

Unbiased Estimates of Variance Components With Bootstrap Procedures

Robert L. Brennan
University of Iowa

This article provides general procedures for obtaining unbiased estimates of variance components for any random-model balanced design under any bootstrap sampling plan, with the focus on designs of the type typically used in generalizability theory. The results reported here are particularly helpful when the bootstrap is used to estimate standard errors of estimated variance components. For the $p \times i$ design, Wiley (2000) provided formulas for correcting for bias in bootstrap estimates of variance components. This article extends Wiley's results to any design and any bootstrap procedure. There are important differences in approach, however. In particular, in this article unbiased estimates of variance components are obtained directly for any bootstrap sample through the use of modified expected T -term (uncorrected sums of squares) equations.

Keywords: *generalizability theory; variance components; bootstrap*

This article provides general procedures for obtaining unbiased estimates of variance components for any random-model balanced design under any bootstrap sampling plan, with the focus on designs of the type typically used in generalizability theory. Without any bootstrapping, well-known procedures exist for obtaining analysis of variance (ANOVA) unbiased estimates of variance components for balanced designs (e.g., Brennan, 2001; Searle, 1971; Searle, Casella, & McCulloch, 1992). So if the only goal is to estimate variance components, the procedures discussed herein are not necessary. However, these procedures are particularly helpful when the bootstrap is used to estimate standard errors of estimated variance components, as discussed more fully in a companion article (Tong & Brennan, 2007).

The most frequently discussed procedure in the literature for estimating standard errors of estimated variance components assumes that score effects are normally distributed. This assumption, however, is often highly suspect in generalizability theory, especially when data are dichotomous. For this reason, 20 years ago

Author's Note: Please address correspondence to Robert L. Brennan, Director, Center for Advanced Studies in Measurement and Assessment (CASMA), 210 Lindquist, College of Education, University of Iowa, Iowa City, IA 52242; e-mail: robert-brennan@uiowa.edu.

Brennan, Harris, and Hanson (1987) studied the possibility of using various bootstrap procedures to estimate standard errors of estimated variance components for the $p \times i$ design with n_p persons and n_i items (see Brennan, 2001, chap. 6, for a summary of Brennan et al., 1987). Among the procedures they considered were

- bootstrap persons (boot- p) by drawing a random sample of n_p persons with replacement from the persons in the data, keeping the items the same;
- bootstrap items (boot- i) by drawing a random sample of n_i items with replacement from the items in the data, keeping the persons the same; and
- bootstrap both persons and items (boot- p, i) by drawing a random sample of n_p persons with replacement and a random sample of n_i items with replacement.

For each of these bootstrap procedures, Brennan et al. (1987) estimated the standard error of each of the variance component estimates as the standard deviation over replications of the ANOVA-like estimates of the variance component under the particular bootstrap procedure. In a simulation study, they found that the resulting estimated standard errors were often poor, no matter what the nature of the underlying data (normal or dichotomous), and they demonstrated that at least part of the explanation was that the bootstrap ANOVA-like estimates were necessarily biased. Brennan et al. (1987) provided ad hoc correction factors that improved the estimated standard errors, but it was not until 13 years later that Wiley (2000) provided rigorous derivations of correction factors for the bootstrap estimates of variance components in the $p \times i$ design (see Brennan, 2001, p. 188, for a summary).

Wiley (2000) also provided correction factors for a few bootstrap estimates for the $p \times i \times h$ design, but otherwise the bias in ANOVA-like estimates of variance components under bootstrap procedures has been studied rigorously for the $p \times i$ design only. In a sense, this article extends Wiley's (2000) results to any balanced design and any bootstrap procedure. There are important differences in approach, however, as discussed next.

Let $\hat{\sigma}^2(\alpha)$ be the usual ANOVA unbiased estimates of the variance components for the various effects, α . Also, let $\hat{\sigma}^2(\alpha|\lambda)$ be the ANOVA-like estimates that result from a particular replication of boot- λ , where λ is the set of m facets that are bootstrapped. Here, sometimes these estimates will be referred to as "bootstrap estimates." Both Wiley (2000) and Brennan et al. (1987) viewed the solution to the "bias problem" as one of finding linear functions of bootstrap estimates that gave the $\hat{\sigma}^2(\alpha)$. Also, Wiley (2000) approached the problem by focusing on mean squares to estimate variance components.

By contrast, the approach taken here is to estimate $\sigma^2(\alpha)$ directly from the data for any bootstrap sample using modified versions of the no-bootstrapping expected T -terms equations, $ET(\alpha)$. (T terms are uncorrected sums of squares; e.g., see Brennan, 2001). Replacing parameters with estimates, the modified expected T -term

equations, $ET(\alpha|\lambda)$, can be solved directly for the $\hat{\sigma}^2(\alpha)$. The principal purpose of this article is to explain and justify a relatively simple rule for obtaining these modifications. It is also shown that the modified T -term equations can be used to obtain other results such as a general formula for expressing expected mean square equations under boot- λ as well as equations for $\hat{\sigma}^2(\alpha)$ in terms of bootstrap estimates. More detailed results are provided by Brennan (2006).

Throughout this article, no distinction is made between measurement facets and the “facet” that represents the objects of measurement. That is, here there are as many facets as there are indexes used to represent the design. Also, the model under consideration is always assumed to be random, and the design is balanced.

The next section provides a brief review of the $p \times i$ design without bootstrapping, with particular attention given to how T terms can be used to estimate variance components. For the same design, the subsequent section discusses derivations that give expected T -term equations for boot- p , boot- i , and boot- p, i . The following section extends these results to the $p \times (i:h)$ design for various bootstrap procedures. Then, general procedures and formulas are provided for any balanced design and any bootstrap procedure. With minor exceptions, the notational conventions are those used in Brennan (2001).

The $p \times i$ Design Without Bootstrapping

For the random-model $p \times i$ design, the linear model is

$$X_{pi} = \mu + v_p + v_i + v_{pi},$$

where the last term is confounded with other sources of error, and all effects have an expectation (E) of zero. Also, all pairs of effects are uncorrelated, which means that

$$Ev_p v_i = Ev_p v_{pi} = Ev_i v_{pi} = 0,$$

and

$$Ev_p v_{p'} = Ev_i v_{i'} = Ev_{pi} v_{p'i} = Ev_{pi} v_{p'i'} = Ev_{pi} v_{p'i'} = 0. \quad (1)$$

For the $p \times i$ design, the T terms are

$$T(p) = n_i \sum \bar{X}_p^2, \quad T(i) = n_p \sum \bar{X}_i^2, \quad T(pi) = \sum \sum X_{pi}^2, \text{ and } T(\mu) = n_p n_i \bar{X}^2,$$

and their expected values are

$$\begin{aligned} ET(p) &= n_p n_i \mu^2 + n_p \sigma^2(pi) + n_p \sigma^2(i) + n_p n_i \sigma^2(p) \\ ET(i) &= n_p n_i \mu^2 + n_i \sigma^2(pi) + n_p n_i \sigma^2(i) + n_i \sigma^2(p) \\ ET(pi) &= n_p n_i \mu^2 + n_p n_i \sigma^2(pi) + n_p n_i \sigma^2(i) + n_p n_i \sigma^2(p) \\ ET(\mu) &= n_p n_i \mu^2 + \sigma^2(pi) + n_p \sigma^2(i) + n_i \sigma^2(p). \end{aligned} \quad (2)$$

If we replace the $\sigma^2(\alpha)$ with $\hat{\sigma}^2(a)$ and we replace the $ET(\alpha)$ with actual T terms, then we have four equations in four unknowns. Using standard algebraic or matrix procedures, these equations can be solved for unbiased estimates of the $\sigma^2(\alpha)$:

$$\begin{aligned}\hat{\sigma}^2(p) &= \frac{1}{n_i} \left[\frac{n_i T(p) - n_i T(\mu) - T(pi) + T(i)}{(n_p - 1)(n_i - 1)} \right] \\ \hat{\sigma}^2(i) &= \frac{1}{n_p} \left[\frac{n_p T(i) - n_p T(\mu) - T(pi) + T(p)}{(n_p - 1)(n_i - 1)} \right] \\ \hat{\sigma}^2(pi) &= \frac{T(pi) - T(p) - T(i) + T(\mu)}{(n_p - 1)(n_i - 1)}.\end{aligned}\quad (3)$$

We can also obtain these results using the mean squares:

$$\begin{aligned}MS(p) &= \frac{T(p) - T(\mu)}{n_p - 1} \\ MS(i) &= \frac{T(i) - T(\mu)}{n_i - 1} \\ MS(pi) &= \frac{T(pi) - T(p) - T(i) + T(\mu)}{(n_p - 1)(n_i - 1)}.\end{aligned}\quad (4)$$

It is well known that the expected mean square equations are

$$\begin{aligned}EMS(p) &= \sigma^2(pi) + n_i \sigma^2(p) \\ EMS(i) &= \sigma^2(pi) + n_p \sigma^2(i) \\ EMS(pi) &= \sigma^2(pi).\end{aligned}\quad (5)$$

If we replace the $\sigma^2(\alpha)$ with $\hat{\sigma}^2(\alpha)$ and we replace the $EMS(\alpha)$ with actual mean squares, then it is easy to show that

$$\begin{aligned}\hat{\sigma}^2(p) &= \frac{MS(p) - MS(pi)}{n_i} \\ \hat{\sigma}^2(i) &= \frac{MS(i) - MS(pi)}{n_p} \\ \hat{\sigma}^2(pi) &= MS(pi).\end{aligned}\quad (6)$$

The estimators of variance components are the same in Equation Sets 3 and 6, as they must be because the estimators are based on the same quadratic forms.

The $p \times i$ Design With Bootstrapping

The uncorrelated effects assumptions in Equation 1 are crucial to the derivation of the expected T -term equations in Equation Set 2. At least some of these assumptions are violated, however, under a bootstrap procedure. Consider, for example,

boot- i . When two bootstrap samples result in at least one common item, none of the following can be zero: $E v_i v_{i'}$, $E v_{pi} v_{pi'}$, and $E v_{pi} v_{p'i'}$. When we do not make any of the assumptions in Equation 1, then

$$\begin{aligned}
 ET(p) &= n_p n_i \mu^2 + n_p n_i \sigma^2(p) + \frac{n_p}{n_i} E \left(\sum_{i=1}^{n_i} v_i \right)^2 + \frac{n_p}{n_i} E \left(\sum_{i=1}^{n_i} v_{pi} \right)^2 \\
 ET(i) &= n_p n_i \mu^2 + \frac{n_i}{n_p} E \left(\sum_{p=1}^{n_p} v_p \right)^2 + n_p n_i \sigma^2(i) + \frac{n_i}{n_p} E \left(\sum_{p=1}^{n_p} v_{pi} \right)^2 \\
 ET(pi) &= n_p n_i \mu^2 + n_p n_i \sigma^2(p) + n_p n_i \sigma^2(i) + n_p n_i \sigma^2(pi) \\
 ET(\mu) &= n_p n_i \mu^2 + \frac{n_i}{n_p} E \left(\sum_{p=1}^{n_p} v_p \right)^2 + \frac{n_p}{n_i} E \left(\sum_{i=1}^{n_i} v_i \right)^2 \\
 &\quad + \frac{1}{n_p n_i} E \left(\sum_{p=1}^{n_p} \sum_{i=1}^{n_i} v_{pi} \right)^2.
 \end{aligned} \tag{7}$$

Boot- i

Under boot- i , the terms in Equation Set 7 involving a squared sum over i do not lead to the random model results because each of the squared sums involves nonzero expected values for the cross-product terms, as discussed next.

Results for $(\sum_i v_i)^2$. The third term in both $ET(p)$ and $ET(\mu)$ is $(n_p/n_i) E(\sum_i v_i)^2$. We will call $E(\sum_i v_i)^2$ the kernel of this term. It is

$$E \left(\sum_{i=1}^{n_i} v_i \right)^2 = n_i \sigma^2(i) + n_i(n_i - 1) E(v_i v_{i'}). \tag{8}$$

Figure 1 provides 3 of the possible 256 replications for boot- i when $n_i = 4$. The diagonal cells (designated with the symbol *) contain $\sigma^2(i)$ even without bootstrapping. They contribute to the first term in Equation 8. Clearly, over all replications the expected number of times the diagonal cells contain $\sigma^2(i)$ is precisely n_i . That is,

$$E(\text{number of diagonal matches}) = n_i. \tag{9}$$

For each of the three replications, the off-diagonal cells in Figure 1 for which $E(v_i v_{i'}) = \sigma^2(i)$ are designated with the symbol i , reflecting the fact that they are nonzero solely as a result of bootstrapping items. How frequently is it expected that this will happen? Under sampling with replacement from a finite pool of n_i items, the probability that a specific item is sampled twice is $1/n_i^2$. Because there are n_i items, the probability of a match in two sampled items is $n_i(1/n_i^2) = 1/n_i$. Now, given n_i items, there are $n_i(n_i - 1)$ opportunities for a match; that is, there

Figure 1
Illustration of $E v_i v_{i'} = \sigma^2(i)$ for Three Possible
Replications of Boot- i With $n_i = 4$

	i_1	i_3	i_3	i_4		i_1	i_1	i_3	i_3		i_1	i_1	i_1	i_3
i_1	*				i_1	*	i			i_1	*	i	i	
i_3		*	i		i_1	i	*			i_1	i	*	i	
i_3			i	*	i_3			*	i	i_1	i	i	*	
i_4				*	i_3			i	*	i_3				*

are $n_i(n_i - 1)$ off-diagonal elements in any replication. It follows that

$$E(\text{number of off-diagonal matches}) = \frac{1}{n_i} n_i(n_i - 1) = n_i - 1. \quad (10)$$

Adding Equations 9 and 10 gives

$$E(\text{number of matches}) = 2n_i - 1, \quad (11)$$

which means that

$$E\left(\sum_{i=1}^{n_i} v_i\right)^2 = (2n_i - 1) \sigma^2(i), \quad (12)$$

and

$$\frac{n_p}{n_i} E\left(\sum_{i=1}^{n_i} v_i\right)^2 = n_p s_i \sigma^2(i), \quad (13)$$

where $n_p \sigma^2(i)$ is the no-bootstrapping result (see Equation Set 2), and

$$s_i = \frac{2n_i - 1}{n_i}. \quad (14)$$

That is, under boot- i , the no-bootstrapping result $n_p \sigma^2(i)$ is multiplied by s_i .

Results for $(\sum_i v_{pi})^2$. The same basic logic applies to the v_{pi} term in $ET(p)$. That is,

$$\frac{n_p}{n_i} E\left(\sum_{i=1}^{n_i} v_{pi}\right)^2 = n_p s_i \sigma^2(pi). \quad (15)$$

Results for $(\sum_p \sum_i v_{pi})^2$. When only items are bootstrapped, the v_{pi} term in $ET(\mu)$ (the fourth term in the fourth equation of Equation Set 7) is

$$\frac{1}{n_p n_i} E \left(\sum_{p=1}^{n_p} \sum_{i=1}^{n_i} v_{pi} \right)^2 = s_i \sigma^2(pi). \quad (16)$$

This is illustrated in Figure 2 for a single replication of boot- i with $n_p = 3$ and $n_i = 4$. We will say that the large cells in Figure 2 that involve two persons (possibly the same) are “major” cells. There are two crucial points to note:

- Because only items are bootstrapped, each major off-diagonal cell involves a different pair of persons, and in such cases $E v_{pi} v_{p'i'} = 0$ whether or not $i = i'$; and
- Each of the n_p major diagonal cells has the same form as that discussed in the derivation of $E(\sum_i v_i)^2$ in Equation 12.

It follows that

$$\frac{1}{n_p n_i} E \left(\sum_{p=1}^{n_p} \sum_{i=1}^{n_i} v_{pi} \right)^2 = \frac{1}{n_i} E \left(\sum_{i=1}^{n_i} v_{pi} \right)^2 = s_i \sigma^2(pi). \quad (17)$$

For a more mathematically rigorous proof, see Brennan (2006).

Using T Terms to Estimate $\sigma^2(\alpha)$. In short, the expected T terms under boot- i are

$$\begin{aligned} ET(p|i) &= n_p n_i \mu^2 + n_p s_i \sigma^2(pi) + n_p s_i \sigma^2(i) + n_p n_i \sigma^2(p) \\ ET(i|i) &= n_p n_i \mu^2 + n_i \sigma^2(pi) + n_p n_i \sigma^2(i) + n_i \sigma^2(p) \\ ET(pi|i) &= n_p n_i \mu^2 + n_p n_i \sigma^2(pi) + n_p n_i \sigma^2(i) + n_p n_i \sigma^2(p) \\ ET(\mu|i) &= n_p n_i \mu^2 + s_i \sigma^2(pi) + n_p s_i \sigma^2(i) + n_i \sigma^2(p). \end{aligned} \quad (18)$$

Clearly, these four equations can be used to estimate the variance components with respect to the $T(\alpha|i)$. Doing so gives

$$\begin{aligned} \hat{\sigma}^2(p) &= \frac{n_i T(p|i) - n_i T(\mu|i) - s_i T(pi|i) + s_i T(i|i)}{n_i(n_i - s_i)(n_p - 1)} \\ \hat{\sigma}^2(i) &= \frac{n_p T(i|i) - n_p T(\mu|i) - T(pi|i) + T(p|i)}{n_p(n_i - s_i)(n_p - 1)} \\ \hat{\sigma}^2(pi) &= \frac{T(pi|i) - T(p|i) - T(i|i) + T(\mu|i)}{(n_i - s_i)(n_p - 1)}. \end{aligned} \quad (19)$$

These are the desired unbiased estimates, which are occasionally called the “bias-adjusted” estimates in the bootstrap literature on variance components. Provided next are other related results that are sometimes of interest.

Figure 2
Illustration of $Ev_{pi}v_{p'i'} = \sigma^2(pi)$ for One
Possible Replication of Boot- i With $n_p = 3$ and $n_i = 4$

		p_1				p_2				p_3			
		i_1	i_3	i_3	i_4	i_1	i_3	i_3	i_4	i_1	i_3	i_3	i_4
p_1	i_1	*											
	i_3		*	i									
	i_3		i	*									
	i_4				*								
p_2	i_1					*							
	i_3						*	i					
	i_3						i	*					
	i_4								*				
p_3	i_1									*			
	i_3										*	i	
	i_3										i	*	
	i_4												*

Note: * $\rightarrow$ necessarily equals $\sigma^2(pi)$; $i \rightarrow \sigma^2(pi)$ as a chance occurrence resulting from boot- i .

Using Mean Squares to Estimate $\sigma^2(\alpha)$. The mean squares for boot- i are

$$\begin{aligned} MS(p|i) &= \frac{T(p|i) - T(\mu|i)}{n_p - 1} \\ MS(i|i) &= \frac{T(i|i) - T(\mu|i)}{n_i - 1} \\ MS(pi|i) &= \frac{T(pi|i) - T(p|i) - T(i|i) + T(\mu|i)}{(n_p - 1)(n_i - 1)}. \end{aligned} \tag{20}$$

Given Equation Set 18, the expected mean squares are

$$\begin{aligned} EMS(p|i) &= s_i \sigma^2(pi) + n_i \sigma^2(p) \\ EMS(i|i) &= t_i \sigma^2(pi) + t_i n_p \sigma^2(i) \\ EMS(pi|i) &= t_i \sigma^2(pi), \end{aligned} \tag{21}$$

where

$$t_i = \frac{n_i - s_i}{n_i - 1} = \frac{n_i - 1}{n_i}. \quad (22)$$

It is easy to use Equation Set 21 to obtain expressions for $\hat{\sigma}^2(\alpha)$ in terms of the mean squares that result from a bootstrap replication $MS(\alpha|i)$:

$$\begin{aligned} \hat{\sigma}^2(p) &= \frac{t_i MS(p|i) - s_i MS(pi|i)}{t_i n_i} \\ \hat{\sigma}^2(i) &= \frac{MS(i|i) - MS(pi|i)}{t_i n_p} \\ \hat{\sigma}^2(pi) &= \frac{MS(pi|i)}{t_i}. \end{aligned} \quad (23)$$

These equations give identical results to those in Equation Set 19, which they must because both sets of equations are based on the same fundamental set of quadratic forms.

Expressions for $\hat{\sigma}^2(\alpha)$ in terms of $\hat{\sigma}^2(\alpha|i)$. Sometimes it is useful to have expressions for $\hat{\sigma}^2(\alpha)$ in terms of the boot- i estimators, $\hat{\sigma}^2(\alpha|i)$. To obtain such expressions, we use Equation Set 21 in conjunction with the boot- i version of Equation Set 6; namely,

$$\begin{aligned} \hat{\sigma}^2(p|i) &= \frac{MS(p|i) - MS(pi|i)}{n_i} \\ \hat{\sigma}^2(i|i) &= \frac{MS(i|i) - MS(pi|i)}{n_p} \\ \hat{\sigma}^2(pi|i) &= MS(pi|i). \end{aligned} \quad (24)$$

A bit of algebra gives

$$\begin{aligned} \hat{\sigma}^2(p) &= \hat{\sigma}^2(p|i) - \frac{\hat{\sigma}^2(pi|i)}{n_i - 1} \\ \hat{\sigma}^2(i) &= \frac{\hat{\sigma}^2(i|i)}{t_i} \\ \hat{\sigma}^2(pi) &= \frac{\hat{\sigma}^2(pi|i)}{t_i}. \end{aligned} \quad (25)$$

Boot- p

The symmetry between p and i in the $p \times i$ design can be exploited to obtain results for boot- p . Simply replace p with i , and replace i with p , everywhere in the boot- i section.

Boot- p, i

Boot- p, i involves the independent application of boot- p and boot- i . It follows that under boot- p, i , the boot- i results in Equations 13 and 15 still apply. The corresponding results for boot- p also apply. However,

$$\frac{1}{n_p n_i} \left(\sum_{p=1}^{n_p} \sum_{i=1}^{n_i} v_{pi} \right)^2$$

is not given by $\sigma^2(pi)$ (no bootstrapping result), nor by $s_i \sigma^2(pi)$ (boot- i result), nor by $s_p \sigma^2(pi)$ (boot- p result). Rather, here it is shown that under boot- p, i ,

$$\frac{1}{n_p n_i} \left(\sum_{p=1}^{n_p} \sum_{i=1}^{n_i} v_{pi} \right)^2 = s_p s_i \sigma^2(pi). \quad (26)$$

The crux of the matter is to show that

$$\left(\sum_{p=1}^{n_p} \sum_{i=1}^{n_i} v_{pi} \right)^2 = (2n_p - 1)(2n_i - 1) \sigma^2(pi). \quad (27)$$

Figure 3 provides a matrix display of possible results for a particular replication of boot- p, i with $n_p = 3$ persons and $n_i = 4$ items. In Figure 3, the entry for all nonblank cells is $\sigma^2(pi)$. These nonblank cells are instances in which $p = p'$ and $i = i'$, which will be called a “match.” There are nine major cells in Figure 3, three of which are diagonal and six of which are off-diagonal.

Note, in particular, that for any of the nine major cells, the items are the same, as they must be for a given replication of boot- p, i . From the discussion of boot- i , it necessarily follows that for any major diagonal cell the expected number of matches is $2n_i - 1$. Thus, over all major diagonal cells,

$$E(\text{number of matches in major diagonal cells}) = n_p (2n_i - 1). \quad (28)$$

A match can occur for a major off-diagonal cell only if boot- p results in two persons being the same. From the boot- p analogue of Equation 10, the expected number of times this occurs is $n_p - 1$. Whenever this occurs, the expected number of matches is $2n_i - 1$ (see Equation 11). It follows that

$$E(\text{number of matches in major off-diagonal cells}) = (n_p - 1)(2n_i - 1). \quad (29)$$

Adding Equations 28 and 29 gives

$$E(\text{number of matches}) = (2n_p - 1)(2n_i - 1). \quad (30)$$

For a more mathematically rigorous proof of Equation 26, see Brennan (2006).

Figure 3
Illustration of $Ev_{pi}v_{p'i'} = \sigma^2(pi)$ for One Possible Replication
of Boot- p, i With $n_p = 3$ and $n_i = 4$

		p_1				p_1				p_3					
		i_1	i_3	i_3	i_4	i_1	i_3	i_3	i_4	i_1	i_3	i_3	i_4		
p_1	i_1	*				p									
	i_3		*		i		p		p, i						
	i_3			i	*		p, i		p						
	i_4				*				p						
p_1	i_1	p				*									
	i_3		p		p, i		*		i						
	i_3			p, i	p		i		*						
	i_4				p				*						
p_3	i_1									*					
	i_3										*	i			
	i_3														
	i_4												*		

Note: $*$ $\rightarrow \sigma^2(pi)$ with or without bootstrapping; $i \rightarrow \sigma^2(pi)$ as a chance occurrence resulting from boot- i only; $p \rightarrow \sigma^2(pi)$ as a chance occurrence resulting from boot- p only; $p, i \rightarrow \sigma^2(pi)$ as a chance occurrence resulting from both boot- p and boot- i .

Rule

Let λ be the set of facets that are bootstrapped (e.g., p and/or i), with each of them denoted λ_j . Then, the $ET(\alpha|\lambda)$ terms for the $p \times i$ design can all be obtained using the following rule.

T-terms rule: For each λ_j consider each of the no-bootstrapping $ET(\alpha)$ equations. If α does not contain λ_j , locate the variance components that do contain λ_j , and multiply their no-bootstrapping T -term coefficients by s_{λ_j} .

The resulting set of equations can be solved to obtain the estimated variance components, $\hat{\sigma}^2(\alpha)$. As discussed in the rest of this article, this basic rule also applies to any multifaceted balanced design.

The $p \times (i:h)$ Design

For the $p \times (i:h)$ design, the T terms are

$$T(p) = n_i n_h \sum \bar{X}_p^2, \quad T(h) = n_p n_i \sum \bar{X}_h^2, \quad T(i:h) = n_p \sum \sum \bar{X}_{i:h}^2, \\ T(ph) = n_i \sum \sum \bar{X}_{ph}^2, \quad T(pi:h) = \sum \sum \sum X_{pi:h}^2, \quad \text{and} \quad T(\mu) = n_p n_i n_h \bar{X}^2.$$

Without bootstrapping, Table 1 provides the coefficients of the variance components for the expected values of these T terms. (These coefficients can be obtained using formulas in Brennan, 2001, p. 219, which are provided later.) Replacing expected T terms with actual T terms, and replacing $\sigma^2(\alpha)$ with $\hat{\sigma}^2(\alpha)$, gives a set of equations that can be solved for unbiased estimates of the variance components.

Mean squares with respect to T terms for the $p \times (i:h)$ design are

$$MS(p) = \frac{T(p) - T(\mu)}{n_p - 1} \\ MS(h) = \frac{T(h) - T(\mu)}{n_h - 1} \\ MS(i:h) = \frac{T(i:h) - T(h)}{n_h(n_i - 1)} \\ MS(ph) = \frac{T(ph) - T(p) - T(h) + T(\mu)}{(n_p - 1)(n_h - 1)} \\ MS(pi:h) = \frac{T(pi:h) - T(ph) - T(i:h) + T(h)}{n_h(n_p - 1)(n_i - 1)}. \quad (31)$$

The expected values of the mean squares are

$$EMS(p) = \sigma^2(pi:h) + n_i \sigma^2(ph) + n_i n_h \sigma^2(p) \\ EMS(h) = \sigma^2(pi:h) + n_i \sigma^2(ph) + n_p \sigma^2(i:h) + n_i n_p \sigma^2(h) \\ EMS(i:h) = \sigma^2(pi:h) + n_p \sigma^2(i:h) \\ EMS(ph) = \sigma^2(pi:h) + n_i \sigma^2(ph) \\ EMS(pi:h) = \sigma^2(pi:h). \quad (32)$$

When expected mean squares are replaced with actual mean squares, the resulting equations can be solved for the estimated variance components. Doing so gives the following:

$$\hat{\sigma}^2(p) = \frac{MS(p) - MS(ph)}{n_i n_h} \\ \hat{\sigma}^2(h) = \frac{MS(h) - MS(i:h) - MS(ph) + MS(pi:h)}{n_p n_i}$$

Table 1
Coefficients of μ^2 and Variance Components in Expected Values of T
Terms for Balanced $p \times (i:h)$ Design With No Bootstrapping

<i>ET</i> Term	Coefficients					
	μ^2	$\sigma^2 (pi:h)$	$\sigma^2 (ph)$	$\sigma^2 (i:h)$	$\sigma^2 (h)$	$\sigma^2 (p)$
<i>ET</i> (p)	$n_p n_i n_h$	n_p	$n_p n_i$	n_p	$n_p n_i$	$n_p n_i n_h$
<i>ET</i> (h)	$n_p n_i n_h$	n_h	$n_i n_h$	$n_p n_h$	$n_p n_i n_h$	$n_i n_h$
<i>ET</i> ($i:h$)	$n_p n_i n_h$	$n_i n_h$	$n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$	$n_i n_h$
<i>ET</i> (ph)	$n_p n_i n_h$	$n_p n_h$	$n_p n_i n_h$	$n_p n_h$	$n_p n_i n_h$	$n_p n_i n_h$
<i>ET</i> ($pi:h$)	$n_p n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$
<i>ET</i> (μ)	$n_p n_i n_h$	1	n_i	n_p	$n_p n_i$	$n_i n_h$

$$\begin{aligned}\hat{\sigma}^2(i:h) &= \frac{MS(i:h) - MS(pi:h)}{n_p} \\ \hat{\sigma}^2(ph) &= \frac{MS(ph) - MS(pi:h)}{n_i} \\ \hat{\sigma}^2(pi:h) &= MS(pi:h).\end{aligned}\quad (33)$$

These results are identical to those obtained by solving the T -term equations directly for estimated variance components, as they must be because the mean squares are linear combinations of the T terms.

Boot- p , Boot- i , and Boot- h

Although the T -terms rule was inferred based on bootstrap results for the $p \times i$ design, the rule clearly applies for any single bootstrapped facet, no matter what the design may be. Consider, for example, $ET(p) = n_i n_h E \sum \bar{X}_p^2$ for the $p \times (i:h)$ design. Suppose we focus on boot- h and the v_h term. The bootstrap facet h is not in p , but h is in v_h , which means that the conditions for the rule are met. Now, because $T(p)$ involves the square of average effects over i and h , it follows that the v_h term in $ET(p)$ is

$$n_i n_h E \left[\sum_p \left(\frac{\sum_h \sum_i v_h}{n_i n_h} \right)^2 \right] = \frac{n_p}{n_i n_h} E \left(\sum_h \sum_i v_h \right)^2 = \frac{n_p n_i}{n_h} E \left(\sum_h v_h \right)^2.$$

The form of this result mirrors that of Equation 13 for the v_i effect in $T(p)$ under boot- i in the $p \times i$ design. It follows that

$$\frac{n_p n_i}{n_h} E \left(\sum_h v_h \right)^2 = \left(\frac{n_p n_i}{n_h} \right) (2n_h - 1) \sigma^2(h) = n_p n_i s_h \sigma^2(h),$$

Table 2
Coefficients of μ^2 and Variance Components in Expected Values of T
Terms for Balanced $p \times (i:h)$ Design With Boot- h

<i>ET</i> Term	Coefficients					
	μ^2	$\sigma^2 (pi:h)$	$\sigma^2 (ph)$	$\sigma^2 (i:h)$	$\sigma^2 (h)$	$\sigma^2 (p)$
<i>ET</i> ($p h$)	$n_p n_i n_h$	$n_p s_h$	$n_p n_i s_h$	$n_p s_h$	$n_p n_i s_h$	$n_p n_i n_h$
<i>ET</i> ($h h$)	$n_p n_i n_h$	n_h	$n_i n_h$	$n_p n_h$	$n_p n_i n_h$	$n_i n_h$
<i>ET</i> ($i:h h$)	$n_p n_i n_h$	$n_i n_h$	$n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$	$n_i n_h$
<i>ET</i> ($ph h$)	$n_p n_i n_h$	$n_p n_h$	$n_p n_i n_h$	$n_p n_h$	$n_p n_i n_h$	$n_p n_i n_h$
<i>ET</i> ($pi:h h$)	$n_p n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$	$n_p n_i n_h$
<i>ET</i> (μh)	$n_p n_i n_h$	s_h	$n_i s_h$	$n_p s_h$	$n_p n_i s_h$	$n_i n_h$

where $n_p n_i$ is the coefficient without bootstrapping (see Table 1). The coefficients for the full set of expected T -term equations under boot- h are given in Table 2.

Using the expected T -term equations, the expected mean square equations under boot- h can be derived. They are

$$\begin{aligned}
 EMS(p|h) &= s_h \sigma^2(pi:h) + s_h n_i \sigma^2(ph) + n_i n_h \sigma^2(p) \\
 EMS(h|h) &= t_h \sigma^2(pi:h) + t_h n_i \sigma^2(ph) + t_h n_p \sigma^2(i:h) + t_h n_p n_i \sigma^2(h) \\
 EMS(i:h|h) &= \sigma^2(pi:h) + n_p \sigma^2(i:h) \\
 EMS(ph|h) &= t_h \sigma^2(pi:h) + t_h n_i \sigma^2(ph) \\
 EMS(pi:h|h) &= \sigma^2(pi:h),
 \end{aligned} \tag{34}$$

where $t_h = (n_h - 1)/n_h$. Using these equations, unbiased estimators of variance components in terms of bootstrap estimators can be derived (see Brennan, 2006). They are

$$\begin{aligned}
 \hat{\sigma}^2(p) &= \hat{\sigma}^2(p|h) - \frac{\hat{\sigma}^2(ph|h)}{n_h - 1} - \frac{\hat{\sigma}^2(pi:h|h)}{n_i(n_h - 1)} \\
 \hat{\sigma}^2(h) &= \frac{1}{t_h} \left[\hat{\sigma}^2(h|h) + \frac{\hat{\sigma}^2(i:h|h)}{n_i n_h} \right] \\
 \hat{\sigma}^2(i:h) &= \hat{\sigma}^2(i:h|h) \\
 \hat{\sigma}^2(ph) &= \frac{1}{t_h} \left[\hat{\sigma}^2(ph|h) + \frac{\hat{\sigma}^2(pi:h|h)}{n_i n_h} \right] \\
 \hat{\sigma}^2(pi:h) &= \hat{\sigma}^2(pi:h|h).
 \end{aligned}$$

Note that the T -terms rule applies to boot- i in the $p \times (i:h)$ design even though there is no i effect in that design. That is, although i is nested within h , it is still possible to bootstrap i only.

Boot- p, h and Boot- p, i

When a pair of facets is bootstrapped, the T -terms rule can be applied for both of them independently, as illustrated previously for boot- p, i with the $p \times i$ design. The fact that that derivation was couched in the context of the $p \times i$ design is not restrictive.

In short, we have demonstrated that the T -terms rule applies for single bootstrap facets and for pairs of nonnested bootstrap facets. Next, we show that the T -terms rule also applies to nested bootstrap facets. Subsequently, we show that it applies to more than two bootstrap facets.

Boot- i, h With i Nested Within h

Boot- i, h means bootstrap i and independently bootstrap h . In this section, it is demonstrated that when i is bootstrapped first, the T -terms rule gives the correct results. The crux of the matter is to show that under boot- i, h , the coefficients of $\sigma^2(i:h)$ and $\sigma^2(pi:h)$ in $ET(p)$ and $ET(\mu)$ involve $s_i s_h$.

Consider $ET(p)$ and $v_{i:h}$. $ET(p) = n_i n_h E \sum \bar{X}_p^2$ involves the term

$$n_i n_h E \left[\sum_p \left(\frac{\sum_h \sum_i v_{i:h}}{n_i n_h} \right)^2 \right] = \frac{n_p}{n_i n_h} E \left(\sum_h \sum_i v_{i:h} \right)^2.$$

Focus on the kernel $E(\sum \sum v_{i:h})^2$, and consider Figure 4 in which $n_h = 3$ and $n_i = 4$. The layout of the figure mirrors that of Figure 3 except that the set of items for the third level of h is not the same as that for the first level of h . Note that for the $p \times (i:h)$ design, the items are different for each unique level of h . However, the set of items is the same whenever the levels of h are the same, which is precisely what happens when i is bootstrapped first.

Under these circumstances, the logic discussed previously for bootstrapping two facets still applies, and

$$E \left(\sum_h \sum_i v_{i:h} \right)^2 = (2n_i - 1)(2n_h - 1) \sigma^2(i:h). \quad (35)$$

It follows that

$$\frac{n_p}{n_i n_h} E \left(\sum_h \sum_i v_{i:h} \right)^2 = n_p s_i s_h \sigma^2(i:h), \quad (36)$$

where n_p is the coefficient without bootstrapping (see Table 1).

The same result applies to the $v_{i:h}$ effect in $ET(\mu)$. Also, using the same logic, it can be shown that under boot- i, h the coefficients of $\sigma^2(pi:h)$ in $ET(p)$ and $ET(\mu)$ are obtained by multiplying the respective no-bootstrapping terms by $s_i s_h$.

Figure 4
Illustration of $Ev_{i:h}v_{i':h'} = \sigma^2(i:h)$ for One Possible Replication
of Boot- i , h With $n_h = 3$, $n_i = 4$, and Boot- i Performed First

	h_1				h_1				h_3			
	i_1	i_3	i_3	i_4	i_1	i_3	i_3	i_4	i_1	i_1	i_3	i_3
h_1	i_1	*			h							
	i_3		*	i		h	i, h					
	i_3		i	*		i, h	h					
	i_4			*				h				
h_1	i_1	h			*							
	i_3		h	i, h		*	i					
	i_3		i, h	h		i	*					
	i_4			h				*				
h_3	i_1								*	i		
	i_1								i	*		
	i_3										*	i
	i_3										i	*

Note: * $\rightarrow \sigma^2(i:h)$ with or without bootstrapping; $i \rightarrow \sigma^2(i:h)$ as a chance occurrence resulting from boot- i only; $h \rightarrow \sigma^2(i:h)$ as a chance occurrence resulting from boot- h only; $i, h \rightarrow \sigma^2(i:h)$ as a chance occurrence resulting from both boot- i and boot- h .

Boot- p , i , h

Strictly speaking, it has not yet been demonstrated that the T -terms rule yields the correct result for the simultaneous application of all three bootstrap procedures to the $v_{pi:h}$ term in $ET(\mu) = n_p n_i n_h E\bar{X}^2$. That is, we need to show that

$$n_p n_i n_h E \left(\frac{\sum_p \sum_i \sum_h v_{pi:h}}{n_p n_i n_h} \right)^2 = \frac{1}{n_p n_i n_h} E \left(\sum_p \sum_i \sum_h v_{pi:h} \right)^2 = s_p s_i s_h \sigma^2(pi:h).$$

To demonstrate this result, it is sufficient to show that

$$\left(\sum_p \sum_i \sum_h v_{pi:h} \right)^2 = (2n_h - 1)(2n_p - 1)(2n_i - 1) \sigma^2(pi:h).$$

Figure 5
Obtaining Multiplier of $\sigma^2(pih)$ for Boot- p, i, h

	h_1	h_3	h_3
h_1	Figure 3	Figure 3	Figure 3
h_3	Figure 3	Figure 3	Figure 3
h_3	Figure 3	Figure 3	Figure 3

Suppose $n_p = 3$, $n_i = 4$, $n_h = 3$, and a particular replication of boot- p, i, h results in (p_1, p_1, p_3) , (i_1, i_3, i_3, i_4) , and (h_1, h_3, h_3) . This is represented in Figure 5, where the reference to Figure 3 in each of the cells means that Figure 3 is replicated in each of these cells. We know from previous results that for each of the major diagonal cells in Figure 5, the expected number of matches is $(2n_p - 1)(2n_i - 1)$. Thus, over all major diagonal cells

$$E(\text{number of matches in major diagonal cells}) = n_h [(2n_p - 1)(2n_i - 1)]. \quad (37)$$

A match can occur for a major off-diagonal cell in Figure 5 only if boot- h results in two levels of h being the same. By analogy with previous discussions, the expected number of times this occurs is $n_h - 1$. Whenever this occurs, the expected number of matches is $(2n_p - 1)(2n_i - 1)$. It follows that

$$E(\text{number of matches in major off-diagonal cells}) = (n_h - 1)[(2n_p - 1)(2n_i - 1)]. \quad (38)$$

Adding Equations 37 and 38 gives

$$E(\text{number of matches}) = (2n_h - 1)(2n_p - 1)(2n_i - 1), \quad (39)$$

which implies that

$$\left(\sum_p \sum_i \sum_h v_{pi:h} \right)^2 = (2n_h - 1)(2n_p - 1)(2n_i - 1) \sigma^2(pi:h).$$

General Procedures for Any Balanced Design

The $p \times (i:h)$ design provides a microcosm of the complexities that can arise in the types of designs encountered in generalizability theory. This section provides general procedures and results for any design and bootstrap procedure.

***T* Terms**

For any component α , the T term for a balanced design (see Brennan, 2001, p. 217) is

$$T(\alpha) = \left[\prod n(\sim \alpha) \right] \sum_{\alpha} \bar{X}_{\alpha}^2, \quad (40)$$

where $\prod n(\sim \alpha)$ is the product of the sample sizes for the indices not in α , and the summation is over all of the indices in α .

Expected T Terms for Balanced Designs With No Bootstrapping

Brennan (2001, p. 219, Equation 7.3) provides an equation for obtaining no-bootstrapping expected T terms that applies to both balanced and unbalanced designs. For balanced designs only, the equation is somewhat simpler. Specifically, the coefficient of $\sigma^2(\alpha)$ in the expected value of the T term for β is

$$k[\sigma^2(\alpha), ET(\beta)] = \prod n(\beta) \prod n[\sim (\alpha \cup \beta)], \quad (41)$$

where $\prod n(\beta)$ is to be interpreted as the product of the sample sizes for all indices in β and $\prod n[\sim (\alpha \cup \beta)]$ means the product of the sample sizes for all indices that are not in either α or β .

Expected T Terms Under Boot— λ

Let λ_j be any one of the m indexes in λ , and let

$$s_{\lambda_j} = \frac{2n_{\lambda_j} - 1}{n_{\lambda_j}}. \quad (42)$$

To obtain the coefficients of each of the variance components in the expected T terms for the boot— λ procedure, apply the following rule:

T -terms rule: For each λ_j consider each of the no-bootstrapping $ET(\alpha)$ equations. If α does not contain λ_j , locate the variance components that do contain λ_j , and multiply their no-bootstrapping T -term coefficients by s_{λ_j} .

The result of doing so can be expressed in a single equation:

$$k[\sigma^2(\alpha), ET(\beta|\lambda)] = \prod n(\beta) \prod n[\sim (\alpha \cup \beta)] \prod [s_{\lambda_j} | \lambda_j \in \alpha \cap \lambda_j \notin \beta], \quad (43)$$

where the last term is the product of s_{λ_j} for all λ_j such that $\lambda_j \in \alpha \cap \lambda_j \notin \beta$.

Replacing the left side of the expected T -term equations for boot— λ with actual T terms, and replacing all $\sigma^2(\alpha)$ with $\hat{\sigma}^2(\alpha)$, gives estimation equations that can be solved for the $\hat{\sigma}^2(\alpha)$, which are the so-called ANOVA unbiased estimates of the variance components. Computationally, this is usually the most direct way to

estimate the variance components. However, expected mean squares under boot- λ can be obtained and used to estimate the variance components. Also, researchers sometimes want the $\hat{\sigma}^2(\alpha)$ expressed in terms of the bootstrap estimates, $\hat{\sigma}^2(\alpha|\lambda)$.

Expected Mean Squares Under Boot- λ

There are at least two procedures that can be used to obtain the expected mean square equations under boot- λ , $EMS(\beta|\lambda)$. First, the $EMS(\beta|\lambda)$ equations can be obtained by using the $T(\alpha|\lambda)$ equations with the boot- λ version of the usual formulas for mean squares with respect to T terms (e.g., see Equation Set 20). The algebra required to do so can be tedious, however. Second, the rule discussed next can be used.

For a random model with a balanced design and no bootstrapping, the following is a general expression for the expected mean square equations (see Brennan, 2001, p. 77):

$$EMS(\beta) = \sum \left\{ \left[\prod n(\sim \alpha) \right] \sigma^2(\alpha) \right\}, \quad (44)$$

where the summation is taken over all α that contain at least all of the indexes in β , and $\prod n(\sim \alpha)$ is the product of the sample sizes for the indexes not in α . See, for example, Equation Set 32.

Now, let

$$t_{\lambda_j} = \frac{n_{\lambda_j} - 1}{n_{\lambda_j}}, \quad (45)$$

and let β^* be the set of primary indexes (those prior to any colon) in β . To obtain the coefficients of each of the variance components in the $EMS(\beta|\lambda)$ equations, apply the following rule to each of the coefficients in the $EMS(\beta)$ equations:

EMS rule: Provided λ_j is not a nesting index (i.e., any index after a colon) in both α and β , multiply the coefficient by t_{λ_j} if $\lambda_j \in \alpha \cap \lambda_j \in \beta^*$, or by s_{λ_j} if $\lambda_j \in \alpha \cap \lambda_j \notin \beta^*$.

For example, see Equation Set 34.

Bias-Corrected Estimates of Variance Components

It is possible to use the $EMS(\beta|\lambda)$ equations to solve for unbiased estimates of the variance components, $\hat{\sigma}^2(\alpha)$, in terms of the boot- λ estimates (e.g., see Equation Set 25). The resulting equations are sometimes called the bias-corrected estimates of variance components, where it is understood that the bias is induced by boot- λ . In general, for nested designs the resulting expressions for $\hat{\sigma}^2(\alpha)$ in terms

of $\hat{\sigma}^2(\beta|\lambda)$ do not seem to have any reasonably simple predictable form (e.g., see Brennan, 2006, Appendix B). For fully crossed designs, however, there is a regularity to the resulting equations (e.g., see Brennan, 2006, Appendix C) that can be described by an algorithm and/or a complicated equation provided by Brennan (2006).

Final Comments

Nested designs almost always involve complexities beyond those in crossed designs. That is certainly true in the context of bootstrapping. It is important to note that when one or more facets are nested within one or more other facets, the order of the bootstrapping should mirror the order of the indexes using the notational conventions in Brennan (2001; e.g., primary facets should be bootstrapped first) for Equations 42–45 to be accurate.

Probably the single most important result in this article is the *T*-terms rule (or its companion Equation 43), which provides the basis for specifying the expected *T*-term equations for any design under any bootstrap procedure. These equations can be readily solved for unbiased estimates of the random effects variance components.

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