illustrate this definition using the class of linear functions as an example, as this case is reasonably simple. We are assuming

$$\mathcal{F} = \{f(x) = ax + b \mid a, b \in \mathbb{R}\}.$$

We can now think of our job as drawing the “best” line through the data.

By Definition 9.1.1, we want to find the function  $f(x) = ax + b$  that minimizes

$$\left( \sum_{i=0}^n [y_i - f(x_i)]^2 \right)^{1/2}.$$

This is a minimization problem over two variables,  $x$  and  $y$ . As you may recall from calculus class, it suffices to minimize the sum rather than its square root. That is, it suffices to minimize

$$\sum_{i=0}^n [ax_i + b - y_i]^2.$$

We minimize this function with calculus. We set

$$\begin{aligned} 0 = \frac{\partial \phi}{\partial a} &= \sum_{k=0}^n 2x_k (ax_k + b - y_k) \\ 0 = \frac{\partial \phi}{\partial b} &= \sum_{k=0}^n 2(ax_k + b - y_k) \end{aligned}$$

These are called the *normal equations*. Believe it or not these are two equations in two unknowns. They can be reduced to

$$\begin{aligned} \sum x_k^2 a + \sum x_k b &= \sum x_k y_k \\ \sum x_k a + (n+1)b &= \sum y_k \end{aligned}$$

The solution is found by naïve Gaussian Elimination, and is ugly. Let

$$\begin{aligned} d_{11} &= \sum x_k^2 \\ d_{12} = d_{21} &= \sum x_k \\ d_{22} &= n+1 \\ e_1 &= \sum x_k y_k \\ e_2 &= \sum y_k \end{aligned}$$

We want to solve

$$\begin{aligned} d_{11}a + d_{12}b &= e_1 \\ d_{21}a + d_{22}b &= e_2 \end{aligned}$$

Gaussian Elimination produces

$$\begin{aligned} a &= \frac{d_{22}e_1 - d_{12}e_2}{d_{22}d_{11} - d_{12}d_{21}} \\ b &= \frac{d_{11}e_2 - d_{21}e_1}{d_{22}d_{11} - d_{12}d_{21}} \end{aligned}$$

The answer is not so enlightening as the means of finding the solution.

We should, for a moment, consider whether this is indeed the solution. Our calculations have only shown an extrema at this choice of  $(a, b)$ ; could it not be a maxima?

### 9.1.3 Least Squares from Basis Functions

In many, but not all cases, the class of functions,  $\mathcal{F}$ , is the span of a small set of functions. This case is simpler to explore and we consider it here. In this case  $\mathcal{F}$  can be viewed as a vector space over the real numbers. That is, for  $f, g \in \mathcal{F}$ , and  $\alpha, \beta \in \mathbb{R}$ , then  $\alpha f + \beta g \in \mathcal{F}$ , where the function  $\alpha f$  is that function such that  $(\alpha f)(x) = \alpha f(x)$ .

Now let  $\{g_j(x)\}_{j=0}^m$  be a set of  $m + 1$  linearly independent functions, *i.e.*,

$$c_0g_0(x) + c_1g_1(x) + \dots + c_mg_m(x) = 0 \quad \forall x \quad \Rightarrow \quad c_0 = c_1 = \dots = c_m = 0$$

Then we say that  $\mathcal{F}$  is *spanned* by the functions  $\{g_j(x)\}_{j=0}^m$  if

$$\mathcal{F} = \left\{ f(x) = \sum_j c_j g_j(x) \mid c_j \in \mathbb{R}, j = 0, 1, \dots, m \right\}.$$

In this case the functions  $g_j$  are *basis functions* for  $\mathcal{F}$ . Note the basis functions need not be unique: a given class of functions will usually have more than one choice of basis functions.

**Example 9.1.** The class  $\mathcal{F} = \{f(x) = ax + b \mid a, b \in \mathbb{R}\}$  is spanned by the two functions  $g_0(x) = 1$ , and  $g_1(x) = x$ . However, it is also spanned by the two functions  $\tilde{g}_0(x) = 2x + 1$ , and  $\tilde{g}_1(x) = x - 1$ .

To find the least squares best approximant of  $\mathcal{F}$  for a given set of data, we minimize the square of the  $\ell^2$  norm of the error; that is we minimize the function

$$\phi(c_0, c_1, \dots, c_m) = \sum_{k=0}^n \left[ \left( \sum_j c_j g_j(x_k) \right) - y_k \right]^2 \quad (9.1)$$

Again we set partials to zero and solve

$$0 = \frac{\partial \phi}{\partial c_i} = \sum_{k=0}^n 2 \left[ \left( \sum_j c_j g_j(x_k) \right) - y_k \right] g_i(x_k)$$

This can be rearranged to get

$$\sum_{j=0}^m \left[ \sum_k g_j(x_k) g_i(x_k) \right] c_j = \sum_{k=0}^n y_k g_i(x_k)$$

If we now let

$$d_{ij} = \sum_{k=0}^n g_j(x_k)g_i(x_k), \quad e_i = \sum_{k=0}^n y_k g_i(x_k),$$

Then we have reduced the problem to the linear system (again, called the normal equations):

$$\begin{bmatrix} d_{00} & d_{01} & d_{02} & \cdots & d_{0m} \\ d_{10} & d_{11} & d_{12} & \cdots & d_{1m} \\ d_{20} & d_{21} & d_{22} & \cdots & d_{2m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ d_{m0} & d_{m1} & d_{m2} & \cdots & d_{mm} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} e_0 \\ e_1 \\ e_2 \\ \vdots \\ e_m \end{bmatrix} \quad (9.2)$$

The choice of the basis functions can affect how easy it is to solve this system. We explore this in Section 9.2. Note that we are talking about the basis  $\{g_j\}_{j=0}^m$ , and not exactly about the class of functions  $\mathcal{F}$ .

For example, consider what would happen if the system of normal equations were diagonal. In this case, solving the system would be rather trivial.

**Example Problem 9.2.** Consider the case where  $m = 0$ , and  $g_0(x) = \ln x$ . Find the least squares approximation of the data

|     |           |           |           |          |          |          |          |          |
|-----|-----------|-----------|-----------|----------|----------|----------|----------|----------|
| $x$ | 0.50      | 0.75      | 1.0       | 1.50     | 2.0      | 2.25     | 2.75     | 3.0      |
| $y$ | -1.187098 | -0.452472 | -0.068077 | 0.713938 | 1.165234 | 1.436975 | 1.725919 | 1.841422 |

*Solution:* Essentially we are trying to find the  $c$  such that  $c \ln x$  best approximates the data. The system of equation 9.2 reduces to the 1-D equation:

$$[\sum_k \ln^2 x_k] c = \sum_k y_k \ln x_k$$

For our data, this reduces to:

$$4.0960c = 6.9844$$

so we find  $c = 1.7052$ . The data and the least squares interpolant are shown in Figure 9.1.  $\dashv$

**Example 9.3.** Consider the awfully chosen basis functions:

$$\begin{aligned} g_0(x) &= \left(\frac{\epsilon}{2} - 1\right)x^2 - \frac{\epsilon}{2}x + 1 \\ g_1(x) &= x^3 + \left(\frac{\epsilon}{2} - 1\right)(x^2 + x) + 1 \end{aligned}$$

where  $\epsilon$  is small, around machine precision.

Suppose the data are given at the nodes  $x_0 = 0, x_1 = 1, x_2 = -1$ . We want to set up the normal equations, so we compute some of the  $d_{ij}$ . First we have to evaluate the basis functions at the nodes  $x_i$ . But this example was rigged to give:

$$\begin{aligned} g_0(x_0) &= 1, \quad g_0(x_1) = 0, \quad g_0(x_2) = \epsilon \\ g_1(x_0) &= 1, \quad g_1(x_1) = \epsilon, \quad g_1(x_2) = 0 \end{aligned}$$

After much work we find we want to solve

$$\begin{bmatrix} 1 + \epsilon^2 & 1 \\ 1 & 1 + \epsilon^2 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \begin{bmatrix} y_0 + \epsilon y_2 \\ y_0 + \epsilon y_1 \end{bmatrix}$$



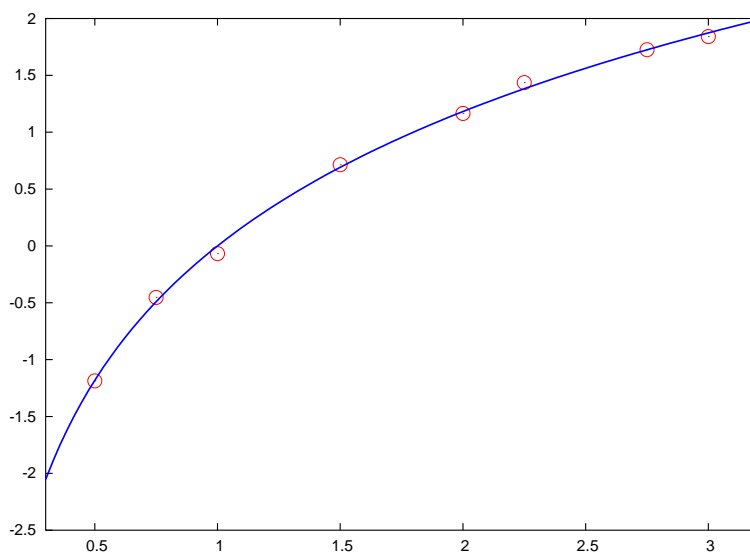


Figure 9.1: The data of Example Problem 9.2 and the least squares interpolant are shown.

However, the computer would only find this if it had infinite precision. Since it does not, and since  $\epsilon$  is rather small, the computer thinks  $\epsilon^2 = 0$ , and so tries to solve the system

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \begin{bmatrix} y_0 + \epsilon y_2 \\ y_0 + \epsilon y_1 \end{bmatrix}$$

When  $y_1 \neq y_2$ , this has no solution. Bummer.

This kind of thing is common in the method of least squares: the coefficients of the normal equations include terms like

$$g_i(x_k)g_j(x_k).$$

When the  $g_i$  are small at the nodes  $x_k$ , these coefficients can get really small, since we are squaring.

Now we draw a rough sketch of the basis functions. We find they do a pretty poor job of discriminating around all the nodes.

## 9.2 Orthonormal Bases

In the previous section we saw that poor choice of basis vectors can lead to numerical problems. Roughly speaking, if  $g_i(x_k)$  is small for some  $i$ 's and  $k$ 's, then some  $d_{ij}$  can have a loss of precision when two small quantities are multiplied together and rounded to zero.

Poor choice of basis vectors can also lead to numerical problems in solution of the normal equations, which will be done by Gaussian Elimination.

Consider the case where  $\mathcal{F}$  is the class of polynomials of degree no greater than  $m$ . For simplicity we will assume that all  $x_i$  are in the interval  $[0, 1]$ . The most obvious choice of basis functions is  $g_j(x) = x^j$ . This certainly gives a basis for  $\mathcal{F}$ , but actually a rather poor one. To see why, look at the graph of the basis functions in Figure 9.3. The basis functions look too much alike on the given interval.

A better basis for this problem is the set of Chebyshev Polynomials of the first kind, *i.e.*,  $g_j(x) = T_j(x)$ , where

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_{i+1}(x) = 2xT_i(x) - T_{i-1}(x).$$

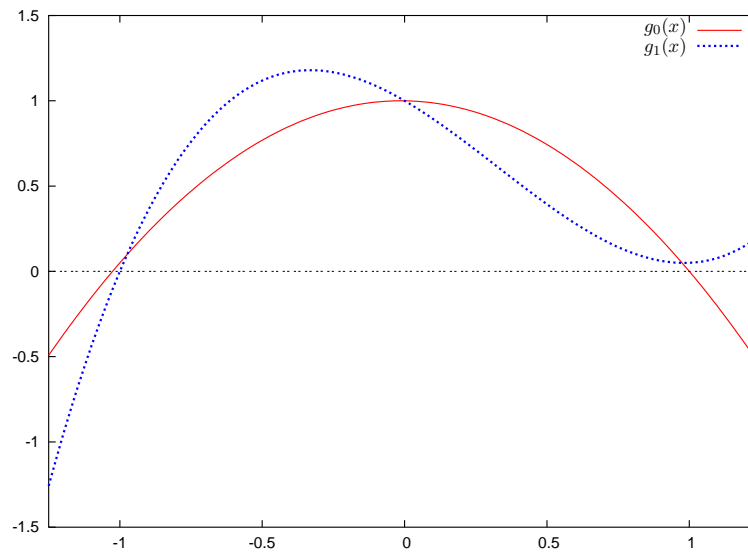


Figure 9.2: The basis functions  $g_0(x) = \left(\frac{\epsilon}{2} - 1\right)x^2 - \frac{\epsilon}{2}x + 1$ , and  $g_1(x) = x^3 + \left(\frac{\epsilon}{2} - 1\right)(x^2 + x) + 1$  are shown for  $\epsilon = 0.05$ . Note that around the three nodes  $0, 1, -1$ , these two functions take nearly identical values. This can lead to a system of normal equations with no solution.

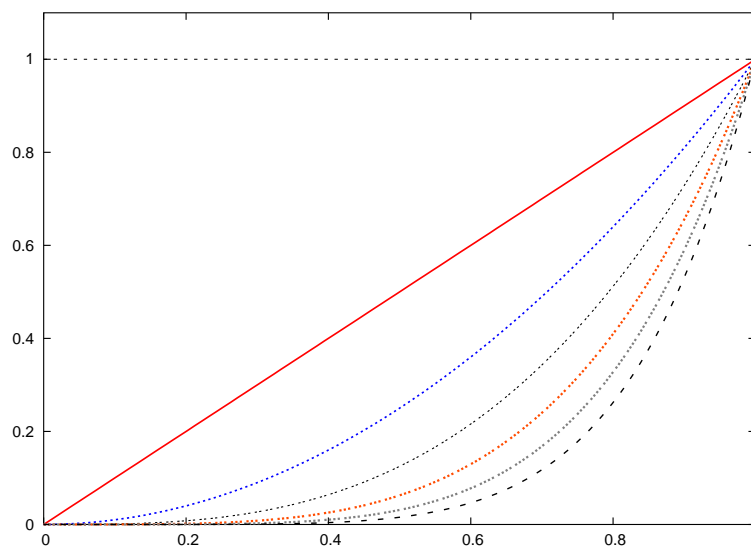


Figure 9.3: The polynomials  $x^i$  for  $i = 0, 1, \dots, 6$  are shown on  $[0, 1]$ . These polynomials make a bad basis because they look so much alike, essentially.

These polynomials are illustrated in Figure 9.4.

### 9.2.1 Alternatives to Normal Equations

It turns out that the Normal Equations method isn't really so great. We consider other methods. First, we define  $\mathbf{A}$  as the  $n \times m$  matrix defined by the entries:

$$a_{ij} = g_j(x_i), \quad i = 0, 1, \dots, n, \quad j = 0, 1, \dots, m.$$

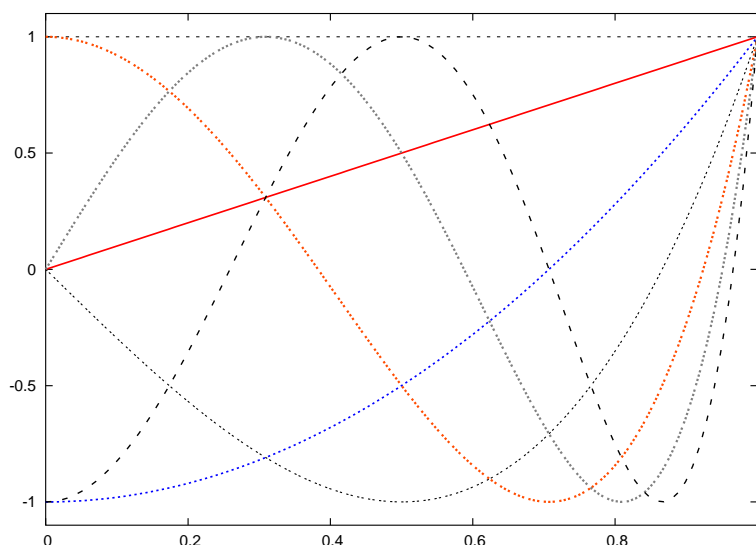


Figure 9.4: The Chebyshev polynomials  $T_j(x)$  for  $j = 0, 1, \dots, 6$  are shown on  $[0, 1]$ . These polynomials make a better basis for least squares because they are orthogonal under some inner product. Basically, they do not look like each other.

That is

$$\mathbf{A} = \begin{bmatrix} g_0(x_0) & g_1(x_0) & g_2(x_0) & \cdots & g_m(x_0) \\ g_0(x_1) & g_1(x_1) & g_2(x_1) & \cdots & g_m(x_1) \\ g_0(x_2) & g_1(x_2) & g_2(x_2) & \cdots & g_m(x_2) \\ g_0(x_3) & g_1(x_3) & g_2(x_3) & \cdots & g_m(x_3) \\ g_0(x_4) & g_1(x_4) & g_2(x_4) & \cdots & g_m(x_4) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ g_0(x_n) & g_1(x_n) & g_2(x_n) & \cdots & g_m(x_n) \end{bmatrix}$$

We write it in this way since we are thinking of the case where  $n \gg m$ , so  $A$  is “tall.”

After some inspection, we find that the Normal Equations can be written as:

$$\boxed{\mathbf{A}^\top \mathbf{A} \mathbf{c} = \mathbf{A}^\top \mathbf{y}.} \quad (9.3)$$

Now let the vector  $\mathbf{c}$  be identified, in the natural way, with a function in  $\mathcal{F}$ . That is  $\mathbf{c}$  is identified with  $f(x) = \sum_{j=0}^m c_j g_j(x)$ . You should now convince yourself that

$$\mathbf{A} \mathbf{c} = f(\mathbf{x}).$$

And thus the residual, or error, of this function is  $\mathbf{r} = \mathbf{y} - \mathbf{A} \mathbf{c}$ .

In our least squares theory we attempted to find that  $\mathbf{c}$  that minimized

$$\|\mathbf{y} - \mathbf{A} \mathbf{c}\|_2^2 = (\mathbf{y} - \mathbf{A} \mathbf{c})^\top (\mathbf{y} - \mathbf{A} \mathbf{c})$$

We can see this as minimizing the Euclidian distance from  $\mathbf{y}$  to  $\mathbf{A} \mathbf{c}$ . For this reason, we will have that the residual is orthogonal to the column space of  $\mathbf{A}$ , that is we want

$$\mathbf{A}^\top \mathbf{r} = \mathbf{A}^\top (\mathbf{y} - \mathbf{A} \mathbf{c}) = \mathbf{0}.$$

This is just the normal equations. We could rewrite this, however, in the following form: find  $\mathbf{c}$ ,  $\mathbf{r}$  such that

$$\begin{bmatrix} \mathbf{I} & \mathbf{A} \\ \mathbf{A}^\top & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{r} \\ \mathbf{c} \end{bmatrix} = \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix}$$

This is now a system of  $n + m$  variables and unknowns, which can be solved by specialized means. This is known as the *augmented form*. We briefly mention that naïve Gaussian Elimination is *not* appropriate to solve the augmented form, as it turns out to be equivalent to using the normal equations method.

### 9.2.2 Ordinary Least Squares in octave/Matlab

The ordinary least squares best approximant is so fundamental that it is hard-wired into octave/Matlab's system solve operator. The general equation we wish to solve is

$$\mathbf{A}\mathbf{c} = \mathbf{y}.$$

This system is overdetermined: there are more rows than columns in  $\mathbf{A}$ , *i.e.*, more equations than unknown variables. However, in octave/Matlab, this is solved just like the case where  $\mathbf{A}$  is square:

```
octave:1> c = A \ y;
```

Thus, unless specifically told otherwise, you should not implement the ordinary least squares solution method in octave/Matlab. Under the hood, octave/Matlab is *not* using the normal equations method, and does not suffer the increased condition number of the normal equations method.

## 9.3 Orthogonal Least Squares

The method described in Section 9.1, sometimes referred to as “ordinary least squares,” assumes that measurement error is found entirely in the dependent variable, and that there is no error in the independent variables.

For example, consider the case of two variables,  $x$  and  $y$ , which are thought to be related by an equation of the form  $y = mx + b$ . A number of measurements are made, giving the two sequences  $\{x_i\}_{i=1}^n$  and  $\{y_i\}_{i=1}^n$ . Ordinary least squares assumes, that

$$y_i = mx_i + b + \epsilon_i,$$

where  $\epsilon_i$ , the error of the  $i^{\text{th}}$  measurement, is a random variable. It is usually assumed that  $E[\epsilon_i] = 0$ , *i.e.*, that the measurements are “unbiased.” Under the further assumption that the errors are independent and have the same variance, the ordinary least squares solution is a very good one.<sup>1</sup>

However, what if it were the case that

$$y_i = m(x_i + \xi_i) + b + \epsilon_i,$$

*i.e.*, that there is actually error in the measurement of the  $x_i$ ? In this case, the orthogonal least squares method is appropriate.

---

<sup>1</sup>This means that the ordinary least squares solution gives an unbiased estimator of  $m$  and  $b$ , and, moreover, gives the estimators with the lowest variance among all linear, *a priori* estimators. For more details on this, locate the Gauss-Markov Theorem in a good statistics textbook.

The difference between the two methods is illustrated in Figure 9.5. In Figure 9.5(a), the ordinary least squares method is shown; it minimizes the sum of the squared lengths of vertical lines from observations to a line, reflecting the assumption of no error in  $x_i$ . The orthogonal least squares method will minimize the sum of the squared distances from observations to a line, as shown in Figure 9.5(b).

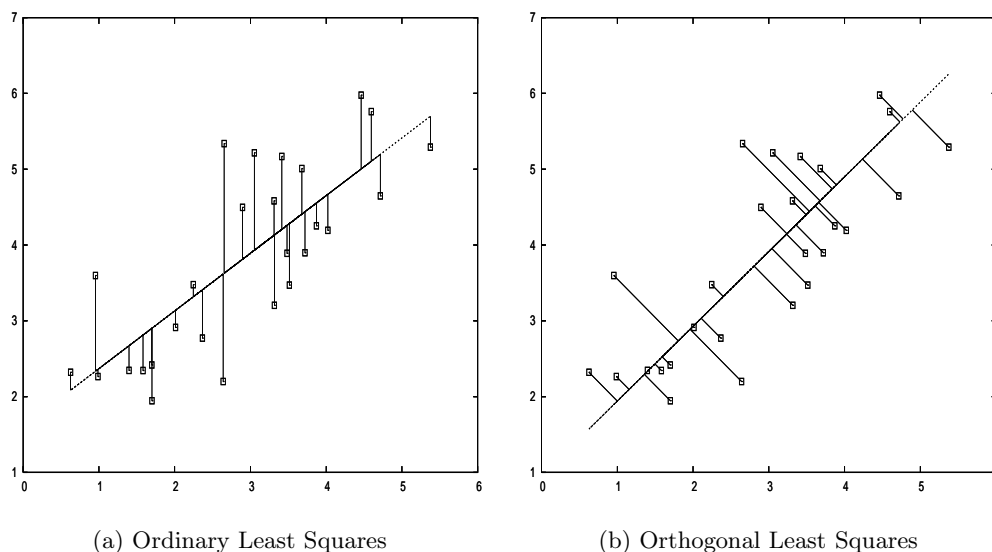


Figure 9.5: The ordinary least squares method, as shown in (a), minimizes the sum of the squared lengths of the vertical lines from the observed points to the regression line. The orthogonal least squares, shown in (b), minimizes the sum of the squared distances from the points to the line. The offsets from points to the regression line in (b) may not look orthogonal due to improper aspect ratio of the figure.

We construct the solution geometrically. Let  $\{\mathbf{x}^{(i)}\}_{i=1}^m$  be the set of observations, expressed as vectors in  $\mathbb{R}^n$ . The problem is to find the vector  $\mathbf{n}$  and number  $d$  such that the hyperplane  $\mathbf{n}^\top \mathbf{x} = d$  is the plane that minimizes the sum of the squared distances from the points to the plane. We can solve this problem using vector calculus.

The function

$$\frac{1}{\|\mathbf{n}\|_2^2} \sum_{i=1}^m \left\| \mathbf{n}^\top \mathbf{x}^{(i)} - d \right\|_2^2.$$

is the one to be minimized with respect to  $\mathbf{n}$  and  $d$ . It gives the sum of the squared distances from the points to the plane described by  $\mathbf{n}$  and  $d$ . To simplify its computation, we will minimize it subject to the constraint that  $\|\mathbf{n}\|_2^2 = 1$ . Thus our problem is to find  $\mathbf{n}$  and  $d$  that solve

$$\min_{\mathbf{n}^\top \mathbf{n} = 1} \sum_{i=1}^m \left\| \mathbf{n}^\top \mathbf{x}^{(i)} - d \right\|_2^2.$$

We can express this as  $\min f(\mathbf{n}, d)$  subject to  $g(\mathbf{n}, d) = 1$ . The solution of this problem uses the Lagrange multipliers technique.

Let  $\mathcal{L}(\mathbf{n}, d, \lambda) = f(\mathbf{n}, d) - \lambda g(\mathbf{n}, d)$ . The Lagrange multipliers theory tells us that a necessary

condition for  $\mathbf{n}, d$  to be the solution is that there exists  $\lambda$  such that the following hold:

$$\begin{cases} \frac{\partial \mathcal{L}}{\partial d}(\mathbf{n}, d, \lambda) = 0 \\ \nabla_{\mathbf{n}} \mathcal{L}(\mathbf{n}, d, \lambda) = \mathbf{0} \\ g(\mathbf{n}, d) = 1 \end{cases}$$

Let  $\mathbf{X}$  be the  $m \times n$  matrix whose  $i^{\text{th}}$  row is the vector  $\mathbf{x}^{(i)\top}$ . We can rewrite the Lagrange function as

$$\begin{aligned} \mathcal{L}(\mathbf{n}, d, \lambda) &= (\mathbf{X}\mathbf{n} - d\mathbf{1}_m)^\top (\mathbf{X}\mathbf{n} - d\mathbf{1}_m) - \lambda \mathbf{n}^\top \mathbf{n} \\ &= \mathbf{n}^\top \mathbf{X}^\top \mathbf{X} \mathbf{n} - 2d \mathbf{1}_m^\top \mathbf{X} \mathbf{n} + d^2 \mathbf{1}_m^\top \mathbf{1}_m - \lambda \mathbf{n}^\top \mathbf{n} \end{aligned}$$

We solve the necessary condition on  $\frac{\partial \mathcal{L}}{\partial d}$ .

$$0 = \frac{\partial \mathcal{L}}{\partial d}(\mathbf{n}, d, \lambda) = 2d \mathbf{1}_m^\top \mathbf{1}_m - 2 \mathbf{1}_m^\top \mathbf{X} \mathbf{n} \quad \Rightarrow \quad d = \mathbf{1}_m^\top \mathbf{X} \mathbf{n} / \mathbf{1}_m^\top \mathbf{1}_m$$

This essentially tells us that we will zero the first moment of the data around the line. Note that this determination of  $d$  requires knowledge of  $\mathbf{n}$ . However, since this is a necessary condition, we can plug it into the gradient equation:

$$\mathbf{0} = \nabla_{\mathbf{n}} \mathcal{L}(\mathbf{n}, d, \lambda) = 2\mathbf{X}^\top \mathbf{X} \mathbf{n} - 2d \left( \mathbf{1}_m^\top \mathbf{X} \right)^\top - 2\lambda \mathbf{n} = 2 \left[ \mathbf{X}^\top \mathbf{X} \mathbf{n} - \frac{\mathbf{1}_m^\top \mathbf{X} \mathbf{n}}{\mathbf{1}_m^\top \mathbf{1}_m} \left( \mathbf{1}_m^\top \mathbf{X} \right)^\top - \lambda \mathbf{n} \right]$$

The middle term is a scalar times a vector, so the multiplication can be commuted, this gives

$$\mathbf{0} = \left[ \mathbf{X}^\top \mathbf{X} \mathbf{n} - \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} \mathbf{n} - \lambda \mathbf{n} \right] = \left[ \mathbf{X}^\top \mathbf{X} - \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} - \lambda \mathbf{I} \right] \mathbf{n}$$

Thus  $\mathbf{n}$  is an eigenvector of the matrix

$$\mathbf{M} = \mathbf{X}^\top \mathbf{X} - \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m}$$

The final condition of the three Lagrange conditions is that  $g(\mathbf{n}, d) = \mathbf{n}^\top \mathbf{n} = 1$ . Thus if  $\mathbf{n}$  is a minimizer, then it is a unit eigenvector of  $\mathbf{M}$ .

It is not clear which eigenvector is the right one, so we might have to check *all* the eigenvectors. However, further work tells us which eigenvector it is. First we rewrite the function to be minimized, when the optimal  $d$  is used:  $\hat{f}(\mathbf{n}) = f(\mathbf{n}, \mathbf{1}_m^\top \mathbf{X} \mathbf{n} / \mathbf{1}_m^\top \mathbf{1}_m)$ . We have

$$\begin{aligned} \hat{f}(\mathbf{n}) &= \mathbf{n}^\top \mathbf{X}^\top \mathbf{X} \mathbf{n} - 2 \frac{\mathbf{1}_m^\top \mathbf{X} \mathbf{n}}{\mathbf{1}_m^\top \mathbf{1}_m} \mathbf{1}_m^\top \mathbf{X} \mathbf{n} + \left( \frac{\mathbf{1}_m^\top \mathbf{X} \mathbf{n}}{\mathbf{1}_m^\top \mathbf{1}_m} \right)^2 \mathbf{1}_m^\top \mathbf{1}_m \\ &= \mathbf{n}^\top \mathbf{X}^\top \mathbf{X} \mathbf{n} - 2 \frac{\mathbf{n}^\top \mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X} \mathbf{n}}{\mathbf{1}_m^\top \mathbf{1}_m} + \frac{\mathbf{n}^\top \mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X} \mathbf{n} \mathbf{1}_m^\top \mathbf{1}_m}{\mathbf{1}_m^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{1}_m} \\ &= \mathbf{n}^\top \mathbf{X}^\top \mathbf{X} \mathbf{n} - 2 \frac{\mathbf{n}^\top \mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X} \mathbf{n}}{\mathbf{1}_m^\top \mathbf{1}_m} + \frac{\mathbf{n}^\top \mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X} \mathbf{n}}{\mathbf{1}_m^\top \mathbf{1}_m} \\ &= \mathbf{n}^\top \mathbf{X}^\top \mathbf{X} \mathbf{n} - \frac{\mathbf{n}^\top \mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X} \mathbf{n}}{\mathbf{1}_m^\top \mathbf{1}_m} \\ &= \mathbf{n}^\top \left[ \mathbf{X}^\top \mathbf{X} - \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} \right] \mathbf{n} \\ &= \mathbf{n}^\top \mathbf{M} \mathbf{n} \end{aligned}$$

This sequence of equations only required that the  $d$  be the optimal  $d$  for the given  $\mathbf{n}$ , and used the fact that a scalar is its own transpose, thus  $\mathbf{1}_m^\top \mathbf{X} \mathbf{n} = \mathbf{n}^\top \mathbf{X}^\top \mathbf{1}_m$ .

Now if  $\mathbf{n}$  is a unit eigenvector of  $\mathbf{M}$ , with corresponding eigenvalue  $\lambda$ , then  $\mathbf{n}^\top \mathbf{M} \mathbf{n} = \lambda$ . Note that because  $f(\mathbf{n}, d)$  is defined as  $\mathbf{w}^\top \mathbf{w}$ , for some vector  $\mathbf{w}$ , then the matrix  $\mathbf{M}$  must be positive definite, *i.e.*,  $\lambda$  must be positive. However, we want to minimize  $\lambda$ . Thus we take  $\mathbf{n}$  to be the unit eigenvector associated with the smallest eigenvalue.

Note that, by roundoff, you may compute that  $\mathbf{M}$  has some negative eigenvalues, though they are small in magnitude. Thus one should select, as  $\mathbf{n}$ , the unit eigenvector associated with the smallest eigenvalue in absolute value.

**Example Problem 9.4.** Find the equation of the line which best approximates the 2D data  $\{(x_i, y_i)\}_{i=1}^m$ , by the orthogonal least squares method.

*Solution:* In this case the matrix  $\mathbf{X}$  is

$$\begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \\ \vdots & \vdots \\ x_m & y_m \end{bmatrix}$$

Thus we have that

$$\begin{aligned} \mathbf{M} &= \mathbf{X}^\top \mathbf{X} - \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m}, \\ &= \begin{bmatrix} \sum x_i^2 & \sum x_i y_i \\ \sum x_i y_i & \sum y_i^2 \end{bmatrix} - \frac{1}{m} \begin{bmatrix} (\sum x_i)^2 & \sum x_i \sum y_i \\ \sum x_i \sum y_i & (\sum y_i)^2 \end{bmatrix}, \\ &= \begin{bmatrix} \sum x_i^2 & \sum x_i y_i \\ \sum x_i y_i & \sum y_i^2 \end{bmatrix} - m \begin{bmatrix} \bar{x}^2 & \bar{x}\bar{y} \\ \bar{x}\bar{y} & \bar{y}^2 \end{bmatrix}, \\ &= \begin{bmatrix} \sum x_i^2 - m\bar{x}^2 & \sum x_i y_i - m\bar{x}\bar{y} \\ \sum x_i y_i - m\bar{x}\bar{y} & \sum y_i^2 - m\bar{y}^2 \end{bmatrix} \\ &= \begin{bmatrix} 2\alpha & \beta \\ \beta & 2\gamma \end{bmatrix}. \end{aligned} \tag{9.4}$$

where we use  $\bar{x}, \bar{y}$ , to mean, respectively, the mean of the  $x$ - and  $y$ -values. The characteristic polynomial of the matrix, whose roots are the eigenvalues of the matrix is

$$p(\lambda) = \det \begin{bmatrix} 2\alpha - \lambda & \beta \\ \beta & 2\gamma - \lambda \end{bmatrix} = 4\alpha\gamma - \beta^2 - 2(\alpha + \gamma)\lambda + \lambda^2.$$

The roots of this polynomial are given by the quadratic equation

$$\lambda_{\pm} = \frac{2(\alpha + \gamma) \pm \sqrt{4(\alpha + \gamma)^2 - 4(4\alpha\gamma - \beta^2)}}{2} = (\alpha + \gamma) \pm \sqrt{(\alpha - \gamma)^2 + \beta^2}$$

We want the smaller eigenvalue,  $\lambda_- = (\alpha + \gamma) - \sqrt{(\alpha - \gamma)^2 + \beta^2}$ . The associated eigenvector is in the null space of the matrix

$$\mathbf{0} = \begin{bmatrix} 2\alpha - \lambda_- & \beta \\ \beta & 2\gamma - \lambda_- \end{bmatrix} \mathbf{v} = \begin{bmatrix} 2\alpha - \lambda_- & \beta \\ \beta & 2\gamma - \lambda_- \end{bmatrix} \begin{bmatrix} -k \\ 1 \end{bmatrix} = \begin{bmatrix} \beta - k(2\alpha - \lambda_-) \\ -k\beta + 2\gamma - \lambda_- \end{bmatrix}$$

This is solved by

$$\begin{aligned} k &= \frac{2\gamma - \lambda_-}{\beta} = \frac{(\gamma - \alpha) + \sqrt{(\gamma - \alpha)^2 + \beta^2}}{\beta} \\ &= \frac{\sum(y_i^2 - x_i^2) - m(\bar{y}^2 - \bar{x}^2) + \sqrt{(\sum(y_i^2 - x_i^2) - m(\bar{y}^2 - \bar{x}^2))^2 + 4(\sum x_i y_i - m\bar{x}\bar{y})^2}}{2\sum x_i y_i - m\bar{x}\bar{y}}. \end{aligned} \quad (9.5)$$

Thus the best plane through the data is of the form

$$-kx + 1y = d \quad \text{or} \quad y = kx + d$$

Note that the eigenvector,  $\mathbf{v}$ , that we used is *not* a unit vector. However it is parallel to the unit vector we want, and can still use the regular formula to compute the optimal  $d$ .

$$\begin{aligned} d &= \mathbf{1}_m^\top \mathbf{X} \mathbf{n} / \mathbf{1}_m^\top \mathbf{1}_m = \frac{1}{m} \mathbf{1}_m^\top \mathbf{X} \begin{bmatrix} -k \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} \bar{x} & \bar{y} \end{bmatrix} \begin{bmatrix} -k \\ 1 \end{bmatrix} = \bar{y} - k\bar{x} \end{aligned}$$

Thus the optimal line through the data is

$$y = kx + d = k(x - \bar{x}) + \bar{y} \quad \text{or} \quad y - \bar{y} = k(x - \bar{x}),$$

with  $k$  defined in equation 9.5.

+

### 9.3.1 Computing the Orthogonal Least Squares Approximant

Just as the Normal Equations equation 9.3 define the solution to the ordinary least squares approximant, but are not normally used to solve the problem, so too is the above described means of computing the orthogonal least squares not a good idea.

First we define

$$\mathbf{W} = \mathbf{X} - \frac{\mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m}.$$

Now note that

$$\begin{aligned} \mathbf{W}^\top \mathbf{W} &= \left( \mathbf{X} - \frac{\mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} \right)^\top \left( \mathbf{X} - \frac{\mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} \right) = \mathbf{X}^\top \mathbf{X} - 2 \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} + \frac{(\mathbf{1}_m \mathbf{1}_m^\top \mathbf{X})^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{(\mathbf{1}_m^\top \mathbf{1}_m)^2} \\ &= \mathbf{X}^\top \mathbf{X} - 2 \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} + \frac{\mathbf{X}^\top \mathbf{1}_m (\mathbf{1}_m^\top \mathbf{1}_m) \mathbf{1}_m^\top \mathbf{X}}{(\mathbf{1}_m^\top \mathbf{1}_m)^2} = \mathbf{X}^\top \mathbf{X} - 2 \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} + \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} \\ &= \mathbf{X}^\top \mathbf{X} - \frac{\mathbf{X}^\top \mathbf{1}_m \mathbf{1}_m^\top \mathbf{X}}{\mathbf{1}_m^\top \mathbf{1}_m} = \mathbf{M}. \end{aligned}$$

We now need some linear algebra magic:

**Definition 9.3.1.** A square matrix  $\mathbf{U}$  is called *unitary* if its inverse is its transpose, *i.e.*,

$$\mathbf{U}^\top \mathbf{U} = \mathbf{I} = \mathbf{U} \mathbf{U}^\top.$$

From the first equation, we see that the columns of  $\mathbf{U}$  form a collection of orthonormal vectors. The second equation tells that the rows of  $\mathbf{U}$  are also such a collection.



**Definition 9.3.2.** Every  $m \times n$  matrix  $\mathbf{B}$  can be decomposed as

$$\mathbf{B} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\top},$$

where  $\mathbf{U}$  and  $\mathbf{V}$  are unitary matrices,  $\mathbf{U}$  is  $m \times m$ ,  $\mathbf{V}$  is  $n \times n$ , and  $\mathbf{\Sigma}$  is  $m \times n$ , and has nonzero elements only on its diagonal. The values of the diagonal of  $\mathbf{\Sigma}$  are the *singular values* of  $\mathbf{B}$ . The column vectors of  $\mathbf{V}$  span the row space of  $\mathbf{B}$ , and the column vectors of  $\mathbf{U}$  contain the column space of  $\mathbf{B}$ .

The singular value decomposition generalizes the notion of eigenvalues and eigenvectors to the case of nonsquare matrices. Let  $\mathbf{u}^{(i)}$  be the  $i^{\text{th}}$  column vector of  $\mathbf{U}$ ,  $\mathbf{v}^{(i)}$  the  $i^{\text{th}}$  column of  $\mathbf{V}$ , and let  $\sigma_i$  be the  $i^{\text{th}}$  element of the diagonal of  $\mathbf{\Sigma}$ . Then if  $\mathbf{x} = \sum_i \alpha_i \mathbf{v}^{(i)}$ , we have

$$\mathbf{B}\mathbf{x} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\top} \sum_i \alpha_i \mathbf{v}^{(i)} = \mathbf{U}\mathbf{\Sigma} [\alpha_1 \alpha_2 \dots \alpha_n]^{\top} = \mathbf{U} \begin{bmatrix} \sigma_1 \alpha_1 & 0 & \dots & 0 \\ 0 & \sigma_2 \alpha_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \alpha_n \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix} = \sum_i \sigma_i \alpha_i \mathbf{u}^{(i)}.$$

Thus  $\mathbf{v}^{(i)}$  and  $\mathbf{u}^{(i)}$  act as an “eigenvector pair” with “eigenvalue”  $\sigma_i$ .

The singular value decomposition is computed by the octave/Matlab command  $[\mathbf{U}, \mathbf{S}, \mathbf{V}] = \text{svd}(\mathbf{B})$ . The decomposition is computed such that the diagonal elements of  $\mathbf{S}$ , the singular values, are positive, and decreasing with increasing index.

Now we can use the singular value decomposition on  $\mathbf{W}$ :

$$\mathbf{W} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\top}.$$

Thus

$$\mathbf{M} = \mathbf{W}^{\top}\mathbf{W} = \mathbf{V}\mathbf{\Sigma}^{\top}\mathbf{U}^{\top}\mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\top} = \mathbf{V}\mathbf{\Sigma}^{\top}|\mathbf{\Sigma}\mathbf{V}^{\top} = \mathbf{V}\mathbf{S}^2\mathbf{V}^{\top},$$

where  $\mathbf{S}^2$  is the  $n \times n$  diagonal matrix whose  $i^{\text{th}}$  diagonal is  $\sigma_i^2$ . Thus we see that the solution to the orthogonal least squares problem, the eigenvector associated with the smallest eigenvalue of  $\mathbf{M}$ , is the column vector of  $\mathbf{V}$  associated with the smallest, in absolute value, singular value of  $\mathbf{W}$ . In octave/Matlab, this is  $\mathbf{V}(:, \mathbf{n})$ .

This may not appear to be a computational savings, but if  $\mathbf{M}$  is computed up front, and its eigenvectors are computed, there is loss of precision in its smallest eigenvalues which might lead us to choose the wrong normal direction (especially if there is more than one!). On the other hand,  $\mathbf{M}$  is a  $n \times n$  matrix, whereas  $\mathbf{W}$  is  $m \times n$ . If storage is at a premium, and the method is being reapplied with new observations, it may be preferable to keep  $\mathbf{M}$ , rather than keeping  $\mathbf{W}$ . That is, it may be necessary to trade conditioning for space.

### 9.3.2 Principal Component Analysis

The above analysis leads us to the topic of Principal Component Analysis. Suppose the  $m \times n$  matrix  $\mathbf{X}$  represents  $m$  noisy observations of some process, where each observation is a vector in  $\mathbb{R}^n$ . Suppose the observations nearly lie in some  $k$ -dimensional subspace of  $\mathbb{R}^n$ , for  $k < n$ . How can you find an approximate value of  $k$ , and how do you find the  $k$ -dimensional subspace?

As in the previous subsection, let

$$W = X - \frac{\mathbf{1}_m \mathbf{1}_m^\top X}{\mathbf{1}_m^\top \mathbf{1}_m} = X - \mathbf{1}_m \bar{X}, \quad \text{where } \bar{X} = \mathbf{1}_m^\top X / \mathbf{1}_m^\top \mathbf{1}_m.$$

Now note that  $\bar{X}$  is the mean of the  $m$  observations, as a row vector in  $\mathbb{R}^n$ . Under the assumption that the noise is approximately the same for each observation, we should think that  $\bar{X}$  is likely to be in or very close to the  $k$ -dimensional subspace. Then each row of  $W$  should be like a vector which is contained in the subspace. If we take some vector  $\mathbf{v}$  and multiply  $W\mathbf{v}$ , we expect the resultant vector to have small norm if  $\mathbf{v}$  is not in the  $k$ -dimensional subspace, and to have a large norm if it is in the subspace.

You should now convince yourself that this is related to the singular value decomposition of  $W$ . Decomposing  $\mathbf{v} = \sum_i \alpha_i \mathbf{v}^{(i)}$ , we have  $W\mathbf{v} = \sum_i \sigma_i \alpha_i \mathbf{u}^{(i)}$ , and thus product vector has small norm if the  $\alpha_i$  associated with large  $\sigma_i$  are small, and large norm otherwise. That is the principal directions of the “best”  $k$ -dimensional subspace associated with  $X$  are the  $k$  columns of  $V$  associated with the largest singular values of  $W$ .

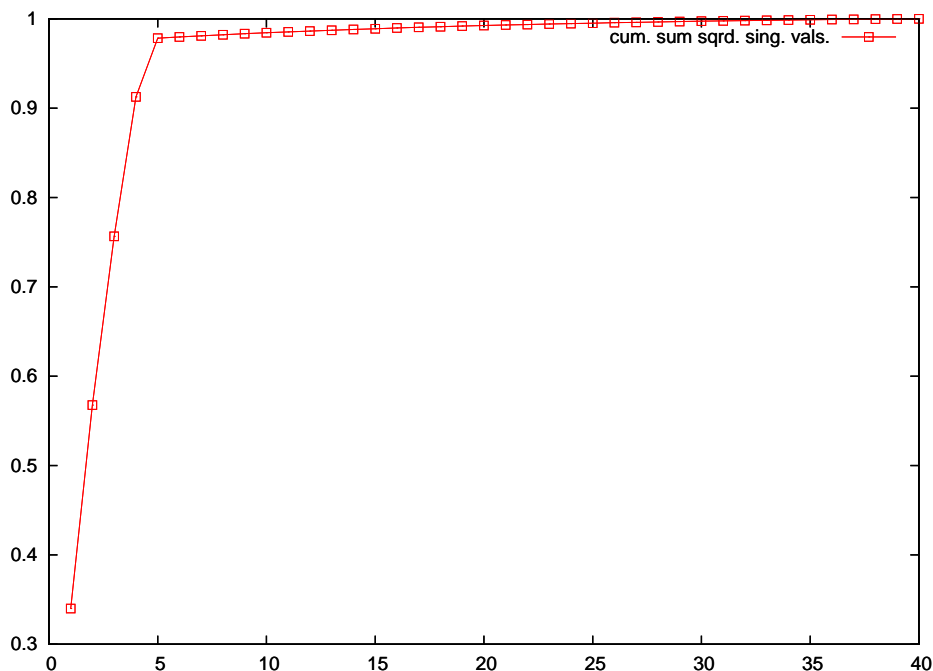


Figure 9.6: Noisy 5-dimensional data lurking in  $\mathbb{R}^{40}$  are treated to Principal Component Analysis. This figure shows the normalized cumulative sum of squared singular values of  $W$ . There is a sharp “elbow” at  $k = 5$ , which indicates the data is actually 5-dimensional.

If  $k$  is unknown *a priori*, a good value can be obtained by eyeing a graph of the cumulative sum of squared singular values of  $W$ , and selecting the  $k$  that makes this appropriately large. This is illustrated in Figure 9.6, with data generated by the following octave/Matlab code:

```
octave:1> X = rand(150,5);
octave:2> sawX = (X * randn(5,40)) + kron(ones(150,1),randn(1,40));
octave:3> sawX += 0.1 * randn(150,40);
octave:4> wun = ones(150,1);
```

```
octave:5> W = sawX - (wun * wun' * sawX) / (wun' * wun);
octave:6> [U,S,V] = svd(W);
octave:7> eigs = diag(S'*S);
octave:8> cseig = cumsum(eigs) ./ sum(eigs);
octave:9> plot ((1:40)',cseig,'xr-0;cum. sum sqrd. sing. vals.');
```

## EXERCISES

- (9.1) How do you know that the choice of constants  $c_i$  in our least squares analysis actually find a minimum of equation 9.1, and not, say, a maximum?
- (9.2) Our “linear” least squares might be better called the “affine” least squares. In this exercise you will find the best linear function which approximates a set of data. That is, find the function  $f(x) = cx$  which is the ordinary least squares best approximant to the given data

$$\frac{x \parallel x_0 \mid x_1 \mid \dots \mid x_n}{y \parallel y_0 \mid y_1 \mid \dots \mid y_n}$$

- (9.3) Find the constant that best approximates, in the ordinary least squares sense, the given data  $\mathbf{x}, \mathbf{y}$ . (*Hint:* you can use equation 9.2 or equation 9.3 using a single basis function  $g_0(x) = 1$ .) Do the  $x_i$  values affect your answer?
- (9.4) Find the function  $f(x) = c$  which best approximates, in the ordinary least squares sense, the data

$$\frac{x \parallel 1 \mid -2 \mid 5}{y \parallel 1 \mid -2 \mid 4}$$

- (9.5) Find the function  $ax + b$  that best approximates the data

$$\frac{x \parallel 0 \mid -1 \mid 2}{y \parallel 0 \mid 1 \mid -1}$$

Use the ordinary least squares method.

- (9.6) Find the function  $ax + b$  that best approximates the data of the previous problem using the orthogonal least squares method.
- (9.7) Find the function  $ax^2 + b$  that best approximates the data

$$\frac{x \parallel 0 \mid 1 \mid 2}{y \parallel 0.3 \mid 0.1 \mid 0.5}$$

- (9.8) Prove that the least squares solution is the solution of the normal equations, equation 9.3, and thus takes the form

$$\mathbf{c} = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{y}.$$

- (9.9) For ordinary least squares regression to the line  $y = mx + b$ , express the approximate  $m$  in terms of the  $\alpha, \beta$ , and  $\gamma$  parameters from equation 9.4. Compare this to that found in equation 9.5.
- (9.10) Any symmetric positive definite matrix,  $\mathbf{G}$  can be used to define a norm in the following way:

$$\|\mathbf{v}\|_{\mathbf{G}} =_{\text{df}} \sqrt{\mathbf{v}^\top \mathbf{G} \mathbf{v}}$$

The *weighted* least squares method for  $\mathbf{G}$  and data  $\mathbf{A}$  and  $\mathbf{y}$ , finds the  $\hat{\mathbf{c}}$  that solves

$$\min_{\mathbf{c}} \|\mathbf{A}\mathbf{c} - \mathbf{y}\|_{\mathbf{G}}^2$$

Prove that the normal equations form of the solution of this problem is

$$\mathbf{A}^\top \mathbf{G} \mathbf{A} \hat{\mathbf{c}} = \mathbf{A}^\top \mathbf{G} \mathbf{y}.$$

- (9.11) (Continuation) Let the symmetric positive definite matrix  $\mathbf{G}$  have Cholesky Factorization  $\mathbf{G} = \mathbf{L}\mathbf{L}^\top$ , where  $\mathbf{L}$  is a lower triangular matrix. Show that the solution to the weighted least squares method is the  $\hat{\mathbf{c}}$  that is the ordinary (unweighted) least squares best approximate solution to the problem

$$\mathbf{L}^\top \mathbf{A} \mathbf{c} = \mathbf{L}^\top \mathbf{y}.$$

- (9.12) The  $r^2$  statistic is often used to describe the “goodness-of-fit” of the ordinary least squares approximation to data. It is defined as

$$r^2 = \frac{\|\mathbf{A}\hat{\mathbf{c}}\|_2^2}{\|\mathbf{y}\|_2^2},$$

where  $\hat{\mathbf{c}}$  is the approximant  $\mathbf{A}^\top \mathbf{A}^{-1} \mathbf{A}^\top \mathbf{y}$ .

- (a) Prove that we also have

$$r^2 = 1 - \frac{\|\mathbf{A}\hat{\mathbf{c}} - \mathbf{y}\|_2^2}{\|\mathbf{y}\|_2^2}.$$

- (b) Prove that the  $r^2$  parameter is “scale-invariant,” that is, if we change the units of our data, the parameter is unchanged (although the value of  $\hat{\mathbf{c}}$  may change.)
- (c) Devise a similar statistic for the orthogonal least squares approximation which is scale-invariant and rotation-invariant.
- (9.13) As proved in Example Problem 9.4, the orthogonal least squares best approximate line for data  $\{(x_i, y_i)\}_{i=1}^m$  goes through the point  $(\bar{x}, \bar{y})$ . Does the same thing hold for the ordinary least squares best approximate line?
- (9.14) Find the constant  $c$  such that  $f(x) = \ln(cx)$  best approximates, in the least squares sense, the given data

$$\begin{array}{c|c|c|c|c} x & x_0 & x_1 & \dots & x_n \\ \hline y & y_0 & y_1 & \dots & y_n \end{array}$$

(Hint: You cannot use basis functions and equation 9.2 to solve this. You must use the Definition 9.1.1.) The *geometric mean* of the numbers  $a_1, a_2, \dots, a_n$  is defined as  $(\prod a_i)^{1/n}$ . How does your answer relate to the geometric mean?

- (9.15) Write code to find the function  $ae^x + be^{-x}$  that best interpolates, in the least squares sense, a set of data  $\{(x_i, y_i)\}_{i=0}^n$ . Your m-file should have header line like:

```
function [a,b] = lsqrexp(xys)
```

where  $\mathbf{xys}$  is the  $(n+1) \times 2$  matrix whose rows are the  $n+1$  tuples  $(x_i, y_i)$ . Use the normal equations method. This should reduce the problem to solving a  $2 \times 2$  linear system; let octave/Matlab solve that linear system for you. (Hint: To find  $\mathbf{x}$  such that  $\mathbf{M}\mathbf{x} = \mathbf{b}$ , use  $\mathbf{x} = \mathbf{M} \setminus \mathbf{b}$ .)

- (a) What do you get when you try the following?

```
octave:1> xs = [-1 -0.5 0 0.5 1]';
octave:2> ys = [1.194 0.430 0.103 0.322 1.034]';
octave:3> xys = [xs ys];
octave:4> [a,b] = lsqrexp(xys)
```

- (b) Try the following:

```
octave:5> xys = xys = [-0.00001 0.3; 0 0.6; 0.00001 0.7];
octave:6> [a,b] = lsqrexp(xys)
```

Does something unexpected happen? Why?

- (9.16) Write code to find the plane  $\mathbf{n}^\top \mathbf{x}^{(i)} = d$  that best interpolates, in the least squares sense, a set of data  $\{\mathbf{x}^{(i)}\}_{i=0}^m$ . Your m-file should have header line like:

```
function [n,d] = orthlsq(X)
```

where  $X$  is the  $m \times n$  matrix whose rows are the  $m$  tuples  $(x_1, x_2, \dots, x_n)$ . Use the octave/Matlab `eig` function, which returns the eigenvalues and vectors of a matrix.

- (a) Create artificially planar data by the following:

```
octave:1> m = 100;n = 5;epsi = 0.1;offs = 2;
octave:2> Xsub = rand(m,(n-1));
octave:3> T = rand(n-1,n);
octave:4> X = Xsub * T;
octave:5> X += offs .* ones(size(X));
octave:6> X += epsi .* randn(size(X));
```

Now  $X$  contains data which are approximately on a  $(n - 1)$ -dimensional hyperplane in  $\mathbb{R}^n$ . The data, when centered, lay in the rowspace of  $T$ . Now test your code.

```
octave:7> [n,d] = orthlsq(X);
```

You should have that the vector  $n$  is orthogonal to the rows of  $T$ . Check this:

```
octave:8> disp(norm(T * n));
```

What do you get? Try again with `epsi` very small ( $1 \times 10^{-5}$ ) or zero.

- (b) Compare the orthogonal least squares technique to the ordinary least squares in a two dimensional setting. Consider  $x, y$  data nearly on the line  $y = mx + b$ :

```
octave:1> obs = 100;xeps = 1.0;yeps = 1.0;m = 0.375;b = 1;
octave:2> Xtrue = randn(obs,1);Ytrue = m .* Xtrue .+ b;
octave:3> XSaw = Xtrue + xeps * randn(size(Xtrue));
octave:4> YSaw = Ytrue + yeps * randn(size(Ytrue));
octave:5> lsmb = [XSaw, ones(obs,1)] \ YSaw;
octave:6> lsm = lsmb(1); lsb = lsmb(2);
octave:7> [n,d] = orthlsq([XSaw, YSaw]);
octave:8> orthm = -n(1) / n(2);orthb = d / n(2);
```

Compare the estimated coefficients from both solutions. Plot the two regression lines.

```
octave:9> hold off;
octave:10> plot(XSaw,YSaw,"*;observed data;");
octave:11> hold on;
octave:12> plot(XSaw,m*XSaw .+ b,"r-;true line;");
octave:13> plot(XSaw,lsm*XSaw .+ lsb,"g-;ordinary least squares;");
octave:14> plot(XSaw,orthm*XSaw .+ orthb,"b-;orthogonal least squares;");
octave:15> hold off;
```

Try this again with different values of `xeps` and `yeps`, which control the sizes of the errors in the  $x$  and  $y$  dimensions. Try with `xeps = 0.1, yeps = 1.0`, and with `xeps = 1.0, yeps = 0.1`. Under which situations does orthogonal least squares outperform ordinary least squares? Do they give equally erroneous results in some situations? Can you think of a way of “reweighting” channel data to make the orthogonal least squares method more robust in cases of unequal error variance?

## Chapter 10

# Ordinary Differential Equations

Ordinary Differential Equations, or ODEs, are used in approximating some physical systems. Some classical uses include simulation of the growth of populations and trajectory of a particle. They are usually easier to solve or approximate than the more general Partial Differential Equations, PDEs, which can contain partial derivatives.

Much of the background material of this chapter should be familiar to the student of calculus. We will focus more on the approximation of solutions, than on analytical solutions. For more background on ODEs, see any of the standard texts, *e.g.*, [8].

### 10.1 Elementary Methods

A one-dimensional ODE is posed as follows: find some function  $x(t)$  such that

$$\begin{cases} \frac{dx(t)}{dt} = f(t, x(t)), \\ x(a) = c. \end{cases} \quad (10.1)$$

In calculus classes, you probably studied the case where  $f(t, x(t))$  is independent of its second variable. For example the ODE given by

$$\begin{cases} \frac{dx(t)}{dt} = t^2 - t, \\ x(a) = c. \end{cases}$$

has solution  $x(t) = \frac{1}{3}t^3 - \frac{1}{2}t^2 + K$ , where  $K$  is chosen such that  $x(a) = c$ .

A more general case is when  $f(t, x)$  is separable, that is  $f(t, x) = g(t)h(x)$  for some functions  $g, h$ . You may recall that the solution to such a separable ODE usually involved the following equation:

$$\int \frac{dx}{h(x)} = \int g(t) dt$$

Finding an analytic solution can be considerably more difficult in the general case, thus we turn to approximation schemes.

### 10.1.1 Integration and ‘Stepping’

We attempt to solve the ODE by integrating both sides. That is

$$\begin{aligned}\frac{dx(t)}{dt} &= f(t, x(t)), \quad \text{yields} \\ \int_t^{t+h} dx &= \int_t^{t+h} f(r, x(r)) dr, \quad \text{thus} \\ x(t+h) &= x(t) + \int_t^{t+h} f(r, x(r)) dr.\end{aligned}\tag{10.2}$$

If we can approximate the integral then we have a way of ‘stepping’ from  $t$  to  $t+h$ , *i.e.*, if we have a good approximate of  $x(t)$  we can approximate  $x(t+h)$ . Note that this means that all the work we have put into approximating integrals can be used to approximate the solution of ODEs.

Using stepping schemes we can approximate  $x(t_{final})$  given  $x(t_{initial})$  by taking a number of steps. For simplicity we usually use the same step size,  $h$ , for each step, though nothing precludes us from varying the step size.

If we apply the left-hand rectangle rule for approximating integrals to equation 10.2, we get

$$\boxed{x(t+h) \approx x(t) + hf(t, x(t))}.\tag{10.3}$$

This is called *Euler’s Method*. Note this is essentially the same as the ‘forward difference’ approximation we made to the derivative, equation 7.1.

Trapezoid rule gives

$$x(t+h) \approx x(t) + \frac{h}{2} [f(t, x(t)) + f(t+h, x(t+h))].$$

But we cannot evaluate this exactly, since  $x(t+h)$  appears on both sides of the equation. And it is embedded on the right hand side. Bummer. But if we could approximate it, say by using Euler’s Method, maybe the formula would work. This is the idea behind the Runge-Kutta Method (see Section 10.2).

### 10.1.2 Taylor’s Series Methods

We see that our more accurate integral approximations will be useless since they require information we do not know, *i.e.*, evaluations of  $f(t, x)$  for yet unknown  $x$  values. Thus we fall back on Taylor’s Theorem (Theorem 1.1). We can also view this as using integral approximations where all information comes from the left-hand endpoint.

By Taylor’s theorem, if  $x$  has at least  $m+1$  continuous derivatives on the interval in question, we can write

$$x(t+h) = x(t) + hx'(t) + \frac{1}{2}h^2x''(t) + \dots + \frac{1}{m!}h^m x^{(m)}(t) + \frac{1}{(m+1)!}h^{m+1}x^{(m+1)}(\tau),$$

where  $\tau$  is between  $t$  and  $t+h$ . Since  $\tau$  is essentially unknown, our best calculable approximation to this expression is

$$x(t+h) \approx x(t) + hx'(t) + \frac{1}{2}h^2x''(t) + \dots + \frac{1}{m!}h^m x^{(m)}(t).$$

This approximate solution to the ODE is called a *Taylor’s series method of order  $m$* . We also say that this approximation is a *truncation* of the Taylor’s series. The difference between the actual



value of  $x(t+h)$ , and this approximation is called the *truncation error*. The truncation error exists independently from any error in computing the approximation, called roundoff error. We discuss this more in Subsection 10.1.5.

### 10.1.3 Euler's Method

When  $m = 1$  we recover Euler's Method:

$$x(t+h) = x(t) + hx'(t) = x(t) + hf(t, x(t)).$$

**Example 10.1.** Consider the ODE

$$\begin{cases} \frac{dx(t)}{dt} = x, \\ x(0) = 1. \end{cases}$$

The actual solution is  $x(t) = e^t$ . Euler's Method will underestimate  $x(t)$  because the curvature of the actual  $x(t)$  is positive, and thus the function is always above its linearization. In Figure 10.1, we see that eventually the Euler's Method approximation is very poor.

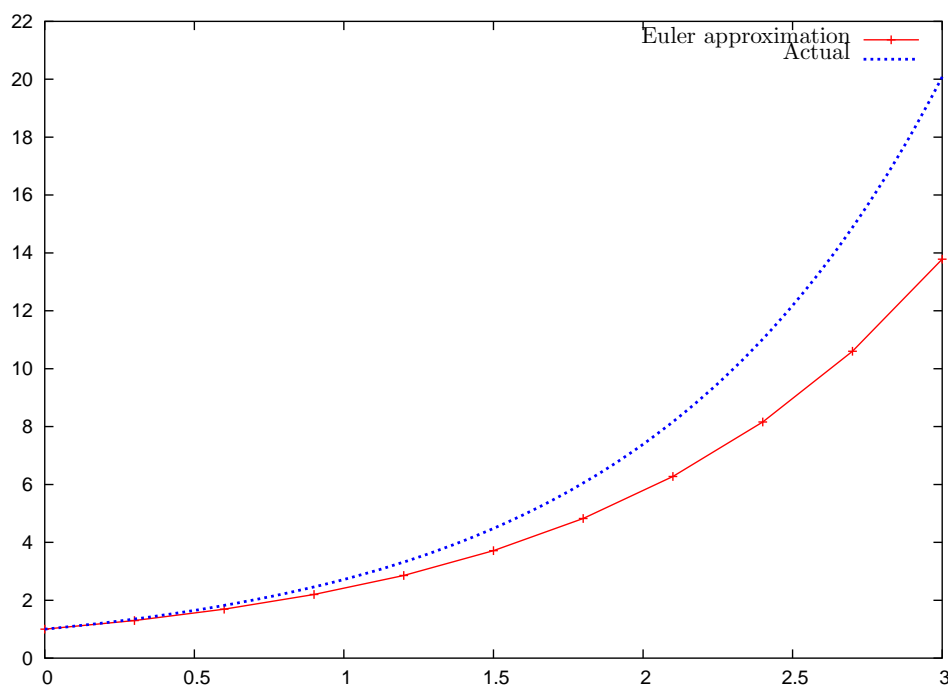


Figure 10.1: Euler's Method applied to approximate  $x' = x$ ,  $x(0) = 1$ . Each step proceeds on the linearization of the curve, and is thus an underestimate, as the actual solution,  $x(t) = e^t$  has positive curvature. Here step size  $h = 0.3$  is used.

### 10.1.4 Higher Order Methods

Higher order methods are derived by taking more terms of the Taylor's series expansion. Note however, that they will require information about the higher derivatives of  $x(t)$ , and thus may not be appropriate for the case where  $f(t, x)$  is given as a "black box" function.

**Example Problem 10.2.** Derive the Taylor's series method for  $m = 3$  for the ODE

$$\begin{cases} \frac{dx(t)}{dt} = x + e^x, \\ x(0) = 1. \end{cases}$$

*Solution:* By simple calculus:

$$\begin{aligned} x'(t) &= x + e^x \\ x''(t) &= x' + e^x x' \\ x'''(t) &= x''(1 + e^x) + x' e^x x' \end{aligned}$$

We can then write our step like a program:

$$\begin{aligned} x'(t) &\leftarrow x(t) + e^{x(t)} \\ x''(t) &\leftarrow x'(t) \left(1 + e^{x(t)}\right) \\ x'''(t) &\leftarrow x''(t) \left(1 + e^{x(t)}\right) + (x'(t))^2 e^{x(t)} \\ x(t+h) &\approx x(t) + hx'(t) + \frac{1}{2}h^2x''(t) + \frac{1}{6}h^3x'''(t) \end{aligned}$$

+

### 10.1.5 Errors

There are two types of errors: truncation and roundoff. Truncation error is the error of truncating the Taylor's series after the  $m^{\text{th}}$  term. You can see that the truncation error is  $\mathcal{O}(h^{m+1})$ . Roundoff error occurs because of the limited precision of computer arithmetic.

While it is possible these two kinds of error could cancel each other, given our pessimistic worldview, we usually assume they are additive. We also expect some tradeoff between these two errors as  $h$  varies. As  $h$  is made smaller, the truncation error presumably decreases, while the roundoff error increases. This results in an optimal  $h$ -value for a given method. See Figure 10.2. Unfortunately, the optimal  $h$ -value will usually depend on the given ODE and the approximation method. For an ODE with unknown solution, *it is generally impossible to predict the optimal  $h$* . We have already observed this kind of behaviour, when analyzing approximate derivatives—*cf.* Example Problem 7.5.

Both of these kinds of error can accumulate: Since we step from  $x(t)$  to  $x(t+h)$ , an error in the value of  $x(t)$  can cause a greater error in the value of  $x(t+h)$ . It turns out that for some ODEs and some methods, this does not happen. This leads to the topic of stability.

### 10.1.6 Stability

Suppose you had an exact method of solving an ODE, but had the wrong data. That is, you were trying to solve

$$\begin{cases} \frac{dx(t)}{dt} = f(t, x(t)), \\ x(a) = c, \end{cases}$$

but instead fed the wrong data into the computer, which then solved exactly the ODE

$$\begin{cases} \frac{dx(t)}{dt} = f(t, x(t)), \\ x(a) = c + \epsilon. \end{cases}$$

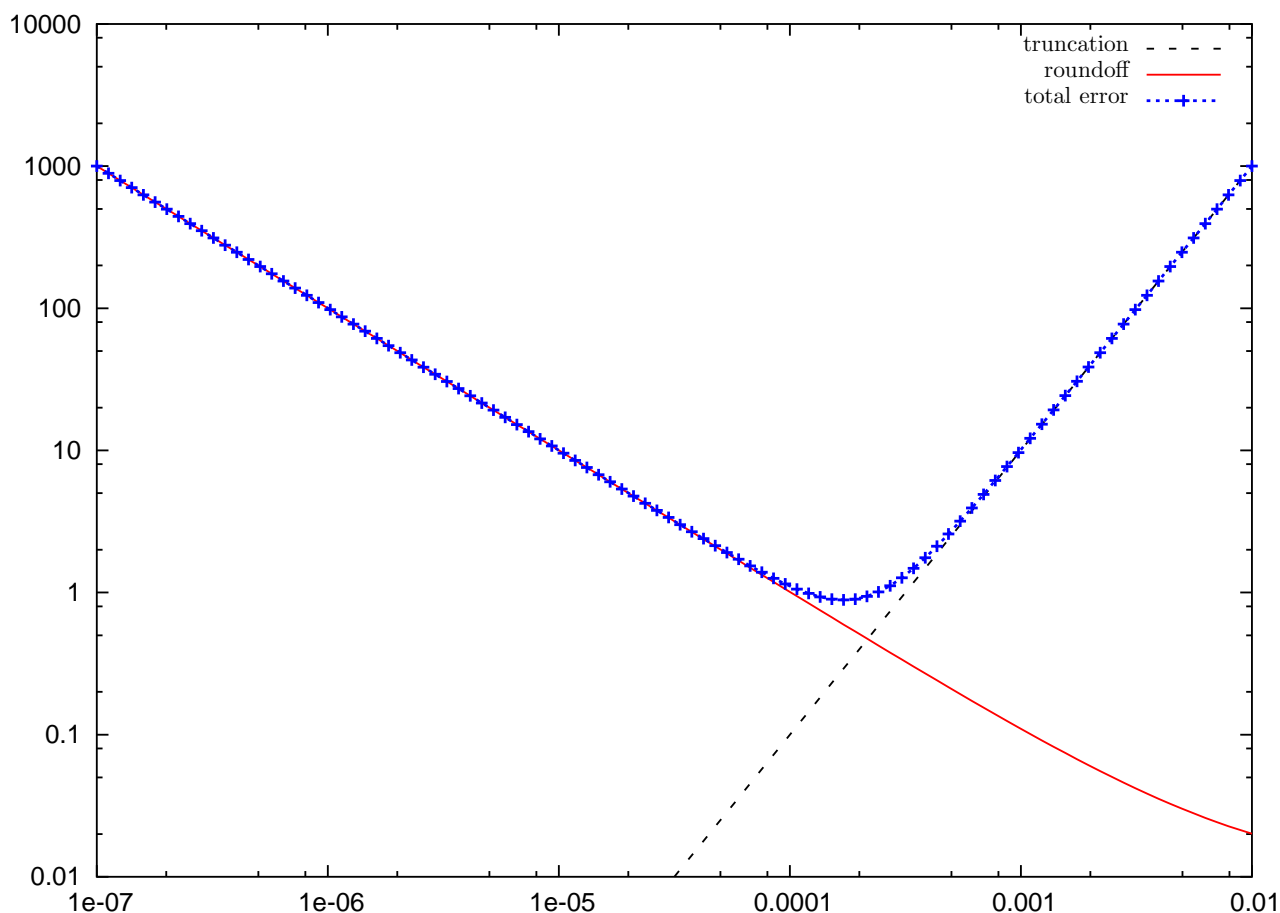


Figure 10.2: The truncation, roundoff, and total error for a fictional ODE and approximation method are shown. The total error is apparently minimized for an  $h$  value of approximately 0.0002. Note that the truncation error appears to be  $\mathcal{O}(h)$ , thus the approximation could be Euler’s Method. In reality, we expect the roundoff error to be more “bumpy,” as seen in Figure 7.1.

This solution can diverge from the correct one because of the different starting conditions. We illustrate this with the usual example.

**Example 10.3.** Consider the ODE

$$\frac{dx(t)}{dt} = x.$$

This has solution  $x(t) = x(0)e^t$ . The curves for different starting conditions diverge, as in Figure 10.3(a).

However, if we instead consider the ODE

$$\frac{dx(t)}{dt} = -x,$$

which has solution  $x(t) = x(0)e^{-t}$ , we see that differences in the initial conditions become immaterial, as in Figure 10.3(b).

Thus the latter ODE exhibits stability: roundoff and truncation errors accrued at a given step will become irrelevant as more steps are taken. The former ODE exhibits the opposite behavior—accrued errors will be amplified.

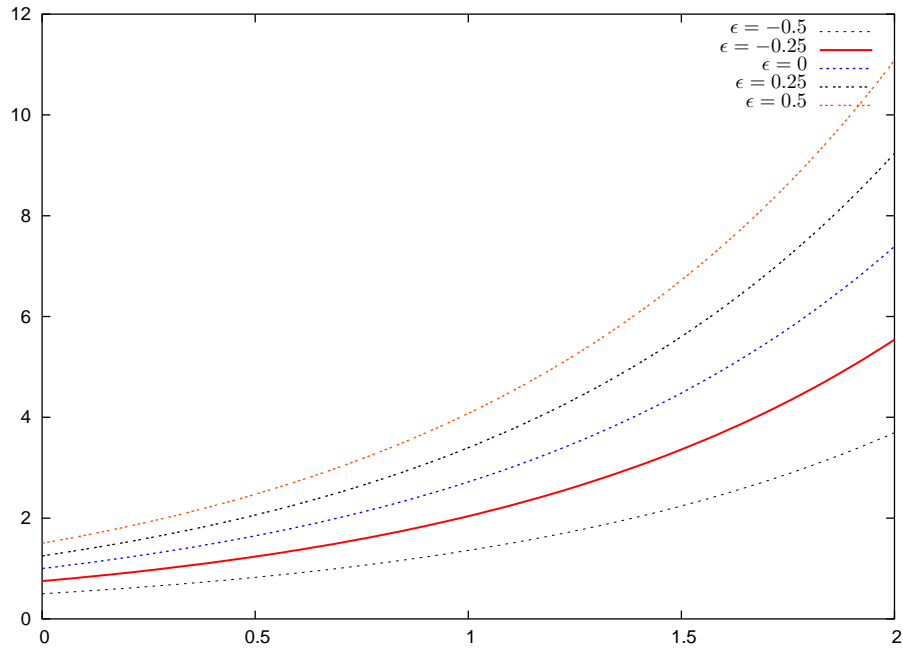
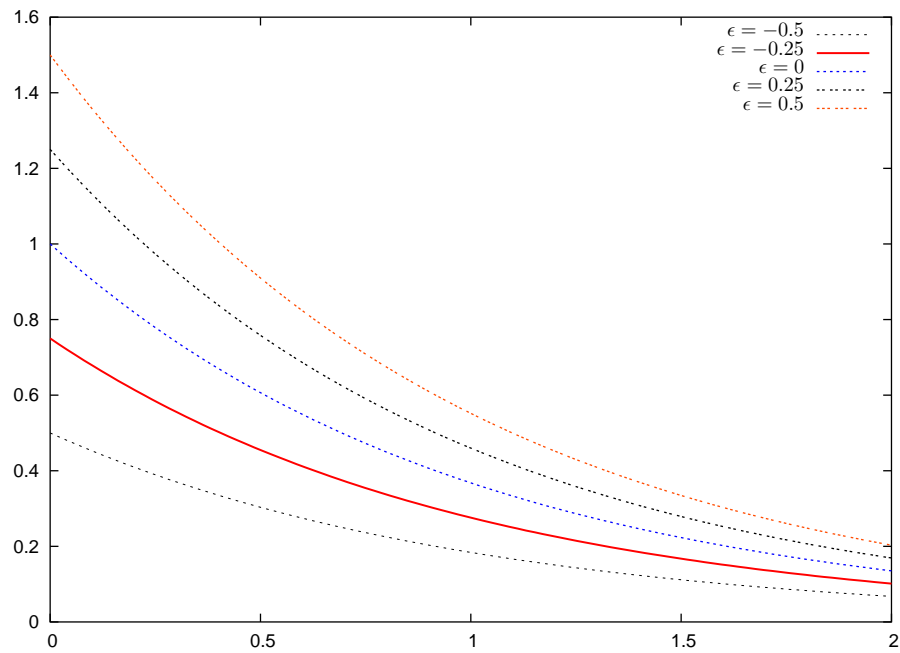
(a)  $(1 + \epsilon)e^t$ (b)  $(1 + \epsilon)e^{-t}$ 

Figure 10.3: Exponential functions with different starting conditions: in (a), the functions  $(1 + \epsilon)e^t$  are shown, while in (b),  $(1 + \epsilon)e^{-t}$  are shown. The latter exhibits stability, while the former exhibits instability.

It turns out there is a simple test for stability. If  $f_x > \delta$  for some positive  $\delta$ , then the ODE is unstable; if  $f_x < -\delta$  for a positive  $\delta$ , the equation is stable. Some ODEs fall through this test, however.

We can prove this without too much pain. Define  $x(t, s)$  to be the solution to

$$\begin{cases} \frac{dx(t)}{dt} = f(t, x(t)), \\ x(a) = s, \end{cases}$$

for  $t \geq a$ .

Then instability means that

$$\lim_{t \rightarrow \infty} \left| \frac{\partial}{\partial s} x(t, s) \right| = \infty.$$

Think about this in terms of the curves for our simple example  $x' = x$ .

If we take the derivative of the ODE we get

$$\begin{aligned} \frac{\partial}{\partial t} x(t, s) &= f(t, x(t, s)), \\ \frac{\partial}{\partial s} \frac{\partial}{\partial t} x(t, s) &= \frac{\partial}{\partial s} f(t, x(t, s)), \quad i.e., \\ \frac{\partial}{\partial s} \frac{\partial}{\partial t} x(t, s) &= f_t(t, x(t)) \frac{\partial t}{\partial s} + f_x(t, x(t, s)) \frac{\partial x(t, s)}{\partial s}. \end{aligned}$$

By the independence of  $t, s$  the first part of the RHS is zero, so

$$\frac{\partial}{\partial s} \frac{\partial}{\partial t} x(t, s) = f_x(t, x(t, s)) \frac{\partial x(t, s)}{\partial s}.$$

We use continuity of  $x$  to switch the orders of differentiation:

$$\frac{\partial}{\partial t} \frac{\partial}{\partial s} x(t, s) = f_x(t, x(t, s)) \frac{\partial}{\partial s} x(t, s).$$

Defining  $u(t) = \frac{\partial}{\partial s} x(t, s)$ , and  $q(t) = f_x(t, x(t, s))$ , we have

$$\frac{\partial}{\partial t} u(t) = q(t)u(t).$$

The solution is  $u(t) = ce^{Q(t)}$ , where

$$Q(t) = \int_a^t q(r) dr.$$

If  $q(r) = f_x(r, x(r, s)) \geq \delta > 0$ , then  $\lim Q(t) = \infty$ , and so  $\lim u(t) = \infty$ . But note that  $u(t) = \frac{\partial}{\partial s} x(t, s)$ , and thus we have instability.

Similarly if  $q(r) \leq -\delta < 0$ , then  $\lim Q(t) = -\infty$ , and so  $\lim u(t) = 0$ , giving stability.

### 10.1.7 Backwards Euler's Method

Euler's Method is the most basic numerical technique for solving ODEs. However, it may suffer from instability, which may make the method inappropriate or impractical. However, it can be recast into a method which may have superior stability at the cost of limited applicability.

This method, the so-called Backwards Euler's Method, is a stepping method: given a reasonable approximation to  $x(t)$ , it calculates an approximation to  $x(t+h)$ . As usual, Taylor's Theorem is the starting point. Letting  $t_f = t+h$ , Taylor's Theorem states that

$$x(t_f - h) = x(t_f) + (-h)x'(t_f) + \frac{(-h)^2}{2}x''(t_f) + \dots,$$

for an analytic function. Assuming that  $x$  has two continuous derivatives on the interval in question, the second order term is truncated to give

$$x(t) = x(t+h-h) = x(t_f - h) \approx x(t_f) + (-h)x'(t_f)$$

and so,  $x(t+h) \approx x(t) + hx'(t+h)$

The complication with applying this method is that  $x'(t+h)$  may not be computable if  $x(t+h)$  is not known, thus cannot be used to calculate an approximation for  $x(t+h)$ . Since this approximation may contain  $x(t+h)$  on both sides, we call this method an *implicit method*. In contrast, Euler's Method, and the Runge-Kutta methods in the following section are *explicit methods*: they can be used to directly compute an approximate step. We make this clear by examples.

**Example 10.4.** Consider the ODE

$$\begin{cases} \frac{dx(t)}{dt} = \cos x, \\ x(0) = 2\pi. \end{cases}$$

In this case, if we wish to approximate  $x(0+h)$  using Backwards Euler's Method, we have to find  $x(h)$  such that  $x(h) = x(0) + \cos x(h)$ . This is equivalent to finding a root of the equation

$$g(y) = 2\pi + \cos y - y = 0$$

The function  $g(y)$  is nonincreasing ( $g'(y)$  is nonpositive), and has a zero between 6 and 8, as seen in Figure 10.4. The techniques of Chapter 4 are needed to find the zero of this function.

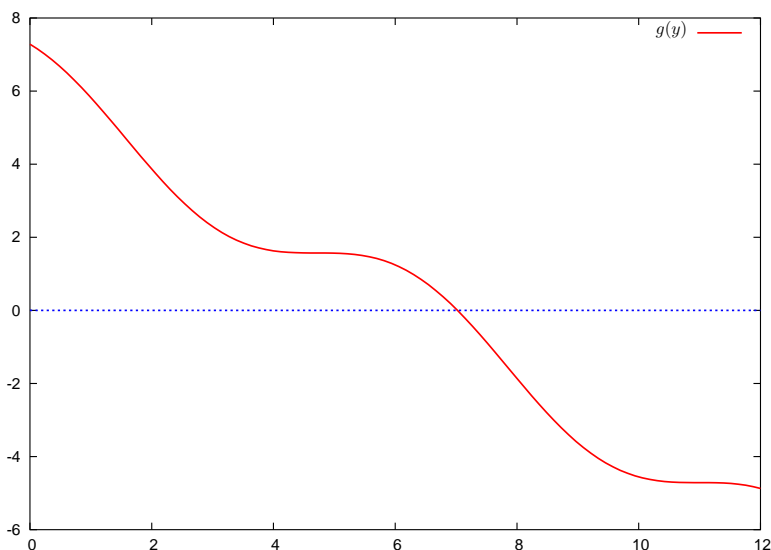


Figure 10.4: The nonincreasing function  $g(y) = 2\pi + \cos y - y$  is shown.

**Example 10.5.** Consider the ODE from Example 10.1:

$$\begin{cases} \frac{dx(t)}{dt} = x, \\ x(0) = 1. \end{cases}$$

The actual solution is  $x(t) = e^t$ . Euler's Method underestimates  $x(t)$ , as shown in Figure 10.1. Using Backwards Euler's Method, gives the approximation:

$$\begin{aligned} x(t+h) &= x(t) + hx(t+h), \\ x(t+h) &= \frac{x(t)}{1-h}. \end{aligned}$$

Using Backwards Euler's Method gives an *overestimate*, as shown in Figure 10.5. This is because each step proceeds on the tangent line to a curve  $ke^t$  to a point on that curve. Generally Backwards Euler's Method is preferred over vanilla Euler's Method because it gives equivalent stability for larger stepsize  $h$ . This effect is not evident in this case.

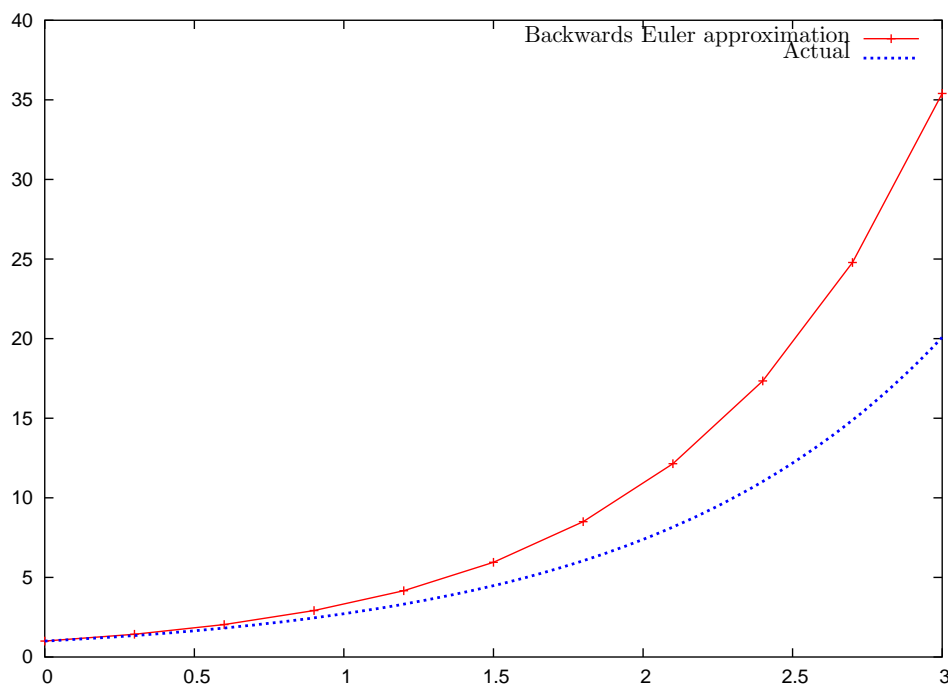


Figure 10.5: Backwards Euler's Method applied to approximate  $x' = x$ ,  $x(0) = 1$ . The approximation is an overestimate, as each step is to a point on a curve  $ke^t$ , through the tangent at that point. Compare this figure to Figure 10.1, which shows the same problem approximated by Euler's Method, with the same stepsize,  $h = 0.3$ .

## 10.2 Runge-Kutta Methods

Recall the ODE problem: find some  $x(t)$  such that

$$\begin{cases} \frac{dx(t)}{dt} = f(t, x(t)), \\ x(a) = c, \end{cases}$$

where  $f, a, c$  are given.

Recall that the Taylor's series method has problems: either you are using the first order method (Euler's Method), which suffers inaccuracy, or you are using a higher order method which requires evaluations of higher order derivatives of  $x(t)$ , *i.e.*,  $x''(t), x'''(t)$ , etc. This makes these methods less useful for the general setting of  $f$  being a blackbox function. The Runge-Kutta Methods (don't ask me how it's pronounced) seek to resolve this.

### 10.2.1 Taylor's Series Redux

We fall back on Taylor's series, in this case the 2-dimensional version:

$$f(x+h, y+k) = \sum_{i=0}^{\infty} \frac{1}{i!} \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \right)^i f(x, y).$$

The thing in the middle is an operator on  $f(x, y)$ . The partial derivative operators are interpreted exactly as if they were algebraic terms, that is:

$$\begin{aligned} \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \right)^0 f(x, y) &= f(x, y), \\ \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \right)^1 f(x, y) &= h \frac{\partial f(x, y)}{\partial x} + k \frac{\partial f(x, y)}{\partial y}, \\ \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \right)^2 f(x, y) &= h^2 \frac{\partial^2 f(x, y)}{\partial x^2} + 2hk \frac{\partial^2 f(x, y)}{\partial x \partial y} + k^2 \frac{\partial^2 f(x, y)}{\partial y^2}, \\ &\vdots \end{aligned}$$

There is a truncated version of Taylor's series:

$$f(x+h, y+k) = \sum_{i=0}^n \frac{1}{i!} \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \right)^i f(x, y) + \frac{1}{(n+1)!} \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \right)^{n+1} f(\bar{x}, \bar{y}).$$

where  $(\bar{x}, \bar{y})$  is a point on the line segment with endpoints  $(x, y)$  and  $(x+h, y+k)$ .

For practice, we will write this for  $n = 1$ :

$$f(x+h, y+k) = f(x, y) + hf_x(x, y) + kf_y(x, y) + \frac{1}{2} (h^2 f_{xx}(\bar{x}, \bar{y}) + 2hk f_{xy}(\bar{x}, \bar{y}) + k^2 f_{yy}(\bar{x}, \bar{y}))$$

### 10.2.2 Deriving the Runge-Kutta Methods

We now introduce the Runge-Kutta Method for stepping from  $x(t)$  to  $x(t+h)$ . We suppose that  $\alpha, \beta, w_1, w_2$  are fixed constants. We then compute:

$$\begin{aligned} K_1 &\leftarrow hf(t, x) \\ K_2 &\leftarrow hf(t + \alpha h, x + \beta K_1). \end{aligned}$$

Then we approximate:

$$x(t+h) \leftarrow x(t) + w_1 K_1 + w_2 K_2.$$

We now examine the "proper" choices of the constants. Note that  $w_1 = 1, w_2 = 0$  corresponds to Euler's Method, and does not require computation of  $K_2$ . We will pick another choice.



Also notice that the definition of  $K_2$  should be related to Taylor's theorem in two dimensions. Let's look at it:

$$\begin{aligned} K_2/h &= f(t + \alpha h, x + \beta K_1) \\ &= f(t + \alpha h, x + \beta h f(t, x)) \\ &= f + \alpha h f_t + \beta h f f_x + \frac{1}{2} (\alpha^2 h^2 f_{tt}(\bar{t}, \bar{x}) + \alpha \beta h^2 f_{tx}(\bar{t}, \bar{x}) + \beta^2 h^2 f^2 f_{xx}(\bar{t}, \bar{x})). \end{aligned}$$

Now reconsider our step:

$$\begin{aligned} x(t+h) &= x(t) + w_1 K_1 + w_2 K_2 \\ &= x(t) + w_1 h f + w_2 h f + w_2 \alpha h^2 f_t + w_2 \beta h^2 f f_x + \mathcal{O}(h^3). \\ &= x(t) + (w_1 + w_2) h x'(t) + w_2 h^2 (\alpha f_t + \beta f f_x) + \mathcal{O}(h^3). \\ &= x(t) + (w_1 + w_2) h x'(t) + w_2 h^2 (\alpha f_t + \beta f f_x) + \mathcal{O}(h^3). \end{aligned}$$

If we happen to choose our constants such that

$$w_1 + w_2 = 1, \quad \alpha w_2 = \frac{1}{2} = \beta w_2,$$

then we get

$$\begin{aligned} x(t+h) &= x(t) + h x'(t) + \frac{1}{2} h^2 (f_t + f f_x) + \mathcal{O}(h^3) \\ &= x(t) + h x'(t) + \frac{1}{2} h^2 x''(t) + \mathcal{O}(h^3), \end{aligned}$$

*i.e.*, our choice of the constants makes the approximate  $x(t+h)$  good up to a  $\mathcal{O}(h^3)$  term, because we end up with the Taylor's series expansion up to that term. cool.

The usual choice of constants is  $\alpha = \beta = 1, w_1 = w_2 = \frac{1}{2}$ . This gives the *second order Runge-Kutta Method* :

$$x(t+h) \leftarrow x(t) + \frac{h}{2} f(t, x) + \frac{h}{2} f(t+h, x + h f(t, x)).$$

This can be written (and evaluated) as

$$\boxed{\begin{aligned} K_1 &\leftarrow h f(t, x) \\ K_2 &\leftarrow h f(t+h, x + K_1) \\ x(t+h) &\leftarrow x(t) + \frac{1}{2} (K_1 + K_2). \end{aligned}} \quad (10.4)$$

Another choice is  $\alpha = \beta = 2/3, w_1 = 1/4, w_2 = 3/4$ . This gives

$$x(t+h) \leftarrow x(t) + \frac{h}{4} f(t, x) + \frac{3h}{4} f\left(t + \frac{2h}{3}, x + \frac{2h}{3} f(t, x)\right).$$

The Runge-Kutta Method of order two has error term  $\mathcal{O}(h^3)$ . Sometimes this is not enough and higher-order Runge-Kutta Methods are used. The next Runge-Kutta Method is the order four method:

$$\boxed{\begin{aligned} K_1 &\leftarrow h f(t, x) \\ K_2 &\leftarrow h f(t+h/2, x + K_1/2) \\ K_3 &\leftarrow h f(t+h/2, x + K_2/2) \\ K_4 &\leftarrow h f(t+h, x + K_3) \\ x(t+h) &\leftarrow x(t) + \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4). \end{aligned}} \quad (10.5)$$

This method has order  $\mathcal{O}(h^5)$ . (See <http://mathworld.wolfram.com/Runge-KuttaMethod.html>)

The Runge-Kutta Method can be extrapolated to even higher orders. However, the number of function evaluations grows faster than the accuracy of the method. Thus the methods of order higher than four are normally not used.

We already saw that  $w_1 = 1, w_2 = 0$  corresponds to Euler's Method. We consider now the case  $w_1 = 0, w_2 = 1$ . The method becomes

$$x(t+h) \leftarrow x(t) + hf\left(t + \frac{h}{2}, x + \frac{h}{2}f(t, x)\right).$$

This is called the *modified Euler's Method*. Note this gives a *different* value than if Euler's Method was applied twice with step size  $h/2$ .

### 10.2.3 Examples

**Example 10.6.** Consider the ODE:

$$\begin{cases} x' = (tx)^3 - \left(\frac{x}{t}\right)^2 \\ x(1) = 1 \end{cases}$$

Use  $h = 0.1$  to compute  $x(1.1)$  using both Taylor's Series Methods and Runge-Kutta methods of order 2.

## 10.3 Systems of ODEs

Recall the regular ODE problem: find some  $x(t)$  such that

$$\begin{cases} \frac{dx(t)}{dt} = f(t, x(t)), \\ x(a) = c, \end{cases}$$

where  $f, a, c$  are given.

Sometimes the physical systems we are considering are more complex. For example, we might be interested in the system of ODEs:

$$\begin{cases} \frac{dx(t)}{dt} = f(t, x(t), y(t)), \\ \frac{dy(t)}{dt} = g(t, x(t), y(t)), \\ x(a) = c, \\ y(a) = d. \end{cases}$$

**Example 10.7.** Consider the following system of ODEs:

$$\begin{cases} \frac{dx(t)}{dt} = t^2 - x \\ \frac{dy(t)}{dt} = y^2 + y - t, \\ x(0) = 1, \\ y(0) = 0. \end{cases}$$

You should immediately notice that this is not a system at all, but rather a collection of two ODEs:

$$\begin{cases} \frac{dx(t)}{dt} = t^2 - x \\ x(0) = 1, \end{cases}$$

and

$$\begin{cases} \frac{dy(t)}{dt} = y^2 + y - t, \\ y(0) = 0. \end{cases}$$

These two ODEs can be solved separately. We call such a system *uncoupled*. In an uncoupled system the function  $f(t, x, y)$  is independent of  $y$ , and  $g(t, x, y)$  is independent of  $x$ . A system which is not uncoupled, is, of course, *coupled*. We will not consider uncoupled systems.

### 10.3.1 Larger Systems

There is no need to stop at two functions. We may imagine we have to solve the following problem: find  $x_1(t), x_2(t), \dots, x_n(t)$  such that

$$\begin{cases} \frac{dx_1(t)}{dt} = f_1(t, x_1(t), x_2(t), \dots, x_n(t)), \\ \frac{dx_2(t)}{dt} = f_2(t, x_1(t), x_2(t), \dots, x_n(t)), \\ \vdots \\ \frac{dx_n(t)}{dt} = f_n(t, x_1(t), x_2(t), \dots, x_n(t)), \\ x_1(a) = c_1, x_2(a) = c_2, \dots, x_n(a) = c_n. \end{cases}$$

The idea is to not be afraid of the notation, write everything as vectors, then *do exactly the same thing as for the one dimensional case!* That's right, there is nothing new but notation:

Let

$$\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix}, \quad \mathbf{X}' = \begin{bmatrix} x_1' \\ x_2' \\ \dots \\ x_n' \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} f_1 \\ f_2 \\ \dots \\ f_n \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} c_1 \\ c_2 \\ \dots \\ c_n \end{bmatrix}.$$

Then we want to find  $\mathbf{X}$  such that

$$\begin{cases} \mathbf{X}'(t) = \mathbf{F}(t, \mathbf{X}(t)) \\ \mathbf{X}(a) = \mathbf{C}. \end{cases} \quad (10.6)$$

Compare this to equation 10.1.

### 10.3.2 Recasting Single ODE Methods

We will consider stepping methods for solving higher order ODEs. That is, we know  $\mathbf{X}(t)$ , and want to find  $\mathbf{X}(t+h)$ . Most of the methods we looked at for solving one dimensional ODEs can be rewritten to solve higher dimensional problems.

For example, Euler's Method, equation 10.3 can be written as

$$\boxed{\mathbf{X}(t+h) \leftarrow \mathbf{X}(t) + h\mathbf{F}(t, \mathbf{X}(t)).}$$

As in 1D, this method is derived from approximating  $\mathbf{X}$  by its linearization.

In fact, our general strategy of using Taylor's Theorem also carries through without change. That is we can use the  $k^{\text{th}}$  order method to step as follows:

$$\mathbf{X}(t+h) \leftarrow \mathbf{X}(t) + h\mathbf{X}'(t) + \frac{h^2}{2}\mathbf{X}''(t) + \dots + \frac{h^k}{k!}\mathbf{X}^{(k)}(t).$$

Additionally we can write the Runge-Kutta Methods as follows:

$$\text{Order two: } \begin{cases} \mathbf{K}_1 \leftarrow h\mathbf{F}(t, \mathbf{X}) \\ \mathbf{K}_2 \leftarrow h\mathbf{F}(t+h, \mathbf{X} + \mathbf{K}_1) \\ \mathbf{X}(t+h) \leftarrow \mathbf{X}(t) + \frac{1}{2}(\mathbf{K}_1 + \mathbf{K}_2). \end{cases}$$

$$\text{Order four: } \begin{cases} \mathbf{K}_1 \leftarrow h\mathbf{F}(t, \mathbf{X}) \\ \mathbf{K}_2 \leftarrow h\mathbf{F}\left(t + \frac{1}{2}h, \mathbf{X} + \frac{1}{2}\mathbf{K}_1\right) \\ \mathbf{K}_3 \leftarrow h\mathbf{F}\left(t + \frac{1}{2}h, \mathbf{X} + \frac{1}{2}\mathbf{K}_2\right) \\ \mathbf{K}_4 \leftarrow h\mathbf{F}(t+h, \mathbf{X} + \mathbf{K}_3) \\ \mathbf{X}(t+h) \leftarrow \mathbf{X}(t) + \frac{1}{6}(\mathbf{K}_1 + 2\mathbf{K}_2 + 2\mathbf{K}_3 + \mathbf{K}_4). \end{cases}$$

**Example Problem 10.8.** Consider the system of ODEs:

$$\begin{cases} x_1'(t) = x_2 - x_3^2 \\ x_2'(t) = t + x_1 + x_3 \\ x_3'(t) = x_2 - x_1^2 \\ x_1(0) = 1, \\ x_2(0) = 0, \\ x_3(0) = 1. \end{cases}$$

Approximate  $\mathbf{X}(0.1)$  by taking a single step of size 0.1, for Euler's Method, and the Runge-Kutta Method of order 2.

*Solution:* We write

$$\mathbf{F}(t, \mathbf{X}(t)) = \begin{bmatrix} x_2(t) - x_3^2(t) \\ t + x_1(t) + x_3(t) \\ x_2(t) - x_1^2(t) \end{bmatrix} \quad \mathbf{X}(0) = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

Thus we have

$$\mathbf{F}(0, \mathbf{X}(0)) = \begin{bmatrix} -1 \\ 2 \\ -1 \end{bmatrix}$$

Euler's Method then makes the approximation

$$\mathbf{X}(0.1) \leftarrow \mathbf{X}(0) + 0.1\mathbf{F}(0, \mathbf{X}(0)) = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + \begin{bmatrix} -0.1 \\ 0.2 \\ -0.1 \end{bmatrix} = \begin{bmatrix} 0.9 \\ 0.2 \\ 0.9 \end{bmatrix}$$

The Runge-Kutta Method computes:

$$\mathbf{K}_1 \leftarrow 0.1\mathbf{F}(0, \mathbf{X}(0)) = \begin{bmatrix} -0.1 \\ 0.2 \\ -0.1 \end{bmatrix} \quad \text{and} \quad \mathbf{K}_2 \leftarrow 0.1\mathbf{F}(0.1, \mathbf{X}(0) + \mathbf{K}_1) = \begin{bmatrix} -0.061 \\ 0.19 \\ -0.061 \end{bmatrix}$$

Then

$$\mathbf{X}(0.1) \leftarrow \mathbf{X}(0) + \frac{1}{2}(\mathbf{K}_1 + \mathbf{K}_2) = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + \begin{bmatrix} -0.0805 \\ 0.195 \\ -0.0805 \end{bmatrix} = \begin{bmatrix} 0.9195 \\ 0.195 \\ 0.9195 \end{bmatrix}$$

+

### 10.3.3 It's Only Systems

The fact we can simply solve systems of ODEs using old methods is good news. It allows us to solve higher order ODEs. For example, consider the following problem: given  $f, a, c_0, c_1, \dots, c_n$ , find  $x(t)$  such that

$$\begin{cases} x^{(n)}(t) = f(t, x(t), x'(t), \dots, x^{(n-1)}(t)), \\ x(a) = c_0, x'(a) = c_1, x''(a) = c_2, \dots, x^{(n-1)}(a) = c_{n-1}. \end{cases}$$

We can put this in terms of a system by letting

$$x_0 = x, x_1 = x', x_2 = x'', \dots, x_{n-1} = x^{(n-1)}.$$

Then the ODE plus these  $n - 1$  equations can be written as

$$\begin{cases} x'_{n-1}(t) = f(t, x_0(t), x_1(t), x_2(t), \dots, x_{n-1}(t)) \\ x'_0(t) = x_1(t) \\ x'_1(t) = x_2(t) \\ \vdots \\ x'_{n-2}(t) = x_{n-1}(t) \\ x_0(a) = c_0, x_1(a) = c_1, x_2(a) = c_2, \dots, x_{n-1}(a) = c_{n-1}. \end{cases}$$

This is just a system of ODEs that we can solve like any other.

Note that this trick also works on systems of higher order ODEs. That is, we can transform any system of higher order ODEs into a (larger) system of first order ODEs.

**Example Problem 10.9.** Rewrite the following system as a system of first order ODEs:

$$\begin{cases} x''(t) = (t/y(t)) + x'(t) - 1 \\ y'(t) = \frac{1}{(x'(t)+y(t))} \\ x(0) = 1, x'(0) = 0, y(0) = -1 \end{cases}$$

*Solution:* We let  $x_0 = x, x_1 = x', x_2 = y$ , then we can rewrite as

$$\begin{cases} x'_1(t) = (t/x_2(t)) + x_1(t) - 1 \\ x'_0(t) = x_1(t) \\ x'_2(t) = \frac{1}{(x_1(t)+x_2(t))} \\ x_0(0) = 1, x_1(0) = 0, x_2(0) = -1 \end{cases}$$

+

### 10.3.4 It's Only Autonomous Systems

In fact, we can use a similar trick to get rid of the time-dependence of an ODE. Consider the first order system

$$\begin{cases} x'_1 = f_1(t, x_1, x_2, \dots, x_n), \\ x'_2 = f_2(t, x_1, x_2, \dots, x_n), \\ x'_3 = f_3(t, x_1, x_2, \dots, x_n), \\ \vdots \\ x'_n = f_n(t, x_1, x_2, \dots, x_n), \\ x_1(a) = c_1, x_2(a) = c_2, \dots, x_n(a) = c_n. \end{cases}$$

We can get rid of the time dependence and thus make the system *autonomous* by making  $t$  another variable function to be found. We do this by letting  $x_0 = t$ , then adding the equations  $x'_0 = 1$ , and  $x_0(a) = a$ , to get the system:

$$\begin{cases} x'_0 = 1, \\ x'_1 = f_1(x_0, x_1, x_2, \dots, x_n), \\ x'_2 = f_2(x_0, x_1, x_2, \dots, x_n), \\ x'_3 = f_3(x_0, x_1, x_2, \dots, x_n), \\ \vdots \\ x'_n = f_n(x_0, x_1, x_2, \dots, x_n), \\ x_0(a) = a, x_1(a) = c_1, x_2(a) = c_2, \dots, x_n(a) = c_n. \end{cases}$$

An autonomous system can be written in the more elegant form:

$$\begin{cases} \mathbf{X}' = \mathbf{F}(\mathbf{X}) \\ \mathbf{X}(a) = \mathbf{C}. \end{cases}$$

Moreover, we can consider the *phase curve* of an autonomous system.

One can consider  $\mathbf{X}$  to be the position of a particle which moves through  $\mathbb{R}^n$  over time. For an autonomous system of ODEs, the movement of the particle is dependent only on its current position and not on time.<sup>1</sup> A phase curve is a flow line in the vector field  $\mathbf{F}$ . You can think of the vector field  $\mathbf{F}$  as being the velocity, at a given point, of a river, the flow of which is time independent. Under this analogy, the phase curve is the path of a vessel placed in the river. In our deterministic world, phase curves never cross. This is because at the point of crossing, there would have to be two different values of the tangent of the curve, *i.e.*, the vector field would have to have two different values at that point.

The following example illustrates the idea of phase curves for autonomous ODE.

**Example 10.10.** Consider the autonomous system of ODEs, without an initial value:

$$\begin{cases} x'_1(t) = -2(x_2 - 2.4) \\ x'_2(t) = 3(x_1 - 1.2) \end{cases}$$

We can rewrite this ODE as

$$\mathbf{X}'(t) = \mathbf{F}(\mathbf{X}(t)).$$

---

<sup>1</sup>Note that if you have converted a system of  $n$  equations with a time dependence to an autonomous system, then the autonomous system should be considered a particle moving through  $\mathbb{R}^{n+1}$ . In this case time becomes one of the dimensions, and thus we speak of position, instead of time.

This is an autonomous ODE. The associated vector field can be expressed as

$$\mathbf{F}(\mathbf{X}) = \begin{bmatrix} 0 & -2 \\ 3 & 0 \end{bmatrix} \mathbf{X} + \begin{bmatrix} 4.8 \\ -3.6 \end{bmatrix}.$$

This vector field is plotted in Figure 10.6.

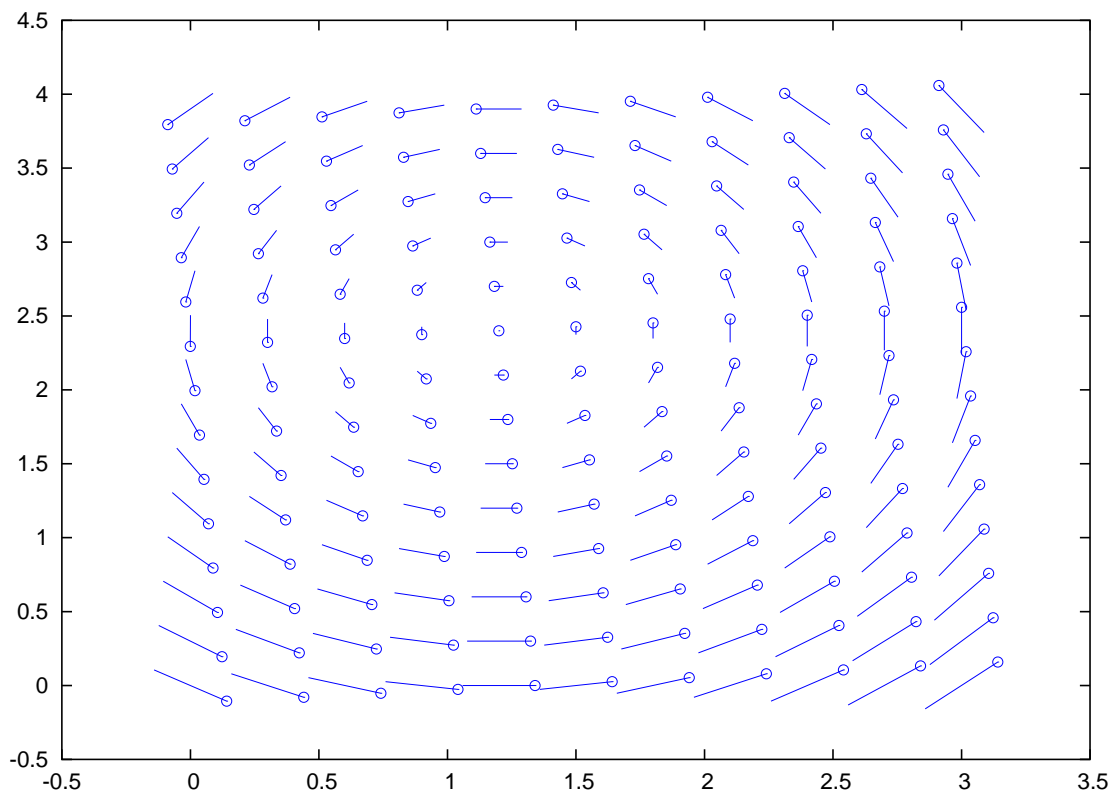


Figure 10.6: The vector field  $\mathbf{F}(\mathbf{X})$  is shown in  $\mathbb{R}^2$ . The tips of the vectors are shown as circles. (Due to budget restrictions, arrowheads were not available for this figure.)

You should verify that this ODE is solved by

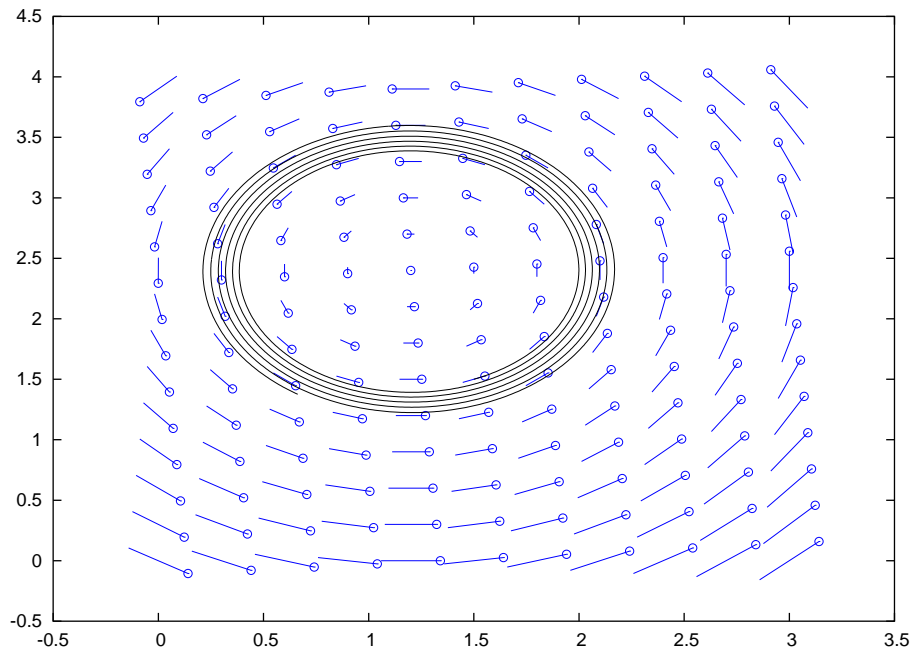
$$\mathbf{X}(t) = r \begin{bmatrix} \sqrt{2} \cos(\sqrt{6}t + t_0) \\ \sqrt{3} \sin(\sqrt{6}t + t_0) \end{bmatrix} + \begin{bmatrix} 1.2 \\ 2.4 \end{bmatrix},$$

for any  $r \geq 0$ , and  $t_0 \in (0, 2\pi]$ . Given an initial value, the parameters  $r$  and  $t_0$  are uniquely determined. Thus the trajectory of  $\mathbf{X}$  over time is that of an ellipse in the plane.<sup>2</sup> Thus the family of such ellipses, taking all  $r \geq 0$ , form the phase curves of this ODE. *We would expect the approximation of an ODE to never cross a phase curve.* This is because the phase curve represents the

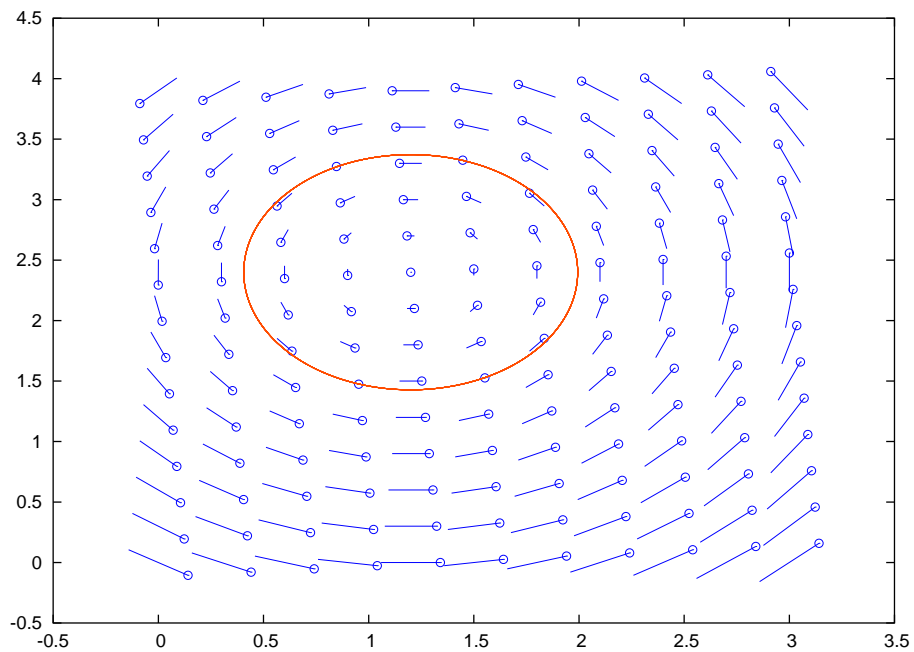
Euler's Method and the second order Runge-Kutta Method were used to approximate the ODE with initial value

$$\mathbf{X}(0) = \begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix}.$$

<sup>2</sup>In the case  $r = 0$ , the ellipse is the "trivial" ellipse which consists of a point.



(a) Euler's Method



(b) Runge-Kutta Method

Figure 10.7: The simulated phase curves of the system of Example 10.10 are shown for (a) Euler's Method and (b) the Runge-Kutta Method of order 2. The Runge-Kutta Method used larger step size, but was more accurate. The actual solution to the ODE is an ellipse, thus the "spiralling" observed for Euler's Method is spurious.



Euler's Method was used for step size  $h = 0.005$  for 3000 steps. The Runge-Kutta Method was employed with step size  $h = 0.015$  for 3000 steps. The approximations are shown in Figure 10.7.

Given that the actual solution of this initial value problem is an ellipse, we see that Euler's Method performed rather poorly, spiralling out from the ellipse. This must be the case for *any* step size, since Euler's Method steps in the direction tangent to the actual solution; thus every step of Euler's Method puts the approximation on an ellipse of larger radius. Smaller stepsize minimizes this effect, but at greater computational cost.

The Runge-Kutta Method performs much better, and for larger step size. At the given resolution, no spiralling is observable. Thus the Runge-Kutta Method outperforms Euler's Method, and at lesser computational cost.<sup>3</sup>

---

<sup>3</sup>Because the Runge-Kutta Method of order two requires two evaluations of  $\mathbf{F}$ , whereas Euler's Method requires only one, per step, it is expected that they would be 'evenly matched' when Runge-Kutta Method uses a step size twice that of Euler's Method.

## EXERCISES

(10.1) Given the ODE:

$$\begin{cases} x'(t) = t^2 - x^2 \\ x(1) = 1 \end{cases}$$

Approximate  $x(1.1)$  by using one step of Euler's Method. Approximate  $x(1.1)$  using one step of the second order Runge-Kutta Method.

(10.2) Given the ODE:

$$\begin{cases} x_1'(t) = x_1x_2 + t \\ x_2'(t) = 2x_2 - x_1^2 \\ x_1(1) = 0 \\ x_2(1) = 3 \end{cases}$$

Approximate  $\mathbf{X}(1.1)$  by using one step of Euler's Method. Approximate  $\mathbf{X}(1.1)$  using one step of the second order Runge-Kutta Method.

(10.3) Consider the separable ODE

$$x'(t) = x(t)g(t),$$

for some function  $g$ . Use backward's Euler (or, alternatively, the right endpoint rule for approximating integrals) to derive the approximation scheme

$$x(t+h) \leftarrow \frac{x(t)}{1 - hg(t+h)}.$$

What could go wrong with using such a scheme?

(10.4) Consider the ODE

$$x'(t) = x(t) + t^2.$$

Using Taylor's Theorem, derive a higher order approximation scheme to find  $x(t+h)$  based on  $x(t)$ ,  $t$ , and  $h$ .

(10.5) Which of the following ODEs can you show are stable? Which are unstable? Which seem ambiguous?

(a)  $x'(t) = -x - \arctan x$  (b)  $x'(t) = 2x + \tan x$  (c)  $x'(t) = -4x - e^x$  (d)  $x'(t) = x + x^3$   
 (e)  $x'(t) = t + \cos x$

(10.6) Rewrite the following higher order ODE as a system of first order ODEs:

$$\begin{cases} x''(t) = x(t) - \sin x'(t), \\ x(0) = 0, \\ x'(0) = \pi. \end{cases}$$

(10.7) Rewrite the system of ODEs as a system of first order ODEs

$$\begin{cases} x''(t) = y(t) + t - x(t), \\ y'(t) = x'(t) + x(t) - 4, \\ x'(0) = 1, \\ x(0) = 2, \\ y(0) = 0. \end{cases}$$

(10.8) Rewrite the following higher order system of ODEs as a system of first order ODEs:

$$\begin{cases} x'''(t) = y''(t) - x'(t), \\ y'''(t) = x''(t) + y'(t), \\ x(0) = x''(0) = y'(0) = -1, \\ x'(0) = y(0) = y''(0) = 1. \end{cases}$$

(10.9) Implement Euler's Method for approximating the solution to

$$\begin{cases} \frac{dx(t)}{dt} = f(t, x(t)), \\ x(a) = c. \end{cases}$$

Your m-file should have header line like:

```
function xfin = euler(f,a,c,h,steps)
```

where `xfin` should be the approximate solution to the ODE at time `a + steps * h`.

- (a) Run your code with  $f(t, x) = -x$ , using  $a = 0 \neq c$ , and using  $h * steps = 1.0$ . In this case the actual solution is

$$x_{fin} = ce^{-1}.$$

This ODE is stable, so your approximation should be good (*cf.* Example 10.3). Experiment with different values of `h`.

- (b) Run your code with  $f(t, x) = x$ , using  $a = 0 \neq c$ , and using  $h * steps = 1.0$ . In this case the actual solution is

$$x_{fin} = ce.$$

Your actual solution may be a rather poor approximation. Prepare a plot of error versus `h` for varying values of `h`. (*cf.* Figure 7.1 and Figure 10.2)

- (c) Run your code with  $f(t, x) = 1/(1 - x)$ , using  $a = 0$ ,  $c = 0.1$ , and using  $h * steps = 2.0$ . Plot your approximations for varying values of `steps`. For example, try `steps` values of 35, 36, and 90, 91. Also try large values of `steps`, like 100, 500, 1000. Can you guess what the actual solution is supposed to look like? Can you explain the poor performance of Euler's Method for this ODE?

(10.10) Implement the Runge-Kutta Method of order two for approximating the solution to

$$\begin{cases} \frac{dx(t)}{dt} = f(t, x(t)), \\ x(a) = c. \end{cases}$$

Your m-file should have header line like:

```
function xfin = rkm(f,a,c,h,steps)
```

where `xfin` should be the approximate solution to the ODE at time `a + steps * h`.

Test your code with the ODEs from the previous problem. Does the Runge-Kutta Method perform any better than Euler's Method for the last ODE?



# Appendix A

## Old Exams

### A.1 First Midterm, Fall 2003

P1 (7 pnts) Clearly state Taylor's Theorem for  $f(x+h)$ . Include all hypotheses, and state the conditions on the variable that appears in the error term.

P2 (7 pnts) Write out the Lagrange Polynomial  $\ell_0(x)$  for nodes  $x_0, x_1, \dots, x_n$ . That is, write the polynomial that has value 1 at  $x_0$  and has value 0 at  $x_1, x_2, \dots, x_n$ .

P3 (7 pnts) Write the Lagrange form of the polynomial of lowest degree that interpolates the following values:

$$\begin{array}{c|c|c} x_k & -1 & 1 \\ \hline y_k & 11 & 17 \end{array}$$

P4 (14 pnts) Use the method of Bisection for finding the zero of the function  $f(x) = x^3 - 3x^2 + 5x - \frac{5}{2}$ . Let  $a_0 = 0$ , and  $b_0 = 2$ . What are  $a_2, b_2$ ?

P5 (21 pnts) • Write out the iteration step of Newton's Method for finding a zero of the function  $f(x)$ . Your iteration should look like

$$x_{k+1} = ??$$

- Write the Newton's Method iteration for finding  $\sqrt{5}$ .
- Letting  $x_0 = 1$ , find the  $x_1$  and  $x_2$  for your iteration. Note that  $\sqrt{5} \approx 2.236$ .

P6 (7 pnts) Write out the iteration step of the Secant Method for finding a zero of the function  $f(x)$ . Your iteration should look like

$$x_{k+1} = ??$$

P7 (21 pnts) Consider the following approximation:

$$f'(x) \approx \frac{f(x+h) - 5f(x) + 4f(x + \frac{h}{2})}{3h}$$

- Derive this approximation using Taylor's Theorem.
- Assuming that  $f(x)$  has bounded derivatives, give the accuracy of the above approximation. Your answer should be something like  $\mathcal{O}(h^2)$ .
- Let  $f(x) = x^2$ . Approximate  $f'(0)$  with this approximation, using  $h = \frac{1}{3}$ .

P8 (21 pnts) Consider the data:

$$\begin{array}{c|c|c|c} k & 0 & 1 & 2 \\ \hline x_k & 3 & 1 & -1 \\ \hline f(x_k) & 5 & 15 & 9 \end{array}$$

- Construct the divided differences table for the data.
- Construct the Newton form of the polynomial  $p(x)$  of lowest degree that interpolates  $f(x)$  at these nodes.
- Suppose that these data were generated by the function  $f(x) = x^3 - 5x^2 + 2x + 17$ . Find a numerical upper bound on the error  $|p(x) - f(x)|$  over the interval  $[-1, 3]$ . Your answer should be a number.

## A.2 Second Midterm, Fall 2003

P1 (6 pts) Write the Trapezoid rule approximation for  $\int_a^b f(x) dx$ , using the nodes  $\{x_i\}_{i=0}^n$ .

P2 (6 pts) Suppose Gaussian Elimination with scaled partial pivoting is applied to the matrix

$$A = \begin{bmatrix} 0.0001 & -0.1 & -0.01 & 0.001 \\ 43 & 91 & -43 & 1 \\ -12 & 26 & -1 & 0 \\ -7 & \frac{1}{2} & -10 & \pi \end{bmatrix}.$$

Which row contains the first pivot? You **must** show your work.

P3 (14 pts) Let  $\phi(n)$  be some quadrature rule that divides an interval into  $2^n$  equal subintervals. Suppose

$$\int_a^b f(x) dx = \phi(n) + a_5 h_n^5 + a_{10} h_n^{10} + a_{15} h_n^{15} + \dots,$$

where  $h_n = \frac{b-a}{2^n}$ . Using evaluations of  $\phi(\cdot)$ , devise a ‘‘Romberg-style’’ quadrature rule that is a  $\mathcal{O}(h_n^{10})$  approximation to the integral.

P4 (14 pts) Compute the LU factorization of the matrix

$$A = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ 2 & 2 & -1 \end{bmatrix}$$

using naïve Gaussian Elimination. Show all your work. Your final answer should be two matrices, L and U. Verify your answer, *i.e.*, verify that  $A = LU$ .

P5 (14 pts) Run one iteration of either Jacobi or Gauss Seidel on the system:

$$\begin{bmatrix} 1 & 3 & 4 \\ -2 & 2 & 1 \\ -1 & 3 & -2 \end{bmatrix} \mathbf{x} = \begin{bmatrix} -3 \\ -3 \\ 1 \end{bmatrix}$$

Start with  $\mathbf{x}^{(0)} = [1 \ 1 \ 1]^T$ . Clearly indicate your answer  $\mathbf{x}^{(1)}$ . Show your work. You **must** indicate *which* of the two methods you are using.

P6 (21 pts) Derive the two-node *Chebyshev Quadrature* rule:

$$\int_{-1}^1 f(x) dx \approx c[f(x_0) + f(x_1)].$$

Make this rule exact for all polynomials of degree  $\leq 2$ .

P7 (28 pts) Consider the quadrature rule:

$$\int_0^1 f(x) dx \approx z_0 f(0) + z_1 f(1) + z_2 f'(0) + z_3 f'(1).$$

- Write four linear equations involving  $z_i$  to make this rule exact for polynomials of the highest possible degree.
- Solve your system for  $z$  using naïve Gaussian Elimination.

### A.3 Final Exam, Fall 2003

P1 (4 **pnts**) Clearly state Taylor's Theorem for  $f(x+h)$ . Include all hypotheses, and state the conditions on the variable that appears in the error term.

P2 (4 **pnts**) State the conditions that characterize  $S(x)$  as a natural cubic spline on the interval  $[a, b]$ . Let the knots be  $a = t_0 < t_1 < t_2 < \dots < t_n = b$ .

P3 (4 **pnts**) Let  $x_0 = 3, x_1 = -5, x_2 = 0$ . Write out the Lagrange Polynomial  $\ell_0(x)$  for these nodes; that is, write the polynomial that has value 1 at  $x_0$  and has value 0 at  $x_1, x_2$ .

P4 (4 **pnts**) Consider the ODE:

$$\begin{cases} x'(t) = f(t, x(t)) \\ x(a) = c \end{cases}$$

Write out the Euler Method to step from  $x(t)$  to  $x(t+h)$ .

P5 (7 **pnts**) Compute the LU factorization of the matrix

$$A = \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & -1 \\ -2 & 0 & 2 \end{bmatrix}$$

using naïve Gaussian Elimination. Show all your work. Your final answer should be two matrices, L and U. Verify your answer, *i.e.*, verify that  $A = LU$ .

P6 (9 **pnts**) Let  $\alpha$  be given. Determine a quadrature rule of the form

$$\int_{-\alpha}^{\alpha} f(x) dx \approx Af(0) + Bf''(-\alpha) + Cf''(\alpha)$$

that is exact for polynomials of highest possible degree. What is the highest degree polynomial for which this rule is exact?

P7 (9 **pnts**) Suppose that  $\phi(n)$  is some computational function that approximates a desired quantity,  $L$ . Furthermore suppose that

$$\phi(n) = L + a_1 n^{-\frac{1}{2}} + a_2 n^{-\frac{2}{2}} + a_3 n^{-\frac{3}{2}} + \dots$$

Combine two evaluations of  $\phi(\cdot)$  in the manner of Richardson to get a  $\mathcal{O}(n^{-1})$  approximation to  $L$ .

P8 (9 **pnts**) Find the least-squares best approximate of the form  $y = \ln(cx)$  to the data

$$\begin{array}{c|c|c|c} x_0 & x_1 & \dots & x_n \\ \hline y_0 & y_1 & \dots & y_n \end{array}$$

*Caution:* this should *not* be done with basis vectors.

P9 (9 **pnts**) Let

$$\mathcal{F} = \{f(x) = c_0 x + c_1 \log x + c_2 \cos x \mid c_0, c_1, c_2 \in \mathbb{R}\}.$$

Set up (*but do not attempt to solve*) the normal equations to find the least-squares best  $f \in \mathcal{F}$  to approximate the data:

$$\begin{array}{c|c|c|c} x_0 & x_1 & \dots & x_n \\ \hline y_0 & y_1 & \dots & y_n \end{array}$$

The normal equations should involve the vector  $\mathbf{c} = [c_0 \ c_1 \ c_2]^\top$ , which uniquely determines a function in  $\mathcal{F}$ .

P10 (9 pts) Consider the following approximation:

$$f''(x) \approx \frac{3f(x-h) - 4f(x) + f(x+3h)}{6h^2}$$

- Derive this approximation using Taylor's Theorem.
- Assuming that  $f(x)$  has bounded derivatives, give the accuracy of the above approximation. Your answer should be something like  $\mathcal{O}(h^?)$ .

P11 (11 pts) Consider the ODE:

$$\begin{cases} x'(t) = x(t)g(t) \\ x(0) = 1 \end{cases}$$

- Use the Fundamental Theorem of Calculus to write a step update of the form:

$$x(t+h) = x(t) + \int_t^{t+h} ??$$

- Approximate the integral using the Trapezoid Rule to get an *explicit* step update of the form

$$x(t+h) \leftarrow Q(t, x(t), h)$$

- Suppose that  $g(t) \geq m > 0$  for all  $t$ . Do you see any problem with this stepping method if  $h > 2/m$ ?

*Hint:* the actual solution to the ODE is

$$x(t) = e^{\int_0^t g(r) dr}.$$

P12 (9 pts) Consider the ODE:

$$\begin{cases} x'(t) = e^{x(t)} + \sin(x(t)) \\ x(0) = 0 \end{cases}$$

Write out the Taylor's series method of order three to approximate  $x(t+h)$  given  $x(t)$ . It is permissible to write the update as a small program like:

$$\begin{aligned} x'(t) &\leftarrow Q_0(x(t)) \\ x''(t) &\leftarrow Q_1(x(t), x'(t)) \\ &\vdots \\ x(t+h) &\leftarrow R(x(t), x'(t), x''(t), \dots) \end{aligned}$$

rather than write the update as a monstrous equation of the form

$$x(t+h) \leftarrow M(x(t)).$$

P13 (15 pts) Consider the data:

|          |      |    |     |
|----------|------|----|-----|
| $k$      | 0    | 1  | 2   |
| $x_k$    | -0.5 | 0  | 0.5 |
| $f(x_k)$ | 5    | 15 | 9   |

- Construct the divided differences table for the data.



- Construct the Newton form of the polynomial  $p(x)$  of lowest degree that interpolates  $f(x)$  at these nodes.
- Suppose that these data were generated by the function  $f(x) = 40x^3 - 32x^2 - 6x + 15$ . Find a numerical upper bound on the error  $|p(x) - f(x)|$  over the interval  $[-0.5, 0.5]$ . Your answer should be a number.

P14 (15 pnts) • Write out the iteration step of Newton's Method for finding a zero of the function  $f(x)$ . Your iteration should look like

$$x_{k+1} = ??$$

- Write the Newton's Method iteration for finding  $\sqrt[3]{25/4}$ .
- Letting  $x_0 = \frac{5}{2}$ , find the  $x_1$  and  $x_2$  for your iteration. Note that  $\sqrt[3]{25/4} \approx 1.842$ .

P15 (15 pnts) • Let  $x$  be some given number, and let  $f(\cdot)$  be a given, "black box" function. Using Taylor's Theorem, derive a  $\mathcal{O}(h)$  approximation to the derivative  $f'(x)$ . Call your approximation  $\phi(h)$ ; the approximation should be defined in terms of  $f(\cdot)$  evaluated at some values, and should probably involve  $x$  and  $h$ .

- Let  $f(x) = x^2 + 1$ . Approximate  $f'(0)$  using your  $\phi(h)$ , for  $h = \frac{1}{2}$ .
- For the same  $f(x)$  and  $h$ , get a  $\mathcal{O}(h^2)$  approximation to  $f'(0)$  using the method of Richardson's Extrapolation; your answer should probably include a table like this:

$$\begin{array}{cc} D(0,0) & \\ D(1,0) & D(1,1) \end{array}$$

## A.4 First Midterm, Fall 2004

[Definitions] Answer *no more than two* of the following.

P1 (12 pnts) Clearly state Taylor's Theorem for  $f(x+h)$ . Include all hypotheses, and state the conditions on the variable that appears in the error term.

P2 (12 pnts) Write the general form of the iterated solution to the problem  $A\mathbf{x} = \mathbf{b}$ . Let  $\mathbf{Q}$  be your "splitting matrix," and use the factor  $\omega$ . Your solution should look something like:

$$??\mathbf{x}^{(k)} = ??\mathbf{x}^{(k-1)} + ?? \quad \text{or} \quad \mathbf{x}^{(k)} = ??\mathbf{x}^{(k-1)} + ??$$

For one of the following variants, describe what  $\mathbf{Q}$  is, in relation to  $\mathbf{A}$  : Richardson's, Jacobi, Gauss-Seidel.

P3 (12 pnts) Write the iteration for Newton's Method *or* the Secant Method for finding a root to the equation  $f(x) = 0$ . Your solution should look something like:

$$x_{k+1} = ?? + \frac{??}{??}$$

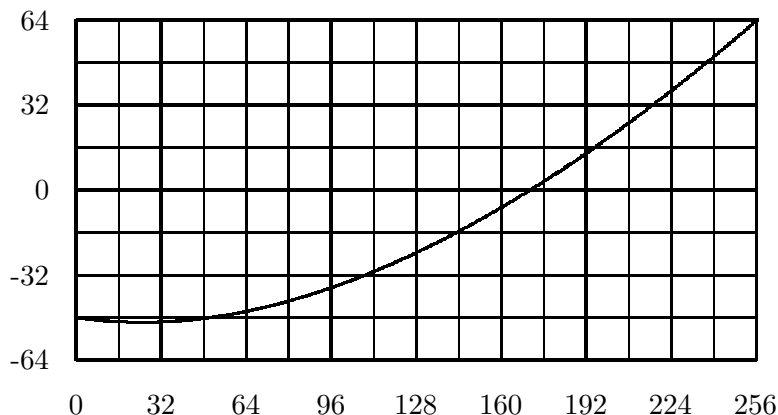
[Problems] Answer *no more than four* of the following.

P1 (14 pnts) Perform bisection on the function graphed below. Let the first interval be  $[0, 256]$ . Give the second, third, fourth, and fifth intervals.

P2 (14 pnts) Give a  $\mathcal{O}(h^4)$  approximation to  $\sin(h + \pi/2)$ . Find a reasonable  $C$  such that the truncation error is no greater than  $Ch^4$ .

P3 (14 pnts) Use Newton's Method to find a good approximation to  $\sqrt[3]{24}$ . Use  $x_0 = 3$ . That is, iteratively define a sequence with  $x_0 = 3$ , such that  $x_k \rightarrow \sqrt[3]{24}$ .

P4 (14 pnts) One of the roots of  $x^2 - bx + c = 0$  as found by the quadratic formula is subject to subtractive cancellation when  $|b| \gg |c|$ . Which root is it? Rewrite the expression for that root to eliminate subtractive cancellation.



P5 (14 pnts) Find the LU decomposition of the following matrix by Gaussian Elimination with naïve pivoting.

$$\begin{bmatrix} 3 & 2 & 4 \\ -6 & 1 & -6 \\ 12 & -12 & 10 \end{bmatrix}$$

P6 (14 pnts) Consider the linear equation:

$$\begin{bmatrix} 6 & 1 & 1 \\ 2 & 4 & 0 \\ 1 & 2 & 6 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 5 \\ -6 \\ 3 \end{bmatrix}$$

Letting  $\mathbf{x}^{(0)} = [1 \ 1 \ 1]^\top$ , find  $\mathbf{x}^{(1)}$  using either the Gauss-Seidel or Jacobi iterative schemes. Use weighting  $\omega = 1$ . You must indicate which scheme you are using. Show all your work.

[Questions] Answer *only one* of the following.

P1 (20 pnts) Suppose that the eigenvalues of  $\mathbf{A}$  are in  $[\alpha, \beta]$  with  $0 < \alpha < \beta$ . Find the  $\omega$  that minimizes  $\|I - \omega \mathbf{A}^2\|_2$ . What is the minimal value of  $\|I - \omega \mathbf{A}^2\|_2$  for this optimal  $\omega$ ? For full credit you need to make some argument *why* this  $\omega$  minimizes this norm.

P2 (20 pnts) Let  $f(x) = 0$  have a unique root  $r$ . Recall that the form of the error for Newton's Method is

$$e_{k+1} = \frac{-f''(\xi_k)}{2f'(x_k)} e_k^2,$$

where  $e_k = r - x_k$ . Suppose that  $f(x)$  has the properties that  $f'(x) \geq m > 0$  for all  $x$ , and  $|f''(x)| \leq M$  for all  $x$ . Find  $\delta > 0$  such that  $|e_k| < \delta$  insures that  $x_n \rightarrow r$ . Justify your answer.

P3 (20 pnts) Suppose that  $f(r) = 0 = f'(r) \neq f''(r)$ , and  $f''(x)$  is continuous. Letting  $e_k = x_k - r$ , show that for Newton's Method,

$$e_{k+1} \approx \frac{1}{2} e_k,$$

when  $|e_k|$  is sufficiently small. (*Hint*: Use Taylor's Theorem twice.) Is this faster or slower convergence than for Newton's Method with a simple root?

## A.5 Second Midterm, Fall 2004

[Definitions] Answer *no more than two* of the following three.

P1 (10 pnts) For a set of distinct nodes  $x_0, x_1, \dots, x_{13}$ , what is the Lagrange Polynomial  $\ell_5(x)$ ? You may write your answer as a product. What degree is this polynomial?

P2 (10 pnts) Complete this statement of the polynomial interpolation error theorem: *Let  $p$  be the polynomial of degree at most  $n$  interpolating function  $f$  at the  $n+1$  distinct nodes  $x_0, x_1, \dots, x_n$  on  $[a, b]$ . Let  $f^{(n+1)}$  be continuous. Then for each  $x \in [a, b]$  there is some  $\xi \in [a, b]$  such that*

$$f(x) - p(x) = \frac{?}{?} \prod_{i=0}^n (?).$$

P3 (10 pnts) State the conditions which define the function  $S(x)$  as a natural cubic spline on the interval  $[a, b]$ .

[Problems] Answer *no more than five of the following six.*

P1 (16 pnts) How large must  $n$  be to interpolate the function  $e^x$  to within 0.001 on the interval  $[0, 2]$  with the polynomial interpolant at  $n$  equally spaced nodes?

P2 (16 pnts) Let  $\phi(h)$  be some computable approximation to the quantity  $L$  such that

$$\phi(h) = L + a_5 h^5 + a_{10} h^{10} + a_{15} h^{15} + \dots$$

Combine evaluations of  $\phi(\cdot)$  to devise a  $\mathcal{O}(h^{10})$  approximation to  $L$ .

P3 (16 pnts) Derive the constants  $A$  and  $B$  which make the quadrature rule

$$\int_{-1}^1 f(x) dx \approx Af\left(-\frac{\sqrt{15}}{5}\right) + Bf(0) + Af\left(\frac{\sqrt{15}}{5}\right)$$

exact for polynomials of degree  $\leq 2$ . Use this quadrature rule to approximate

$$\pi = \int_{-1}^1 \frac{2}{1+x^2} dx$$

P4 (16 pnts) Find the polynomial of degree  $\leq 3$  interpolating the data

$$\begin{array}{c|c|c|c|c} x & -1 & 0 & 1 & 2 \\ \hline y & -2 & 8 & 0 & 4 \end{array}$$

(Hint: using Lagrange Polynomials will probably take too long.)

P5 (16 pnts) Find constants  $\alpha, \beta$  such that the following is a quadratic spline on  $[0, 4]$ .

$$Q(x) = \begin{cases} x^2 - 3x + 4 & : 0 \leq x < 1 \\ \alpha(x-1)^2 + \beta(x-1) + 2 & : 1 \leq x < 3 \\ x^2 + x - 4 & : 3 \leq x \leq 4 \end{cases}$$

P6 (16 pnts) Consider the following approximation:

$$f'(x) \approx \frac{f(x+h) - 5f(x) + 4f(x+\frac{h}{2})}{3h}$$

- Derive this approximation via Taylor's Theorem.
- Assuming that  $f(x)$  has bounded derivatives, give the accuracy of the above approximation. Your answer should be something like  $\mathcal{O}(h^?)$ .
- Let  $f(x) = x^2$ . Approximate  $f'(0)$  with this approximation, using  $h = \frac{1}{3}$ .

## A.6 Final Exam, Fall 2004

[Definitions] Answer *all* of the following.

P1 (10 pnts) Clearly state Taylor's Theorem for  $f(x+h)$ . Include all hypotheses, and state the conditions on the variable that appears in the error term.

P2 (10 pnts) Write the iteration for Newton's Method *or* the Secant Method for finding a root to the equation  $f(x) = 0$ . Your solution should look something like:

$$x_{k+1} = ?? + \frac{??}{??}$$

P3 (10 pnts) Write the general form of the iterated solution to the problem  $\mathbf{Ax} = \mathbf{b}$ . Let  $\mathbf{Q}$  be your "splitting matrix," and use the factor  $\omega$ . Your solution should look something like:

$$??\mathbf{x}^{(k)} = ??\mathbf{x}^{(k-1)} + ?? \quad \text{or} \quad \mathbf{x}^{(k)} = ??\mathbf{x}^{(k-1)} + ??$$

For one of the following variants, describe what  $\mathbf{Q}$  is, in relation to  $\mathbf{A}$ : Richardson's, Jacobi, Gauss-Seidel.

P4 (10 pnts) Define what it means for the function  $f(x) \in \mathcal{F}$  to be the least squares best approximant to the data

$$\begin{array}{c|c|c|c} x_0 & x_1 & \dots & x_n \\ \hline y_0 & y_1 & \dots & y_n \end{array}$$

[Problems] Answer *all* of the following.

P1 (10 pnts) Rewrite this system of higher order ODEs as a system of first order ODEs:

$$\begin{cases} x''(t) = x'(t)[x(t) + ty(t)] \\ y''(t) = y'(t)[y(t) - tx(t)] \\ x'(0) = 1 \\ x(0) = 4 \\ y'(0) = -3 \\ y(0) = -2 \end{cases}$$

P2 (10 pnts) Consider the ODE:

$$\begin{cases} x'(t) = t(x+1)^2 \\ x(2) = 1/2 \end{cases}$$

Use Euler's Method to find an approximate value of  $x(2.1)$  using a single step.

P3 (10 pnts) Let  $\phi(h)$  be some computable approximation to the quantity  $L$  such that

$$\phi(h) = L + a_4h^4 + a_8h^8 + a_{12}h^{12} + \dots$$

Combine evaluations of  $\phi(\cdot)$  to devise a  $\mathcal{O}(h^8)$  approximation to  $L$ .

P4 (15 pnts) Consider the approximation

$$f'(x) \approx \frac{9f(x+h) - 8f(x) - f(x-3h)}{12h}$$

- Derive this approximation using Taylor's Theorem.
- Assuming that  $f(x)$  has bounded derivatives, give the accuracy of the above approximation. Your answer should be something like  $\mathcal{O}(h^2)$ .

P5 (15 pnts) Find constants,  $\alpha, \beta, \gamma$  such that the following is a natural cubic spline on  $[1, 3]$ .

$$Q(x) = \begin{cases} \alpha(x-1)^3 + \beta(x-1)^2 + 12(x-1) + 1 & : 1 \leq x < 2 \\ \gamma x^3 + 18x^2 - 30x + 19 & : 2 \leq x < 3 \end{cases}$$

P6 (15 pnts) Devise a subroutine that, given an input number  $z$ , calculates an approximate to  $\sqrt[3]{z}$  via Newton's Method. Write your subroutine in pseudo code, Matlab, or C/C++. Include reasonable termination conditions so your subroutine will terminate if it finds a good approximate solution. Your subroutine should use only the basic arithmetic operations of addition, subtraction, multiplication, division; in particular your subroutine should not have access to a cubed root or logarithm operator.

P7 (15 pnts) Consider the ODE:

$$\begin{cases} x'(t) = \cos(x(t)) + \sin(x(t)) \\ x(0) = 1 \end{cases}$$

Use Taylor's theorem to devise a  $\mathcal{O}(h^3)$  approximant to  $x(t+h)$  which is a function of  $x, t$ , and  $h$  only. You may write your answer as a program:

$$\begin{aligned} x'(t) &\leftarrow Q_0(x(t)) \\ x''(t) &\leftarrow Q_1(x(t), x'(t)) \\ &\vdots \\ \tilde{x} &\leftarrow R(x(t), x'(t), x''(t), \dots) \end{aligned}$$

such that  $x(t+h) = \tilde{x} + \mathcal{O}(h^3)$ .

[Questions] Answer *all* of the following.

P1 (20 pnts) Consider the "quadrature" rule:

$$\int_0^1 f(x) dx \approx A_0 f(0) + A_1 f(1) + A_2 f'(1) + A_3 f''(1)$$

- Write four linear equations involving  $A_i$  to make this rule exact for polynomials of the highest possible degree.
- Find the constants  $A_i$  using Gaussian Elimination with naïve pivoting.

P2 (20 pnts) Consider the data:

|          |     |      |     |
|----------|-----|------|-----|
| $k$      | 0   | 1    | 2   |
| $x_k$    | 0   | 0.25 | 0.5 |
| $f(x_k)$ | 1.5 | 1    | 0.5 |

- Construct the divided differences table for the data.
- Construct the Newton form of the polynomial  $p(x)$  of lowest degree that interpolates  $f(x)$  at these nodes.
- What degree is your polynomial? Is this strange?
- Suppose that these data were generated by the function

$$f(x) = 1 + \frac{\cos 2\pi x}{2}.$$

Find an upper bound on the error  $|p(x) - f(x)|$  over the interval  $[0, 0.5]$ . Your answer should be a number.

P3 (20 pnts) Let

$$\mathcal{F} = \{f(x) = c_0\sqrt{x} + c_1\ell(x) + c_2e^x \mid c_0, c_1, c_2 \in \mathbb{R}\},$$

where  $\ell(x)$  is some black box function. We are concerned with finding the least-squares best  $f \in \mathcal{F}$  to approximate the data

$$\begin{array}{c|c|c|c} x_0 & x_1 & \dots & x_n \\ \hline y_0 & y_1 & \dots & y_n \end{array}$$

- (a) Set up (*but do not attempt to solve*) the normal equations to find the the vector  $\mathbf{c} = [c_0 \ c_1 \ c_2]^\top$ , which determines the least squares approximant in  $\mathcal{F}$ .
- (b) Now suppose that the function  $\ell(x)$  happens to be the Lagrange Polynomial associated with  $x_7$ , among the values  $x_0, x_1, \dots, x_n$ . That is,  $\ell(x_j) = \delta_{j7}$ . Prove that  $f(x_7) = y_7$ , where  $f$  is the least squares best approximant to the data.

P4 (10 pnts) State some substantive question which you thought might appear on this exam, but did not. Answer this question (correctly).

# Appendix B

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