Analytic Functions of Matrices

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Abstract

Given an analytic function defined on a domain in the complex plane, a corresponding function on the set of square matrices is defined. Properties of these analytic functions of matrices are studied. Square roots and logarithms of matrices are defined; simple applications to solving matrix equations and ordinary differential equations are given.

Contents

1 Introduction

The purpose of this paper is to define and study certain analytic functions from the set $M_n(\mathbb{C})$ of $n \times n$ matrices over $\mathbb{C}$ to $M_n(\mathbb{C})$. Certain additional structure will be assumed: the structure of the functions studied will reflect the structure of ordinary analytic functions from $\mathbb{C}$ to $\mathbb{C}$. In other words, the goal of this paper is to construct an operator which takes an analytic function $f : \mathbb{C} \to \mathbb{C}$ to a function $f^M : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ which satisfies

$$(f+g)^M = f^M + g^M \tag{1.1}$$

$$(fg)^M = f^M g^M \tag{1.2}$$

$$(f \circ g)^M = f^M \circ g^M. \tag{1.3}$$

This correspondence will translate results concerning analytic functions of a complex variable to results concerning functions of matrices.

The prototype for the class of functions treated in this paper is the class of polynomial functions of matrices, in which the identities $(p+q)(M) = p(M) + q(M)$, $(pq)(M) = p(M)q(M)$, $(p \circ q)(M) = p(q(M))$ are clearly satisfied. This class of polynomial functions of matrices (and the broader class of analytic functions of matrices) does not include functions like $f(M) = AM$ where A is a non-scalar matrix. However, some of the techniques used in this paper can be extended to solve matrix equations such as $AX - XB = C$.

Definitions and results are first provided for polynomials, then for entire functions (power series), and finally for general analytic functions. Functions which are just n times continuously differentiable will be mentioned briefly. Further enlargement of the class of functions under consideration would require restricting the class of matrices under consideration, to self-adjoint matrices for example. See [4] for further discussion of this point.

At first sight, it would appear that analytic functions of matrices could be defined using power series, which would provide (1.1)–(1.3). However the notion of power series is too limited: given a function which is not entire, there is generally a matrix for which no power series for the function converges. For example, $\tan \begin{pmatrix} \pi & 0 \\ 0 & -\pi \end{pmatrix}$ cannot be defined by a power series. But splitting the matrix into diagonal blocks, and applying different power series to each block,

it seems clear that

$$\tan \begin{pmatrix} \pi & 0 \\ 0 & -\pi \end{pmatrix} = \begin{pmatrix} \tan \pi & 0 \\ 0 & \tan -\pi \end{pmatrix} \tag{1.4}$$

should hold. It is possible to define analytic functions of matrices by splitting matrices into blocks this way, but this paper provides a more elegant definition that generalizes to operators on infinite-dimensional spaces.

A simple question helps to illustrate the value of the concept of analytic functions of matrices. We know how to square a matrix; it is natural to ask whether we can we solve the equation $X^2 = A$. Solving equations entails constructing inverses of functions, so solving the equation $X^2 = A$ would mean constructing an inverse to the squaring function on matrices, i.e., a square root function on the set of matrices.

Another application of the notion of functions of matrices is constructing solutions to ordinary differential equations. For example, if e^{At} is defined appropriately, it should be a solution to the system $(d/dt)X(t) = AX(t)$. More general systems such as $(d/dt)X(t) = A(t)X(t)$ and $(d/dt)X(t) = AX(t) - X(t)B$ can be studied.

The prerequisites for this paper are minimal: simple linear algebra (the definitions of trace, determinant, eigenvalue and eigenvector, and Cramer's rule) and the basics of complex analysis (analytic and meromorphic functions, power series, and Cauchy's integral formula). Starred sections are not necessary for the main development of the material and may require more prerequisites. There are a number of exercises which are straightforward, and some problems which are more difficult and may be open-ended. Starred exercises and problems use results from starred sections.

1.1 Philosophy

Before we study the mathematics in detail, let us first consider some "philosophical" notions, meaning principles which reflect certain values. These principles reflect the *kind* of mathematics we wish to do, and provide us with motivation by framing problems in a certain way. It is quite possible to use a different set of principles, perhaps even the exact opposites of the ones discussed below, and arrive at a different kind of mathematics; the Kronecker product studied in Section 7.1 is an example of mathematics motivated by the opposite of Principle 1.6.

Personally, I value the following principles more than their opposites, but we should not try to make an ideology out of any of them; in the end, we want to solve hard problems by whatever means possible.

Principle 1.5. *It is generally best to express results in explicit form, using exact formulas if possible.*

Exact formulas allow us to express our results simply, to check our calculations and results easily, and to make approximations if necessary. If we are

going to calculate exactly, though, we will often find that the list of operators available is not large enough. For example, polynomial equations cannot be solved in general by the standard algebraic operations alone, but can be solved in closed form using theta functions [9]. We will often find that infinite processes are useful additions to our available operators.

Principle 1.6. *Use infinite processes such as limits, derivatives, infinite series and integrals.*

The original meaning of the word *analysis* is "working backwards" or "undoing," in other words the opposite of proof. For many years (until Weierstraß' definition of limit), infinite methods could not be used in rigorous proofs but were valuable techniques for solving problems in terms of exact formulas; infinite methods thus became associated with the word "analysis." Analytical methods can be useful even when they are not legitimate proofs if they give explicit formulas which can be verified by other means.

It is possible to solve most of the problems discussed in this paper without the use of infinite processes, and those solutions lead to other interesting results. However, infinite processes allow us to generalize results to more complicated situations.

Principle 1.7. *There's more than one way to do it.*

Solving problems in several different ways may enhance our understanding; one method may generalize better than others in certain situations; and the interplay between methods is often fruitful.

1.2 An Illustrative Problem

An illustration of the point of view outlined in Section 1.1 is provided by the solution to the following problem [6, page 58].

Problem 1.8. *Suppose two square matrices A and B are given with the property that $I - AB$ is invertible. Show that $I - BA$ is also invertible.*

Solution. Explicitly write

$$(I - AB)^{-1} = I + AB + ABAB + ABABAB + \cdots \tag{1.9}$$

$$(I - BA)^{-1} = I + BA + BABA + BABABA + \cdots . \tag{1.10}$$

These expansions are not necessarily correct, but we will try to find an exact formula for $(I - BA)^{-1}$ which we can directly verify later.

Expressing (1.10) in terms of (1.9),

$$(I - BA)^{-1} = I + B(I + AB + ABAB + \cdots)A \tag{1.11}$$

$$(I - BA)^{-1} = I + B(I - AB)^{-1}A \tag{1.12}$$

which gives the desired explicit expression for $(I - BA)^{-1}$. □

Exercise 1.13. *Show that formula 1.12 does in fact work (in any ring with unit).*

2 Matrices of Functions

Let us begin our study of functions of matrices by switching some terms around and first studying matrices of functions, an easier topic which will be useful later. We write a matrix of functions of a real or complex variable in the form $M(t) = (M_{ij}(t))$.

2.1 Limit Processes for Matrices of Functions

The limit, derivative, integral and contour integral of matrices of functions are defined element-wise:

$$\lim_{t \to a} M(t) = \left(\lim_{t \to a} M_{ij}(t) \right) \tag{2.1}$$

$$\frac{d}{dt} M(t) = \left(\frac{d}{dt} M_{ij}(t) \right) \tag{2.2}$$

$$\int_a^b M(t)\ dt = \left(\int_a^b M_{ij}(t)\ dt \right) \tag{2.3}$$

$$\oint_\gamma M(z)\ dz = \left(\oint_\gamma M_{ij}(z)\ dz \right). \tag{2.4}$$

It is easy to verify the product rule for derivatives:

$$\frac{d}{dt}\left(A(t)B(t)\right) = \left(\frac{d}{dt} A(t) \right) B(t) + A(t) \left(\frac{d}{dt} B(t) \right). \tag{2.5}$$

The rule for derivatives of inverses $A^{-1}(t) = (A(t))^{-1}$ follows from (2.5):

$$\frac{d}{dt} A^{-1}(t) = -A^{-1}(t) \left(\frac{d}{dt} A(t) \right) A^{-1}(t). \tag{2.6}$$

Let $f(t)$ be a scalar function. The following chain rule is an immediate consequence of the definition of derivative:

$$\frac{d}{dt} A(f(t)) = \frac{dA}{dt}(f(t)) \frac{df}{dt}; \tag{2.7}$$

more complicated variations on the chain rule will be possible when analytic functions of matrices are defined.

The trace is a linear function on matrices, so it behaves in a simple way with respect to derivatives and integrals:

$$\operatorname{tr} \frac{d}{dt} A(t) = \frac{d}{dt} \operatorname{tr} A(t) \tag{2.8}$$

$$\operatorname{tr} \int_a^b A(t)\ dt = \int_a^b \operatorname{tr} A(t)\ dt \tag{2.9}$$

$$\operatorname{tr} \oint_\gamma A(z)\ dz = \oint_\gamma \operatorname{tr} A(z)\ dz. \tag{2.10}$$

However, the determinant does not behave so nicely:

$$\frac{d}{dt}\det\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} = \det\begin{pmatrix} a'_{11} & a'_{12} & \cdots & a'_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} + \tag{2.11}$$

$$+\det\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a'_{21} & a'_{22} & \cdots & a'_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} + \cdots + \det\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a'_{n1} & a'_{n2} & \cdots & a'_{nn} \end{pmatrix}$$

(with a similar decomposition by columns).

Exercise 2.12. *Prove (2.11) by expanding the determinant and using the product rule for derivatives.*

Problem 2.13. *Find an expression for* $(d^k/dt^k)\det A(t)$.

2.2 The Determinant of a Sum*

The determinant of a sum and determinant of an integral have rather complicated formulas.

Exercise 2.14. *Show that*

$$\det(A+B) = \sum_{k=0}^{2^n-1} \det\left(b_i(k)A_{ij} + (1-b_i(k))B_{ij}\right) \tag{2.15}$$

where

$$b_i(k) = \text{the } i^{th} \text{ digit in the binary expansion of } k \tag{2.16}$$

i.e., the determinant of a sum of two matrices is equal to the sum of determinants the 2^n *matrices formed by picking some rows from the first matrix and the remaining rows from the second.*

Hint. Write out the determinant in summation notation, expand each of the products obtained into sums of 2^n terms, switch the order of summation, and recombine. □

Exercise 2.17. *Find the determinant of the sum of* m *matrices.*

Exercise 2.18. *Show that the result of Exercise 2.14 can be obtained from the block matrix identity*

$$\begin{pmatrix} A & I \\ B & -I \end{pmatrix}\begin{pmatrix} I & O \\ B & I \end{pmatrix} = \begin{pmatrix} A+B & I \\ O & -I \end{pmatrix} \tag{2.19}$$

and the Laplace expansion of the determinant in minors of order n *in the first* n *columns.*

Problem 2.20. *Modify the method of Exercise 2.18 to work for the sum of m matrices to obtain the result of Exercise 2.17.*

Hint. First assume that $m = 2^l$ and apply (2.19) l times, starting at the largest "scale" and working down. Evaluate the determinant of the leftmost factor in a similar manner, starting with minors of the largest scale. □

Problem 2.21. *Can the Kronecker product (Section 7.1) be used to find the determinant of a sum of matrices?*

The determinant of an integral is like the determinant of a sum.

Problem 2.22. *Use Exercise 2.17 to find a formula for the determinant of an integral.*

However, there is an easier way to compute determinants of integrals:

(2.23)
$$\det \int A(t)\, dt = \det \begin{pmatrix} \int A_{11}(t_1)\, dt_1 & \int A_{12}(t_1)\, dt_1 & \cdots & \int A_{1n}(t_1)\, dt_1 \\ \int A_{21}(t_2)\, dt_2 & \int A_{22}(t_2)\, dt_2 & \cdots & \int A_{2n}(t_2)\, dt_2 \\ \vdots & \vdots & \ddots & \vdots \\ \int A_{n1}(t_n)\, dt_n & \int A_{n2}(t_n)\, dt_n & \cdots & \int A_{nn}(t_n)\, dt_n \end{pmatrix}$$

(2.24)
$$= \cdots$$

(2.25)
$$= \int \cdots \int \det \begin{pmatrix} A_{11}(t_1) & A_{12}(t_1) & \cdots & A_{1n}(t_1) \\ A_{21}(t_2) & A_{22}(t_2) & \cdots & A_{2n}(t_2) \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1}(t_n) & A_{n2}(t_n) & \cdots & A_{nn}(t_n) \end{pmatrix} dt_1 \cdots dt_n .$$

Note the similarity between (2.25) and (2.11).

Exercise 2.26. *Provide the details for the missing step at line (2.24).*

Exercise 2.27. *Obtain (2.11) from (2.25).*

Hint. Write (2.25) using definite integrals and then differentiate. □

The multiple integral may be difficult to work with, so here are some suggestions for simplifying it.

Problem 2.28. *Is there an interpretation of (2.25) in terms of the Jacobian of a change of variables?*

Problem 2.29. *Can the integral over the cube in (2.25) be turned into an integral over a tetrahedron?*

2.3 The Resolvent and Characteristic Polynomial

If z is a scalar and $A \in M_n(\mathbb{C})$, the matrix $zI - A$ is often written $z - A$. The set of z such that $z - A$ is invertible is called the *resolvent set* $\rho(A)$ of A; the complement of the resolvent set is called the *spectrum* $\sigma(A)$ of A. The function $R_z : \rho(A) \to M_n(\mathbb{C})$ given by $R_z = (z - A)^{-1}$ is called the *resolvent* of A.

Exercise 2.30. *Use Cramer's rule to show that R_z is an analytic function of z in the resolvent set. Recall that by Cramer's rule*

$$A^{-1} = \frac{\mathrm{cl}(A)}{\det A} \tag{2.31}$$

where $\mathrm{cl}(A)$ *is the classical adjoint of A;* $\mathrm{cl}(A) = C^T$ *where C is the matrix of cofactors*

$$C_{ij} = (-1)^{i+j} \det \tilde{A}_{ij} \tag{2.32}$$

where $\tilde{A}_{ij}$ is the matrix obtained by removing the ith row and j^{th} column from A. Note that $\mathrm{cl}(A)$ *is a matrix of polynomials in the entries of A.*

The function $\det(z - A)$ is a monic polynomial of degree n, known as the *characteristic polynomial* of the matrix A. The roots of $c_A(z)$ (counted with multiplicity) are called the *eigenvalues* of A. Note that the set of eigenvalues is exactly the spectrum of A. The following notation will be used throughout: j is an index over the μ distinct eigenvalues λ_j of a matrix counted with multiplicity m_j. When the range of summation is clear from the context it will be omitted. For example, $\sum_j m_j\lambda_j = \sum_{j=1}^{\mu} m_j\lambda_j$ is the sum of the eigenvalues of A counted with multiplicity.

Lemma 2.33 (Resolvent Identity). *For any $z, \zeta \in \rho(A)$,*

$$R_z - R_\zeta = (\zeta - z)R_z R_\zeta. \tag{2.34}$$

Proof. Note that

$$(z - A)(\zeta - A) = z\zeta - (z + \zeta)A + A^2 = \zeta z - (\zeta + z)A + A^2 = (\zeta - A)(z - A) \tag{2.35}$$

for any $z, \zeta \in \mathbb{C}$, so $(z - A)^{-1}$ and $(\zeta - A)^{-1}$ commute for any $z, \zeta \in \rho(A)$:

$$\begin{aligned}(z - A)^{-1}(\zeta - A)^{-1} &= ((\zeta - A)(z - A))^{-1} = \\ &= ((z - A)(\zeta - A))^{-1} = (\zeta - A)^{-1}(z - A)^{-1}.\end{aligned} \tag{2.36}$$

It follows that

$$R_z - R_\zeta = (z - A)^{-1} - (\zeta - A)^{-1} \tag{2.37}$$

$$= (\zeta - A)(\zeta - A)^{-1}(z - A)^{-1} - (z - A)(z - A)^{-1}(\zeta - A)^{-1} \tag{2.38}$$

$$= ((\zeta - A) - (z - A))(z - A)^{-1}(\zeta - A)^{-1}. \tag{2.39}$$

□

2.4 Trace and Determinant

Writing the characteristic polynomial in the form

$$c_A(z) = z^n - c_{n-1}z^{n-1} + \cdots + (-1)^{n-1}c_1 z + (-1)^n c_0, \tag{2.40}$$

it is easy to see that $c_0 = \det A$; expanding the determinant $\det(z - A)$ in the first row, it is clear that the coefficient of z^{n-1} in $c_A(z)$ is the same as the coefficient of z^{n-1} in $(z - A_{11}) \cdots (z - A_{nn})$, from which it follows that $c_{n-1} = \sum_{i=1}^n A_{ii} = \operatorname{tr} A$.

Exercise 2.41. *Show that* $\operatorname{tr} A = \sum_j m_j \lambda_j$.

Problem 2.42. *Use Problem 2.13 to compute the derivative* $(d^{n-1}/dz^{n-1})c_A(z)$ *to show* $c_{n-1} = \operatorname{tr} A$.

Suppose A is invertible. Since $\det(A^{-1})\det(A) = \det(A^{-1}A) = \det I = 1$, $\det(A^{-1}) = (\det A)^{-1} = c_0^{-1}$. Thus the characteristic polynomial of the inverse of the invertible matrix A is

$$\begin{aligned}
c_{A^{-1}}(z) &= \det(z - A^{-1}) && (2.43)\\
&= \det(-zA^{-1})\det(-z^{-1}A)\det(z - A^{-1}) && (2.44)\\
&= (-z)^n c_0^{-1}\det(z^{-1} - A) && (2.45)\\
&= (-z)^n c_0^{-1} c_A(z^{-1}) && (2.46)\\
&= z^n - \frac{c_1}{c_0}z^{n-1} + \cdots + (-1)^{n-1}\frac{c_{n-1}}{c_0}z + (-1)^n\frac{1}{c_0}, && (2.47)
\end{aligned}$$

from which it follows that $\operatorname{tr} A^{-1} = c_1/c_0 = \sum_j m_j/\lambda_j$. Finally, note that the eigenvalues of $z - A$ are $z - \lambda_j$ with multiplicity m_j, so the trace of the resolvent is given by

$$\operatorname{tr}(z - A)^{-1} = \sum_j \frac{m_j}{z - \lambda_j}. \tag{2.48}$$

3 Polynomial Functions of Matrices

Polynomials are a simple prototype for the analytic functions which we wish to study. We want functions of matrices to behave sensibly with respect to addition, multiplication and composition of polynomials as in (1.1)–(1.3); combined with the assumptions that constant polynomials go over to the corresponding constant matrix function, and the identity function goes over to the identity function on matrices, polynomial functions of matrices are completely determined.

3.1 Cauchy's Integral Formula

Recall that we can get powers of a complex variable by Cauchy's integral formula

$$\lambda^k = \frac{1}{2\pi i} \oint_\gamma z^k (z-\lambda)^{-1}\, dz \tag{3.1}$$

where γ is a circle in the complex plane winding once around λ. Cauchy's integral formula can be verified easily in this case by expanding $(z-\lambda)^{-1}$ in powers of z and examining the coefficient of z^{-1} (i.e., the *residue* of $z^k(z-\lambda)^{-1}$).

This gives an alternative way of getting powers of matrices: we can get the whole list of powers of the matrix A by the following formula:

$$(z-A)^{-1} = z^{-1}\left(I - \frac{A}{z}\right)^{-1} = z^{-1}\left(I + \frac{A}{z} + \frac{A^2}{z^2} + \cdots\right) \tag{3.2}$$

where z is large enough so that the series converges.

Exercise 3.3. *Show that $\|A\| = n \sup |A_{ij}|$ defines a norm on $M_n(\mathbb{C})$ with the property that $\|AB\| \le \|A\|\,\|B\|$.*

Exercise 3.4. *Show that $|z| > \|A\|$ implies that (3.2) converges.*

Exercise 3.5. *Show that a circle centered at the origin of radius $r > \|A\|$ encloses the spectrum of A.*

Just as in the ordinary theory of functions of a complex variable, if we want to pick out the power A^k of A, we multiply the above series by z^k and integrate over a large enough circle. Of course, now that we have an integral expression we may vary the contour; the only requirement is the topological condition that the contour must wind once about the spectrum of A. This gives the following theorem:

Theorem 3.6. *For any matrix A and any nonnegative integer k,*

$$A^k = \frac{1}{2\pi i} \oint_\gamma z^k (z-A)^{-1}\, dz \tag{3.7}$$

where γ is a contour winding once around the spectrum of A.

3.2 Applications of Cauchy's Integral Formula

Theorem 3.6 can be used to prove a simple result: if a matrix has only 0 as an eigenvalue, it is nilpotent. To be precise,

Proposition 3.8. *If a matrix $N \in M_n(\mathbb{C})$ has only 0 as an eigenvalue, then $N^n = O$.*

Proof. Let γ be the circle of radius r centered at the origin. Then

$$N^n = \frac{1}{2\pi i} \oint_\gamma z^n (z-N)^{-1}\, dz \tag{3.9}$$

$$= \frac{1}{2\pi i} \int_0^{2\pi} r^n e^{in\theta} (re^{i\theta} - N)^{-1} ire^{i\theta}\, d\theta \tag{3.10}$$

$$= \frac{r^{n+1}}{2\pi} \int_0^{2\pi} e^{i(n+1)\theta} (re^{i\theta} - N)^{-1}\, d\theta. \tag{3.11}$$

However, each of the entries of the matrix in the integrand is bounded above in norm by some constant multiple of r^{-n} as $r \to 0$ (by Cramer's rule), so $N^n \to O$ as $r \to 0$. But N^n is independent of r, so $N^n = O$. □

Theorem 3.6 can also be used to compute the trace of A^k.

Proposition 3.12. *Let A have the eigenvalues λ_j with multiplicities m_j. Then for any positive integer k,*

$$\operatorname{tr} A^k = \sum_j m_j \lambda_j^k. \tag{3.13}$$

Proof. Since the trace of a matrix is linear,

$$\operatorname{tr} A^k = \operatorname{tr} \frac{1}{2\pi i} \oint_\gamma z^k (z-A)^{-1}\, dz \tag{3.14}$$

$$= \frac{1}{2\pi i} \oint_\gamma z^k \operatorname{tr}(z-A)^{-1}\, dz \tag{3.15}$$

$$= \frac{1}{2\pi i} \oint_\gamma z^k \sum_j \frac{m_j}{z-\lambda_j}\, dz \tag{3.16}$$

by (2.48); the result follows by Cauchy's integral formula. □

Clearly Theorem 3.6 behaves properly under addition and scalar multiplication, so we have

Theorem 3.17. *For any matrix A and any polynomial p,*

$$p(A) = \frac{1}{2\pi i} \oint_\gamma p(z)(z-A)^{-1}\, dz \tag{3.18}$$

where γ is a contour winding once around the spectrum of A.

The following generalization of Proposition 3.8 is an application of Theorem 3.17:

Theorem 3.19 (Cayley-Hamilton). *A matrix satisfies its own characteristic equation, i.e., $c_A(A) = O$.*

Proof. Let $c_A(z) = \det(z - A)$ be the characteristic polynomial of the matrix A. Recall that the inverse of a matrix is given by Cramer's rule:

$$M^{-1} = \frac{\mathrm{cl}(M)}{\det M} \tag{3.20}$$

where $\mathrm{cl}(M)$ is the classical adjoint of M (see Exercise 2.30). In the special case $M = z - A$ we have $\det(z - A) = c_A(z)$ and the classical adjoint is a matrix of polynomials, so

$$c_A(A) = \frac{1}{2\pi i} \oint_\gamma c_A(z)(z - A)^{-1}\, dz \tag{3.21}$$

$$= \frac{1}{2\pi i} \oint_\gamma c_A(z) \frac{\mathrm{cl}(A)}{c_A(z)}\, dz \tag{3.22}$$

which vanishes since the integrand is (or rather, can be extended to) an analytic function on $\mathbb{C}$. □

Exercise 3.23. *Show that Proposition 3.8 is a consequence of Theorem 3.19.*

Linear operators in infinite-dimensional spaces may have one-sided inverses but not two-sided inverses. The Cayley-Hamilton theorem shows that that cannot happen in finite-dimensional spaces.

Theorem 3.24. *If* $\det A = 0$ *then* A *has no inverse; if* $\det A \neq 0$ *then* A *has a two-sided inverse.*

Proof. If $AB = I$ or $BA = I$ then $\det A \det B = 1$ which implies that $\det A \neq 0$. On the other hand, if $\det A \neq 0$ then

$$c_A(z) = z^n - c_{n-1}z^{n-1} + \cdots + (-1)^{n-1}c_1 z + (-1)^n c_0 \tag{3.25}$$

with $c_0 \neq 0$, and by the Cayley-Hamilton theorem

$$\frac{1}{(-1)^{n+1}c_0}\left(A^{n-1} - c_{n-1}A^{n-2} + \cdots + (-1)^{n-1}c_1\right) \tag{3.26}$$

is the required two-sided inverse. □

Any polynomial in a matrix can be reduced to a polynomial of degree at most $n - 1$ by successive application of the Cayley-Hamilton theorem. The same result follows from "wrapping" polynomial division in the appropriate integral expression.

Theorem 3.27. *Given a matrix* $A \in M_n(\mathbb{C})$*, any polynomial* $p(A)$ *in* A *is equal to a polynomial* $r(A)$ *in* A *of degree at most* $n - 1$*.*

Proof. Apply polynomial division (the Euclidean algorithm) to obtain $p(z) = c_A(z)q(z) + r(z)$ where the quotient $q(z)$ is a polynomial and the remainder $r(z)$ is a polynomial of degree at most $n-1$. Then

$$p(A) = \frac{1}{2\pi i} \oint_\gamma p(z)(z-A)^{-1}\, dz \tag{3.28}$$

$$= \frac{1}{2\pi i} \oint_\gamma (c_A(z)q(z) + r(z))(z-A)^{-1}\, dz \tag{3.29}$$

$$= r(A). \tag{3.30}$$

□

Exercise 3.31. *What does Theorem 3.27 say when $n = 1$?*

Exercise 3.32. *Compute $r^{(u)}(\lambda_j)$ in terms of $p^{(u)}(\lambda_j)$, $u = 0, \ldots, m_j - 1$.*

Hint. Use the following generalization of Cauchy's integral formula:

$$f^{(u)}(\zeta) = \frac{u!}{2\pi i} \oint_\gamma \frac{f(z)}{(z-\zeta)^{u+1}}\, dz \tag{3.33}$$

where γ is a contour winding once around ζ. □

Problem 3.34. *User Exercise 3.32 to obtain explicit formulas for $r(z)$ and $r(A)$.*

Hint. First consider the case in which all the roots of $c_A(z)$ are distinct. □

The idea of Theorem 3.27, that polynomial identities can be multiplied by an appropriate factor and integrated over an appropriate contour to turn them into matrix identities, has many more applications in this paper.

3.3 The Minimal Polynomial*

The fact that $c_A(A) = O$ implies that there exists a monic (i.e., with leading coefficient 1) polynomial $m_A(z)$ of least degree such that $m_A(A) = O$.

Exercise 3.35. *Show that m_A is unique.*

Exercise 3.36. *Show that $m_A(z)$ divides $c_A(z)$; more generally, show that $p(A) = O$ implies $m_A | p$.*

Exercise 3.37. *Show that the characteristic polynomial $c_A(z)$ can be replaced by the minimal polynomial $m_A(z)$ in the proof of Theorem 3.27.*

4 Entire Functions of Matrices

Suppose $f(z) = a_0 + a_1 z + a_2 z^2 + \cdots$ is a function with a power series which converges everywhere in the plane (i.e., f is an *entire function*). Recall our matrix norm $\|A\| = n \sup |A_{ij}|$. Then $\|A^k\| \leq \|A\|^k$, $k = 0, 1, 2, \ldots$, so the infinite series $f(A)$ converges absolutely by the Weierstraß M-test.

Let γ be a circle centered at the origin of radius $r > \|A\|$ (which therefore encloses the spectrum of A. Then by Theorem 3.6,

$$a_k A^k = \frac{1}{2\pi i} \oint_\gamma a_k z^k (z - A)^{-1}\, dz. \tag{4.1}$$

It follows that

$$f(A) = \frac{1}{2\pi i} \oint_\gamma f(z)(z - A)^{-1}\, dz. \tag{4.2}$$

Of course, now that we know the particular contour integral given above converges, we can modify the contour, just as we did in Theorem 3.6:

Theorem 4.3. *For any matrix A and any entire function f, the series $f(A) = \sum_{k=0}^{\infty} a_k A^k$ converges and is equal to*

$$f(A) = \frac{1}{2\pi i} \oint_\gamma f(z)(z - A)^{-1}\, dz \tag{4.4}$$

where γ is a contour winding once around the spectrum of A.

4.1 Constant Coefficient Differential Equations

The contour integral in (4.4) is an integral over a compact set, so limit processes may be passed under the integral sign. This permits us to take certain limits, derivatives and integrals of entire functions of matrices.

Exercise 4.5. *Evaluate* $\lim_{t \to 0} (\sin tA)/(tA)$.

Exercise 4.6. *Evaluate* $\int_0^t \cosh(sA)\, ds$.

One important application of the above idea is the solution of systems of constant coefficient differential equations

$$\frac{d}{dt} X(t) = AX(t), \quad X(0) = I. \tag{4.7}$$

Again, we re-use our knowledge of the behaviour of scalar functions to solve the matrix differential equation (4.7). In particular, we can map the property

$$\frac{d}{dt} e^{zt} = z e^{zt} \tag{4.8}$$

of the exponential function to a property of functions of matrices by wrapping the identity (4.8) in the appropriate contour integral: differentiating the formula

$$e^{At} = \frac{1}{2\pi i} \oint_\gamma e^{zt} (z - A)^{-1}\, dz \tag{4.9}$$

under the integral sign, it follows that

$$\frac{d}{dt} e^{At} = A e^{At}, \tag{4.10}$$

so e^{At} is the (unique) function satisfying the system (4.7).

Exercise 4.11. *Solve the system*

$$\frac{d}{dt} X(t) = AX(t), \quad X(0) = B. \tag{4.12}$$

Problem 4.13. *Use (2.6) to find*

$$\frac{d}{dt} \frac{1}{2\pi i} \oint_\gamma e^{z} (z - At)^{-1}\, dz. \tag{4.14}$$

Is there a version of (3.33) that would help evaluate (4.14)?

An important consequence of (4.10) is the following identity.

Theorem 4.15. *For any matrix A,*

$$\det e^{A} = e^{\operatorname{tr} A}. \tag{4.16}$$

Proof. To differentiate a row of e^{At} we multiply e^{At} on the left by a row of A. Therefore by (2.11),

$$\frac{d}{dt} \det e^{At} = \det \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ 0 & 1 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} e^{At} + \tag{4.17}$$

$$+ \det \begin{pmatrix} 1 & 0 & \cdots & 0 \\ A_{21} & A_{22} & \cdots & A_{2n} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} e^{At} + \cdots + \det \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix} e^{At}.$$

Each of the determinants of the matrices containing A_{ij}'s may be evaluated by expanding in the column containing A_{ii} to obtain A_{ii}. It follows that $x(t) = \det e^{At}$ is a solution to the scalar ordinary differential equation $(d/dt)x(t) = (\operatorname{tr} A)x(t)$, so $\det e^{At} = ke^{\operatorname{tr} At}$. Setting $t = 0$ gives $k = 1$. Setting $t = 1$ gives the result. $\square$

Theorem 4.15 is a special case of *Jacobi's Identity*.

Exercise 4.18 (Jacobi's Identity). *If $X(t)$ is the (unique) solution to the system of linear differential equations*

$$\frac{d}{dt}X(t) = A(t)X(t), \quad X(0) = I \tag{4.19}$$

for $t \in [0, t_0]$ then

$$\det X(t) = e^{\int_0^t \operatorname{tr} A(s)\, ds} \tag{4.20}$$

for $t \in [0, t_0)$.

It follows from Theorem 4.15 that e^A is nonsingular for any matrix A. However, the inverse can be constructed explicitly using the following theorem.

Theorem 4.21. *For entire functions f and g, $(f+g)(M) = f(M) + g(M)$, $(fg)(M) = f(M)g(M)$ and $(f \circ g)(M) = f(g(M))$.*

Proof. These identities hold for power series. □

Thus identities which hold for entire functions can be turned into matrix identities using the above theorem. Let $f(z) = e^z$, $g(z) = e^{-z}$. Since $1 = f(z)g(z)$, it follows that $I = f(A)g(A)$, so $(e^A)^{-1} = e^{-A}$.

Exercise 4.22. *Show that the identity $\sin^2(A) + \cos^2(A) = I$ holds for any matrix A.*

Exercise 4.23. *Show that the identity $e^{iA} = \cos A + i \sin A$ holds for any matrix A.*

Note that identities for functions in two or more variables may not hold for matrices. For example, $e^A e^B$, e^{A+B} and $e^B e^A$ are all different when

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{4.24}$$

Exercise 4.25. *Using power series, show that $e^A e^B = e^{A+B} = e^B e^A$ holds for* commuting *matrices A, B.*

Problem 4.26. *Is it possible to find an integral representation for entire functions of commuting matrices in two or more variables?*

4.2 Interpolation

Recall that for any polynomial p, $p(A) = r(A)$ for some polynomial r of degree $n-1$. It seems likely that a similar theorem may hold for entire functions, but the first argument used to prove Theorem 3.27, that of reducing the degree of a polynomial function by repeatedly applying the Cayley-Hamilton theorem, cannot be used. Fortunately, entire functions may be divided by polynomials. Dividing f by c_A gives the following result.

Theorem 4.27 (Function Division). *Any entire function f may be written*

$$f(z) = c_A(z)q(z) + r(z) \tag{4.28}$$

where $q(z)$ is an entire function,

$$r(z) = \sum_{j=1}^{\mu} \left[\sum_{u=0}^{m_j-1} \frac{1}{u!}\phi_j^{(u)}(\lambda_j)(z-\lambda_j)^u \right] \prod_{\substack{k=1 \\ k\neq j}}^{\mu} (z-\lambda_k)^{m_k}, \tag{4.29}$$

$$\phi_j(z) = \frac{f(z)(z-\lambda_j)^{m_j}}{c_A(z)}, \tag{4.30}$$

and λ_j are the μ distinct roots of $c_A(z)$ with multiplicities m_j.

Proof. By Exercise 4.32 it is sufficient to show that the meromorphic functions

$$q_j(z) = \frac{f(z) - r(z)}{(z-\lambda_j)^{m_j}} \tag{4.31}$$

are actually entire on $\mathbb{C}$. By Exercise 4.36, the first $m_j - 1$ coefficients of the power series expansion of $f(z)-r(z)$ in $(z-\lambda_j)$ vanish and the result follows. □

Exercise 4.32. *Suppose that*

$$\frac{g(z)}{(z-\lambda_1)^{m_1}}, \ldots, \frac{g(z)}{(z-\lambda_\mu)^{m_\mu}} \tag{4.33}$$

are entire functions ($\lambda_1, \ldots, \lambda_\mu$ all distinct). Show that

$$\frac{g(z)}{(z-\lambda_1)^{m_1} \cdots (z-\lambda_\mu)^{m_\mu}} \tag{4.34}$$

is entire.

Hint. Use the partial fractions decomposition of

$$\frac{1}{(z-\lambda_1)^{m_1} \cdots (z-\lambda_\mu)^{m_\mu}}. \tag{4.35}$$

□

Exercise 4.36 (Lagrange-Hermite Interpolation). *Show that the remainder $r(z)$ given by (4.29) satisfies the Lagrange-Hermite interpolation condition*

$$r^{(u)}(\lambda_j) = f^{(u)}(\lambda_j) \quad \text{for } u = 0, \ldots, m_j - 1,\ j = 1, \ldots, \mu. \tag{4.37}$$

Exercise 4.38. *Show that $r(z)$ is the unique polynomial of degree $n-1$ or less which satisfies (4.28) under the condition that $q(z)$ is entire.*

Exercise 4.39. *If f is a polynomial, show that Theorem 4.27 gives an explicit formula for the partial fractions decomposition of $f(z)/c_A(z)$.*

Using Theorem 4.27, it is possible to show that for any entire function f and any matrix A, $f(A) = r(A)$ for some polynomial $r(z)$. To be precise,

Theorem 4.40 (Buchheim's Formula). *Let f be an entire function and let A be a matrix. Then*

$$f(A) = \sum_{j=1}^{\mu} \left[\sum_{u=0}^{m_j-1} \frac{1}{u!} \phi_j^{(u)}(\lambda_j)(A-\lambda_j)^u \right] \prod_{\substack{k=1 \\ k \neq j}}^{\mu} (A-\lambda_k)^{m_k} \tag{4.41}$$

where

$$\phi_j(z) = \frac{f(z)(z-\lambda_j)^{m_j}}{c_A(z)} \tag{4.42}$$

and λ_j are the μ distinct roots of $c_A(z)$ with multiplicities m_j.

Proof.

$$f(A) = \frac{1}{2\pi i} \oint_\gamma f(z)(z-A)^{-1}\, dz \tag{4.43}$$

$$= \frac{1}{2\pi i} \oint_\gamma (c_A(z)q(z) + r(z))(z-A)^{-1}\, dz \tag{4.44}$$

$$= c_A(A)q(A) + r(A) = r(A). \tag{4.45}$$

□

Theorem 4.40 gives an explicit formula even when f is a polynomial; compare with the Euclidean algorithm for polynomial division used in Theorem 3.27.

Exercise* 4.46. *Show that the appropriate modification of Theorem 4.40 holds when $c_A(z)$ is replaced by any polynomial $m(z)$ for which $m(A) = O$.*

Problem* 4.47. *Are there versions of Theorems 4.27 and 4.40 in which $c_A(z)$ is replaced by an entire function $m(z)$ for which $m(A) = O$?*

Hint. See [2, page 339] for a discussion. □

5 Analytic Functions of Matrices

The results of Section 4 can be generalized to analytic functions defined a disk (and therefore given by power series) and for matrices with eigenvalues in the disk. Greater care has to be taken to show that the matrix power series converge, but otherwise the theory is identical to that of Section 4. However, the power series approach fails for functions such as $\tan \begin{pmatrix} \pi & 0 \\ 0 & -\pi \end{pmatrix}$. On the other hand, given the success of the contour integral approach so far, the following definition seems to be appropriate.

Definition 5.1. *Let f be an analytic function defined on the domain $\Omega \subset \mathbb{C}$. Let $A \in M_n(\mathbb{C})$ be a matrix with spectrum contained in Ω. Let γ be a contour in Ω winding once the spectrum of A. Then $f(A)$ is defined by the formula*

$$f(A) = \frac{1}{2\pi i} \oint_\gamma f(z)(z-A)^{-1}\, dz. \tag{5.2}$$

The function $f : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ given by (5.2) is called the *primary matrix function* $f(A)$ corresponding to the *stem function* $f(t)$.

Since $(z-A)^{-1}$ is a matrix of functions analytic outside of the spectrum of A, the integral in (5.2) converges and is well-defined by Cauchy's theorem. By previous results, $f(A)$ agrees with the old notion of $f(A)$ when f is a polynomial or entire function (or when the spectrum of A is contained within the radius of convergence of a power series expansion for f).

5.1 Basic Theorems

We should check that this notion of function satisfies the identities which we expect.

Theorem 5.3. *Let f, g be two analytic functions defined on the domain $\Omega \supset \mathbb{C}$, and let A be a matrix with spectrum contained in Ω. Then*

$$f(A) + g(A) = (f+g)(A), \tag{5.4}$$

$$f(A)g(A) = (fg)(A). \tag{5.5}$$

Proof. Linearity is obvious. The product formula follows from the resolvent identity (Lemma 2.33): Let G and G' be simply connected open sets satisfying $\sigma(A) \subset G, \bar{G} \subset G', \bar{G}' \subset \Omega$, and let $\gamma = \partial G, \gamma' = \partial G'$ oriented counterclockwise. Note that γ and γ' each wind once about $\sigma(A)$. Then

$$f(A)g(A) = \frac{1}{2\pi i} \oint_\gamma f(z)(z-A)^{-1}\, dz \, \frac{1}{2\pi i} \oint_{\gamma'} g(\zeta)(\zeta - A)^{-1}\, d\zeta \tag{5.6}$$

$$= \frac{1}{2\pi i} \oint_{\gamma'} \frac{1}{2\pi i} \oint_\gamma f(z)g(\zeta)(z-A)^{-1}(\zeta - A)^{-1}\, dz\, d\zeta \tag{5.7}$$

$$= \frac{1}{2\pi i} \oint_{\gamma'} \frac{1}{2\pi i} \oint_\gamma f(z)g(\zeta)(\zeta - z)^{-1}\left((z-A)^{-1} - (\zeta - A)^{-1}\right)\, dz\, d\zeta. \tag{5.8}$$

However

$$\int_\gamma f(z)g(\zeta)(\zeta - z)^{-1}(\zeta - A)^{-1}\, dz = 0 \tag{5.9}$$

because the integrand is an analytic function of z in G' ($\zeta \in \gamma'$ lies outside of

G'). Therefore

$$f(A)g(A) = \frac{1}{2\pi i}\oint_{\gamma'} \frac{1}{2\pi i}\oint_{\gamma} f(z)g(\zeta)(\zeta - z)^{-1}(z - A)^{-1}\, dz\, d\zeta \tag{5.10}$$

$$= \frac{1}{2\pi i}\oint_{\gamma} f(z)(z - A)^{-1}\frac{1}{2\pi i}\oint_{\gamma'} g(\zeta)(\zeta - z)^{-1}\, d\zeta\, dz \tag{5.11}$$

$$= \frac{1}{2\pi i}\oint_{\gamma} f(z)(z - A)^{-1}g(z)\, dz \tag{5.12}$$

$$= (fg)(A). \tag{5.13}$$

□

Example 5.14. *Given a nonsingular matrix A, it is possible to make a branch cut in the complex plane from 0 to ∞ which does not intersect the spectrum of A. Let γ be a contour in the cut plane winding once around each eigenvalue of A. Then*

$$A^{-1} = \frac{1}{2\pi i}\oint_{\gamma} z^{-1}(z - A)^{-1}\, dz \tag{5.15}$$

is the inverse of A.

Exercise 5.16. *Show that the integral in (5.15) vanishes when γ is a counter-clockwise oriented circle centered at the origin of large enough radius.*

Exercise 5.17. *Show that when A is invertible*

$$A^{-1} = \lim_{r\to 0}\frac{1}{2\pi i}\oint_{\gamma(r)} z^{-1}(z - A)^{-1}\, dz \tag{5.18}$$

where $\gamma(r)$ is a clockwise oriented circle of radius r centered at the origin. What happens when A is not invertible?

Exercise 5.19. *Show that Buchheim's Formula (Theorem 4.40) continues to hold for arbitrary analytic functions f.*

Problem 5.20. *Show that Buchheim's formula allows us extend the definition of $f(A)$ to functions which are only n times continuously differentiable, not necessarily analytic.*

The theorem for compositions of functions remains to be proven. First, we must investigate the behaviour of the spectrum of a matrix under an analytic map.

Lemma 5.21. *If $\lambda_j \in \sigma(A)$ then $g(\lambda_j) \in \sigma(g(A))$.*

Proof. Using function division,

$$g(\lambda_j) - g(A) = \frac{1}{2\pi i}\oint_{\gamma} (g(\lambda_j) - g(z))(z - A)^{-1}\, dz \tag{5.22}$$

$$= \frac{1}{2\pi i}\oint_{\gamma} (\lambda_j - z)q(z)(z - A)^{-1}\, dz \tag{5.23}$$

$$= (\lambda_j - A)q(A), \tag{5.24}$$

so

$$\det(g(\lambda_j) - g(A)) = \det(\lambda_j - A) \det q(A) = 0. \tag{5.25}$$

□

Lemma 5.21 shows that $g(\sigma(A)) \subset \sigma(g(A))$ but does not provide information on the multiplicities of the eigenvalues; in fact, multiplicities are preserved, but the proof of that fact will be postponed to Theorem 5.55.

Problem 5.26. *Can you show that the reverse inclusion $\sigma(g(A)) \subset g(\sigma(A))$ holds?*

Theorem 5.27. *Let g be an analytic function defined on the domain $\Omega \subset \mathbb{C}$, and let f be an analytic function defined on the domain $\Omega' \subset \mathbb{C}$. Suppose that $\sigma(A) \subset \Omega$, $\sigma(g(A)) \subset \Omega'$. Then*

$$f(g(A)) = (f \circ g)(A). \tag{5.28}$$

Proof. The proof of this theorem is similar to the proof of the product theorem. Let G_2 be a simply connected open set satisfying $\sigma(g(A)) \subset G_2$ and $\bar{G}_2 \subset \Omega$, and let $\gamma_2 = \partial G_2$ oriented counterclockwise. Let γ_1 be a chain consisting of small circles around each point of $\sigma(A)$; by Lemma 5.21, $g(\gamma_1) \subset G_2$ when the circles are small enough. Then

$$f(g(A)) = \frac{1}{2\pi i} \oint_{\gamma_2} f(z)(z - g(A))^{-1}\, dz \tag{5.29}$$

$$= \frac{1}{2\pi i} \oint_{\gamma_2} f(z) \frac{1}{2\pi i} \oint_{\gamma_1} (z - g(\zeta))^{-1} (\zeta - A)^{-1}\, d\zeta\, dz \tag{5.30}$$

$$= \frac{1}{2\pi i} \oint_{\gamma_1} \frac{1}{2\pi i} \oint_{\gamma_2} f(z)(z - g(\zeta))^{-1}\, dz\, (\zeta - A)^{-1}\, d\zeta \tag{5.31}$$

$$= \frac{1}{2\pi i} \oint_{\gamma_1} f(g(\zeta))(\zeta - A)^{-1}\, d\zeta \tag{5.32}$$

$$= (f \circ g)(A). \tag{5.33}$$

□

5.2 Inverse Functions

Solving equations amounts to constructing inverse functions which can now be done with the help of Theorem 5.27.

The square root problem may now be solved, at least partially. Given a nonsingular matrix A, make a branch cut from 0 to ∞ which avoids the spectrum of A, then define a square root function on the cut plane. Let γ be a contour in the cut plane winding once around the spectrum of A. Then

$$X = \frac{1}{2\pi i} \oint_{\gamma} \sqrt{z}\, (z - A)^{-1}\, dz \tag{5.34}$$

is a solution to the equation $X^2 = A$.

Singular matrices may or may not have square roots. For example, $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ has a square root, while $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ does not.

Exercise 5.35. *Verify that* $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ *does not have a square root by explicit calculation.*

An exact criterion for the existence of square roots using more delicate analysis is given in [4, pages 471–472].

A matrix generally has more square roots than those given by Theorem 5.27.

Exercise 5.36. *Use Buchheim's formula (Theorem 4.40) to show that the matrix* $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ *is a square root of the identity matrix which cannot be a primary matrix function of the identity matrix.*

Problem 5.37 (Putnam 1996-B-4). *Prove or disprove: there is a matrix* A *such that* $\sin A = \begin{pmatrix} 1 & 1996 \\ 0 & 1 \end{pmatrix}$.

Solution. The matrix A has eigenvalue 1 which is also a branch point of the function arcsin so we cannot just take the inverse function. However, we do have function identities available. Suppose there is such a matrix A. Then $\sin^2 A + \cos^2 A = I$ so $\cos^2 A = \begin{pmatrix} 0 & -3992 \\ 0 & 0 \end{pmatrix}$. But that is impossible (otherwise $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ would have a square root). So there is no such matrix A. □

It is now also possible to solve the matrix equation $e^X = A$. By Theorem 4.15, e^X is always nonsingular so $e^X = A$ may have a solution only if A is nonsingular. On the other hand, if A is nonsingular, a branch cut from 0 to ∞ may be made which avoids the spectrum of A; a logarithm can then be defined on the cut plane, and $\log A$ satisfies $e^{\log A} = A$ by Theorem 5.27.

Theorem 5.38. *If* A *is nonsingular,*

$$\det A = e^{\operatorname{tr} \log A} \tag{5.39}$$

where $\log A$ *is any logarithm of* A*, i.e., any solution to* $e^X = A$.

Problem 5.40. *Is it possible to write*

$$\log \det A = \operatorname{tr} \log A? \tag{5.41}$$

5.3 Frobenius Covariants

Suppose the matrix A has eigenvalues λ_j, $j = 1, \ldots, \mu$. Let Ω_j be small open disks centered at λ_j satisfying $\Omega_j \cap \Omega_k = \emptyset$ if $j \neq k$. Let γ_j be a contour in Ω_j winding once around λ_j. Let $\Omega = \Omega_1 \cup \cdots \cup \Omega_\mu$, $\gamma = \gamma_1 + \cdots + \gamma_\mu$.

Consider the function

$$1_j(z) = \begin{cases} 1 & \text{if } z \in \Omega_j \\ 0 & \text{if } z \notin \Omega_j \end{cases}. \tag{5.42}$$

Then 1_j is an analytic function in Ω, so $A_j = 1_j(A)$ is well-defined. The matrices A_j are called the *Frobenius covariants* of A [4, page 403] [8, page 494].

Exercise 5.43. *Show that*

(i) $A_1 + \cdots + A_\mu = I$,

(ii) $A_j A_k = 0$ *if* $j \neq k$, *and*

(iii) $A_j^2 = A_j$;

therefore A_j *are disjoint projections.*

Exercise 5.44. *Show that* A_j *are polynomials in* A.

Exercise 5.45 (Schwerdtfeger's Formula). *Show that*

$$f(A) = \sum_{j=1}^{\mu} A_j \sum_{k=0}^{m_j - 1} \frac{1}{k!} f^{(k)}(\lambda_j)(A - \lambda_j)^k. \tag{5.46}$$

Hint. Note that $f(A) = f|_\Omega(A)$ where $f|_\Omega$ is the restriction of f to Ω. Prove a theorem like Theorem 4.27 for $f|_\Omega = 1_1 f|_\Omega + \cdots + 1_\mu f|_\Omega$. □

5.4 Images of Eigenvalues under Analytic Functions

Lemma 5.21 gives a "lower bound" on the spectrum of a function of a matrix. The goal of this section is to obtain precise information on $\sigma(f(A))$ by calculating the characteristic polynomial of $f(A)$.

Let us begin by studying the behaviour of the trace under analytic functions of matrices. The trace is linear so it behaves well.

Theorem 5.47.

$$\operatorname{tr} f(A) = \sum_j m_j f(\lambda_j). \tag{5.48}$$

Proof. Using the linearity of the trace,

$$\operatorname{tr} f(A) = \operatorname{tr} \frac{1}{2\pi i} \oint_\gamma f(z)(z - A)^{-1}\, dz \tag{5.49}$$

$$= \frac{1}{2\pi i} \oint_\gamma f(z) \operatorname{tr}(z - A)^{-1}\, dz. \tag{5.50}$$

By (2.48),

$$\operatorname{tr} f(A) = \frac{1}{2\pi i} \oint_\gamma f(z) \sum_j \frac{m_j}{z - \lambda_j}\, dz = \sum_j m_j f(\lambda_j). \tag{5.51}$$

□

It is much more difficult to handle determinants directly. Indirectly, Theorem 5.38 shows that

$$\det(\lambda - f(A)) = e^{\operatorname{tr}\log(\lambda - f(A))} \tag{5.52}$$

for $\lambda \in \mathbb{C} - \sigma(f(A))$. (The choice of log depends on λ, but the right hand side of (5.52) is independent of the choice of log because of the exponential.) By Theorem 5.47,

$$\operatorname{tr}\log(\lambda - f(A)) = \sum_j m_j \log(\lambda - f(\lambda_j)). \tag{5.53}$$

Exponentiating,

$$\det(\lambda - f(A)) = e^{\sum_j m_j \log(\lambda - f(\lambda_j))} = \prod_j (\lambda - f(\lambda_j))^{m_j} \tag{5.54}$$

for $\lambda \in \mathbb{C} - \sigma(f(A))$. Since the equality between the above two polynomials holds everywhere in $\mathbb{C}$ except for a finite set of points, it holds everywhere in $\mathbb{C}$ which proves the following theorem.

Theorem 5.55. *If the eigenvalues of A are λ_j with multiplicity m_j, the eigenvalues of $f(A)$ are $f(\lambda_j)$ with multiplicity m_j; in other words, the characteristic polynomial of $f(A)$ is $(\lambda - f(\lambda_1))^{m_1} \cdots (\lambda - f(\lambda_\mu))^{m_\mu}$.*

The minimal polynomial may change in a much more complicated way, as we will see in Problem 6.11.

6 Functions of Matrices and Jordan Canonical Form*

There is an easier way to obtain Theorem 5.55 and some of the other results given above. We begin by studying the effect of a change of basis on a matrix function. It is clear that $p(B^{-1}AB) = B^{-1}p(A)B$ for polynomial and entire functions $p(z)$. The same result holds for primary matrix functions in general.

Theorem 6.1. *For any matrices A and B, if $f(AB)$ is defined, then so is $f(BA)$ and*

$$Bf(AB) = f(BA)B. \tag{6.2}$$

Proof. First, note that the spectra of AB and BA are the same by (1.12). (What happens when $0 \in \sigma(AB)$?) Then a simple calculation gives

$$Bf(AB) = \frac{1}{2\pi i} \oint_\gamma f(z)B(z - AB)^{-1}\, dz = \tag{6.3}$$
$$= \frac{1}{2\pi i} \oint_\gamma f(z)(z - BA)^{-1}B\, dz = f(BA)B.$$

□

If B is invertible then setting $A = CB^{-1}$ gives

Theorem 6.4. *If B is invertible and $f(C)$ exists, then $f(BCB^{-1})$ exists and*

$$f(C) = B^{-1}f(BCB^{-1})B. \tag{6.5}$$

Thus we may obtain $f(C)$ knowing the Jordan canonical form of C and the following theorems on the effect of f on Jordan blocks.

Theorem 6.6.

$$f(J_k(\lambda)) = \begin{pmatrix} f(\lambda) & f'(\lambda) & f''(\lambda)/2 & \cdots & f^{(k-1)}(\lambda)/(k-1)! \\ 0 & f(\lambda) & f'(\lambda) & \cdots & f^{(k-2)}(\lambda)/(k-2)! \\ 0 & 0 & f(\lambda) & \cdots & f^{(k-3)}(\lambda)/(k-3)! \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & f(\lambda) \end{pmatrix}. \tag{6.7}$$

Proof. This is an easy calculation using the inverse of a Jordan block and Cauchy's integral formula. □

Theorem 6.8.

$$f(J_1(\lambda_1) \oplus \cdots \oplus J_n(\lambda_n)) = f(J_1(\lambda_1)) \oplus \cdots \oplus f(J_n(\lambda_n)). \tag{6.9}$$

Exercise 6.10. *Use Schwerdtfeger's formula (Exercise 5.45) to obtain Theorems 6.6 and 6.8.*

Theorem 6.6 is sometimes taken to be the definition of the primary matrix function; it holds for functions f which are n times continuously differentiable, not just for analytic functions. Little is gained by defining the primary matrix function in this way, however, since Buchheim's formula gives the same extension of the definition.

What we do gain by this method is that we may easily obtain Theorem 5.55, the result on transformation of the characteristic polynomial, using the Jordan block method. We can also see what may happen to the minimal polynomial: a Jordan block may "split" if derivatives of f vanish at an eigenvalue.

Problem 6.11. *Investigate the possible Jordan block structures of $f(J_k(\lambda))$ and consequently the possible minimal polynomials of $f(J_k(\lambda))$ for various f.*

Problem 6.12. *Find an exact criterion for the existence of square roots of a matrix.*

The product and composition theorems applied to Jordan blocks may also yield useful identities for functions and their derivatives:

Exercise 6.13. *Use the product formula (5.5) and appropriate Jordan blocks to prove Leibniz' formula for the kth derivative of the product of two functions, $k = 0, 1, \ldots$:*

$$\frac{d^k}{dz^k}(fg)(z) = \sum_{j=0}^{k} C_k^j f^{(j)}(z) g^{(k-j)}(z). \tag{6.14}$$

Exercise 6.15. *Use the composition formula (5.28) and appropriate Jordan blocks to prove Faa di Bruno's rule for the kth derivative of the composition of two functions, $k = 1, 2, \ldots$:*

$$\frac{d^k}{dz^k}(f \circ g)(z) = \sum_{m=1}^{k} f^{(m)}(g(z)) \sum_{I(m,k)} \frac{m!}{\alpha_1! \cdots \alpha_k!} \prod_{u=1}^{k} \left[\frac{g^{(u)}(z)}{u!}\right]^{\alpha_u} \tag{6.16}$$

where

$$I(m,k) = \{\alpha_1, \cdots, \alpha_k : \alpha_1 + \cdots + \alpha_k = m, \alpha_1 + 2\alpha_2 + \cdots + k\alpha_k = k\}. \tag{6.17}$$

See [4, page 421] for more information on Faa di Bruno's rule.

Problem 6.18. *Extend the results of Exercises 6.13 and 6.15 to several functions of several variables. In particular, find a formula for multiple partial derivatives of the composition of two functions of several variables. See [1, page 23] for another approach.*

The Jordan block method gives a clear picture of the behaviour of primary matrix functions. The main drawback of the Jordan block method is that it does not generalize well to operators on infinite dimensional spaces. There is also the æsthetic difficulty that it is not expressed in terms of a single formula which applies to any matrix; rather, it depends on Jordan canonical form which is given in terms of an algorithm rather than a formula.

Problem 6.19. *Is there a formula for Jordan canonical form? Note that such a formula could not be continuous: consider the matrices* $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ *and* $\begin{pmatrix} 0 & \epsilon \\ 0 & 0 \end{pmatrix}$. *See [8, pages 20–21] for an interesting proof of Jordan canonical form.*

7 The Equation $AX - XB = C$

The equation $AX - XB = C$ is not of the form $f(X) = A$ of the equations we have considered so far, so some new methods are required to solve it. The

equation is linear in X, but is surprisingly difficult to solve. For the moment, assume that $A, B, C, X \in M_n(\mathbb{C})$.

One clever approach is to write the equation as a block matrix equation:

$$\begin{pmatrix} I & X \\ O & I \end{pmatrix} \begin{pmatrix} A & O \\ O & B \end{pmatrix} \begin{pmatrix} I & -X \\ O & I \end{pmatrix} = \begin{pmatrix} A & C \\ O & B \end{pmatrix}. \tag{7.1}$$

Since

$$\begin{pmatrix} I & -X \\ O & I \end{pmatrix} = \begin{pmatrix} I & X \\ O & I \end{pmatrix}^{-1}, \tag{7.2}$$

equation (7.1) shows that a necessary condition for the solvability of $AX - XB = C$ is that the two matrices $\begin{pmatrix} A & O \\ O & B \end{pmatrix}$ and $\begin{pmatrix} A & C \\ O & B \end{pmatrix}$ are similar. In fact, that condition is sufficient as well [4, page 279–281], but no constructive proof of that fact is known. Two constructive approaches to solving the equation are outlined below.

7.1 The Kronecker Product

Note that the equation $AX - XB = C$ is linear in the elements of X, so we can write it as an ordinary linear system of equations in the vector $\operatorname{vec}(X) = (x_{11}, x_{21}, \cdots, x_{nn})^T$.

Exercise 7.3. *Show that the equation $AXB = C$ on X is equivalent to the block matrix equation*

$$\begin{pmatrix} b_{11}A & b_{21}A & \cdots & b_{n1}A \\ b_{12}A & b_{22}A & \cdots & b_{n2}A \\ \vdots & \vdots & \ddots & \vdots \\ b_{1n}A & b_{2n}A & \cdots & b_{nn}A \end{pmatrix} \operatorname{vec}(X) = \operatorname{vec}(C). \tag{7.4}$$

The matrix

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1}B & a_{n2}B & \cdots & a_{nn}B \end{pmatrix} \tag{7.5}$$

is called the *Kronecker product* of A and B. Thus the matrix equation $AXB = C$ is equivalent to the matrix equation $(B^T \otimes A)\operatorname{vec}(X) = \operatorname{vec}(C)$.

Exercise 7.6. *Show that if μ is an eigenvalue of A and ν is an eigenvalue of B, then $\mu\nu$ is an eigenvalue of $B^T \otimes A$.*

Hint. Given an eigenvector a of A and an eigenvector b of B^T, construct an "eigenmatrix" X of the operator AXB. □

Exercise 7.7. *An algebraic number is a solution to a polynomial with integer coefficients; an algebraic integer is a solution to a monic polynomial with integer coefficients. Use the Kronecker product to show that the product of two algebraic integers is an algebraic integer, and that the product of two algebraic numbers is an algebraic number.*

The equation $AX - XB = C$ is equivalent to the equation

$$(I \otimes A - B^T \otimes I)\,\mathrm{vec}(X) = \mathrm{vec}(C). \tag{7.8}$$

Exercise 7.9. *Show that if μ is an eigenvalue of A and ν is an eigenvalue of B, then $\mu - \nu$ is an eigenvalue of $(I \otimes A - B^T \otimes I)$.*

Exercise 7.10. *Show that the sum of two algebraic numbers is an algebraic number, and the sum of two algebraic integers is an algebraic integer.*

Exercise 7.11. *Show that the spectrum of $(I \otimes A - B^T \otimes I)$ is exactly the set $\{\mu - \nu : \mu \in \sigma(A), \nu \in \sigma(B)\}$.*

Exercise 7.12. *Use Exercise 7.11 to determine a necessary and sufficient condition on A, B for $AX - XB = C$ to have exactly one solution for any C.*

The Kronecker product is a powerful way of solving linear matrix equations, but as with the Jordan canonical form formulation of matrix functions, it does not generalize well to operators on infinite dimensional spaces.

7.2 An Analytic Solution

As we did with nonlinear matrix equations, we may use analytic concepts to attempt to solve $AX - XB = C$. Suppose that X is a solution, and that A is invertible. Then "solving" for X,

$$X = A^{-1}C + A^{-1}XB \tag{7.13}$$

$$= A^{-1}C + A^{-2}CB + A^{-2}XB^2 \tag{7.14}$$

$$= A^{-1}C + A^{-2}CB + A^{-3}CB^2 + \cdots \tag{7.15}$$

In order for the series (7.15) to converge, we should assume that all the eigenvalues of A lie outside a circle of radius r centered at the origin, while all the eigenvalues of B lie inside the same circle. In this case, the series converges to a solution of the equation.

The above restriction on the eigenvalues of A and B is too strong; our experience with entire functions shows that it can be weakened by replacing the sum with a contour integral. Contour integrals pick out the coefficient of order -1 from series, which just happens to be what we get if we divide A and B by z (and multiply by z^{-2}):

$$X = \frac{1}{2\pi i} \oint_\gamma \sum_{j=0}^{\infty} z^{-1} \left(\frac{A}{z}\right)^{-1-j} C z^{-1} \left(\frac{B}{z}\right)^{j} dz \tag{7.16}$$

where γ is the circle of radius r centered at the origin oriented counterclockwise. Now we can add any other powers of z to the integrand without changing the integral, so we may write

$$X = \frac{1}{2\pi i} \oint_\gamma \sum_{j=0}^{\infty} A^{-1} \left(\frac{z}{A}\right)^j C \sum_{k=0}^{\infty} z^{-1} \left(\frac{B}{z}\right)^k \, dz = \tag{7.17}$$

$$= -\frac{1}{2\pi i} \oint_\gamma (z-A)^{-1} C (z-B)^{-1} \, dz$$

which is the expression for X given in [5, Appendix A]. This allows us to change the shape of the contour as long as we preserve its essential topological features, i.e., that the spectrum of B is entirely within the contour while the spectrum of A is entirely outside the contour. This requires that the spectra of A and B are disjoint, which is exactly the condition derived in Exercise 7.12.

Proposition 7.18. *Suppose the spectra of A and B are disjoint. Let γ be a contour winding around each element of the spectrum of B once but not winding around any element of the spectrum of A. Then*

$$X = -\frac{1}{2\pi i} \oint_\gamma (z-A)^{-1} C (z-B)^{-1} \, dz \tag{7.19}$$

is the unique solution to the equation $AX - XB = C$.

Proof. X is a solution:

$$AX - XB = -\frac{1}{2\pi i} \oint_\gamma (z-A)^{-1} (AC - CB)(z-B)^{-1} \, dz \tag{7.20}$$

$$= \frac{1}{2\pi i} \oint_\gamma (z-A)^{-1} (zC - AC + CB - Cz)(z-B)^{-1} \, dz \tag{7.21}$$

$$= \frac{1}{2\pi i} \oint_\gamma \left(C(z-B)^{-1} - (z-A)^{-1} C \right) \, dz \tag{7.22}$$

$$= CI - OC = C \tag{7.23}$$

because the contour encloses all of the eigenvalues of B but none of the eigenvalues of A.

To prove uniqueness, note that the integral (7.19) gives a linear operator $C \to X$ between two vector spaces $M_n(\mathbb{C})$ of equal dimension; the operator is onto since

$$X = -\frac{1}{2\pi i} \oint_\gamma (z-A)^{-1} (AX - XB)(z-B)^{-1} \, dz, \tag{7.24}$$

so it must be 1–1. In other words, suppose that $AX_1 - X_1 B = C = AX_2 - X_2 B$;

then

$$X_1 = -\frac{1}{2\pi i}\oint_\gamma (z-A)^{-1}(AX_1 - X_1B)(z-B)^{-1}\,dz \tag{7.25}$$

$$= -\frac{1}{2\pi i}\oint_\gamma (z-A)^{-1}(AX_2 - X_2B)(z-B)^{-1}\,dz \tag{7.26}$$

$$= X_2. \tag{7.27}$$

The integral operator given by (7.19) may be regarded as the *inverse* of the operator $AX - XB$. □

Exercise 7.28. *Show that*

$$X = \frac{1}{2\pi i}\oint_\gamma (z-A)^{-1}C(z-B)^{-1}\,dz \tag{7.29}$$

is another representation of the solution, where the contour winds once around each eigenvalue of A but not around any eigenvalue of B.

Exercise 7.30. *Show that the above constructions work when $A \in M_m(\mathbb{C})$, $B \in M_n(\mathbb{C})$, $C, X \in M_{m\times n}(\mathbb{C})$.*

Exercise 7.31. *Show that if $B = A^T$, $C = -C^T$ and the spectra of A and B are disjoint, then $X = X^T$.*

Exercise 7.32. *Show that if $B = A^*$, $C = -C^*$ and the spectra of A and B are disjoint, then $X = X^*$.*

Exercise 7.33. *Show that if A, B, C are all real and the spectra of A and B are disjoint, then X is also real.*

7.3 Constant Coefficient Differential Equations Revisited

Just as we studied variations on the matrix equation $AX = B$, we can study variations on the constant coefficient matrix differential equation $(d/dt)X(t) = AX(t)$.

Exercise 7.34. *Use products of exponentials to solve the system*

$$\frac{d}{dt}X(t) = AX(t) - X(t)B, \quad X(0) = C. \tag{7.35}$$

Exercise 7.36. *Calculate the integral*

$$\int_0^\infty X(t)\,dt \tag{7.37}$$

assuming that it exists. Under what conditions does it exist?

Exercise 7.38. *Find a series solution to the system*

$$\frac{d}{dt}X(t) = AX(t)B, \quad X(0) = C \tag{7.39}$$

Exercise 7.40. *Solve (7.39) using the Kronecker product.*

Problem 7.41. *Can you find an integral representation for the solution of (7.39)?*

8 Conclusion

The overall goal of the theory of primary matrix functions is to enable us to "re-use" our knowledge of analytic functions (as solutions to algebraic and differential equations) in the context of matrices. We have succeeded to a large extent by using analytic methods, specifically contour integrals which have turned out to be more versatile than series. (See [3] for another situation in which contour integrals give better results than series.)

On the other hand, we did not obtain every result we asked for, particularly in degenerate cases: we did not get all the square roots of matrices which have square roots, we did not get perfect criteria about which matrices have a square roots and we did not get solutions to $AX - XB = C$ in the degenerate case in which the spectra of A and B overlap.

This dichotomy of good results in typical cases and poor (or no) results in degenerate cases may be a consequence of our use of infinite processes: strong conditions are required if we are to make use of infinite series and integrals, but when they work, they work well.

In any case, even though the results we obtain are partial, the techniques we have developed are beautiful and powerful additions to our collection of tools for solving problems.

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