

Assignable Algorithms Available for Missing Data for Finding MV

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-----ABSTRACT-----

Assignable algorithms for use with missing data are becoming common- place in microcomputer packages. Specifically, 3 Assignable algorithms are currently available in existing software packages: the multiple-group approach, full information Assignable estimation, and the EM algorithm. Although they belong to this family of estimator, confusion appears to exist over the differences among the 3 algorithms. This article provides a comprehensive, nontechnical overview of the 3 Assignable algorithms. Multiple imputations, which is frequently used in conjunction with the EM algorithm, is also discussed.

Key word: Assignable algorithms, EM algorithm, multiple-group analysis, multiple imputation, software packages

I.INRODUCTION

Until recently ,the analysis of data with missing observations has been dominated by list wise (LD) and pair wise (PD) deletion methods (Kim & Curry, 1977; Roth,1994). However, alternative methods for treating missing data have become increasingly common in software packages, leaving applied researchers with a wide range of data analytic options. In particular, three maximum likelihood(ML) estimation algorithms for use with missing data are currently available: the multiple group approach(Allison,1987;Muthén,Kaplan,&Hollis,1987)canbe implemented using existing structural equation modeling (SEM)

software;Amos(Arbuckle,1995)andMx(Neale,1995)offerfull informationmaximumlikelihood(FIML) estimation; and at least three packages, SPSS Missing Values,EMCOV(Graham&Hofer,1993),and NORM(Schafer,1998), incorporate the expectation maximization (EM) algorithm. The latter two programs alsooffer multipleimputation,asoutlinedbyRubin(1987).The theoreticalbenefitsofMLestimationarewidelyknown(Little&Rubin,1987),andsimulationstudieshavesuggestedthatMLalgorithmsmaybesuperiortotraditionalad hocmissingdatatechniques in manycases(Arbuckle,1996;Enders&Bandalos,inpress;Muthénetal.,1987;Wothke,2000).Althoughmuchoftherecentmissing data researchhasbeenintheareaofSEM,agreatdealofconfusion apparentlyexistsoverthedifferencesamongthethreeMLmissing dataalgorithms.Forexample,asearchoftheSEMNETdiscussion grouparchivesrevealedalargenumberofthreadsandrequestsfor clarificationduringrecentyears,andthefrequencyofthese threadsdoesnotappeartobediminishing.Thatconfusionexistsis probablynotasurpriseandiscertainlynotunwarranted;theMLalgorithmsappearfundamentallydifferentinmanyrespects,despit

ebelongingtothesameestimationfamily.Althoughanextensive bodyoftechnicalliteratureexistsonMLmissingdatamethods(Dempster,Laird,&Rubin,1977;Finkbeiner,1979;Hartley&Hocking,1971;Little&Rubin,1987),nosinglereferenceisavailableto appliedresearchersthatsuccinctlysummarizesthesimilaritiesand differencesamongthealgorithms.Thus,thegoalofthisarticleisto provideathorough,nontechnicalprimeronthree widely available ML estimation algorithms for use with missing data: multiple group analysis, FIML, and the EMalgorithm. Multipleimputationalgorithms,whicharefrequentlyusedin conjunctionwiththeEMalgorithm,willalsobediscussed.

II.MULTIPLE-GROUP APPROACH

A nearly methodforobtainingMLparameter estimatesinthepresenceofmissingdatawasgivenbyHartleyandHocking(1971).The applicationofthismethodtoSEM analyseswasoutlinedbyAllison(1987)andMuthénetal.(1987)andhassincebeenreferredtoasthemultiplegroupmethod.Inthisprocedure,asampleisdividedintoGsubgroups,suchthateachsubgroup hasthesamepatternofmissing data. That is, observationswithineachoftheGsubgroupshavethesame setofvariables present and missing. A likelihood function is computed for each of the G groups, and the group wise likelihood functions are accumulated across the entire sample and maximized. Although mathematically unrelated,thisalgorithmislooselyanalogoustoPD;asubgroupgi contributestotheestimationofallparametersthatinvolve the observeddatapointsforthatgroupbutdoesnotcontribute to parameters that involve missing-data points. Assumingmultivariatenormality,theloglikelihoodfunctiongivenbyHartley and Hocking (1971) is

$$-1/2 \sum_{g=1}^G n_g [\log |\Sigma_g| + tr(sg \Sigma_g^{-1}) + tr(Hg \Sigma_g^{-1}) + Cg]$$

where $H_g = (x_g - \mu_g)(x_g - \mu_g)'$. For each of the G sub groups, n_g is the number of observations, Σ_g and S_g are the parameter estimates and sample moments, respectively, C_g is a constant that depends on the data, and H_g contains the vector of mean residuals. Because the G subgroups have different patterns of missing data, this implies that the elements of x_g , μ_g , S_g , and Σ_g are different for each group. To illustrate, consider a simple model comprising three observed variables: $X1$, $X2$, and $X3$. Furthermore, suppose a subgroup, $g1$, has complete data on $X1$ and $X3$, but is missing $X2$. The μ_g and Σ_g terms in the groupwise likelihood function for $g1$ would contain only the parameter estimates that involve $X1$ and $X3$, as follows:

$$\mu = [\mu_1 - 0 - \mu_3] \text{ and } \Sigma = \begin{bmatrix} \sigma_{11} & 0 & \sigma_{13} \\ 0 & 0 & 0 \\ \sigma_{31} & 0 & \sigma_{33} \end{bmatrix}$$

Similarly, x_g and S_g would contain the corresponding sample moment taken from the n_g complete observations in $g1$. Allison (1987) and Muthén et al. (1987) demonstrated how to implement Hartley and Hocking's (1971) algorithm using the LISREL multiple-groups specification, which maximizes the likelihood equation.

$$-1/2 \sum_{g=1}^G n_g [\log |\Sigma_g| + tr(sg \Sigma_g^{-1}) + C_g]$$

This function is clearly similar to Equation 1, but does not include a term for the vector of mean residuals—LISREL does allow for the addition of a mean vector term, however. In the usual SEM multiple group analysis, G groups are formed that represent independently sampled subpopulations (e.g., men and women), and it is typically of interest to determine whether some specified set of parameters or parameter values are common to the G groups. In the missing-data application, the subpopulations correspond to the G patterns of missing data required by Hartley and Hocking's algorithm. The additional information from the groups with partially recorded data is incorporated by the specification of parameter equality constraints across the G groups. Despite the wide availability of the LISREL program at the time, the multiple group method of missing data analysis had practical limitations that prevented its widespread use. As pointed out by Arbuckle (1996), the LISREL specification for the multiple group approach required an exceptional level of expertise and thus was practically limited to situations in which there are only a small number of missing-data patterns. Muthén et al. (1987) and Kaplan (1995) described situations in which this might occur (e.g., BIB spiraled designs), but the number of distinct missing-data patterns is often quite large in applied settings, making the method difficult to implement.

Despite the technical difficulties associated with its implementation, the multiple group approach does have advantages. First, the method can be used to estimate both just-identified (e.g., correlation, regression) and overidentified (e.g., SEM) model parameters. This is a point of contrast with the EM algorithm, which cannot currently be used to directly estimate linear model parameters. Second, it is important to note that the multiple-group approach does not estimate, or impute, missing observations, but yields direct estimates of model parameters and standard errors. This is an advantage, as additional corrective procedures are not necessary to obtain standard error estimates. Third, the multiple-group approach yields the usual chi-square test statistic for model fit, although the degrees of freedom and accompanying p value are incorrect due to the use of dummy values in the input covariance matrices of subsamples with missing variance-covariance elements. However, this is easily remedied by subtracting the number of pseudo values from the degrees of freedom term. Finally, as a byproduct of the multiple groups specification, the chi-square statistic can also be used to test the MCAR assumption. If the MCAR assumption holds, parameter estimates across subgroups should be equal. Thus, the chi-square difference test of the equality constraints imposed across the G subgroups is also a test of the MCAR assumption; a statistically significant χ^2 value suggests that data are not MCAR.

III. FIML

Two structural equation modeling software packages currently offer FIML estimation routines for missing data: AMOS (Arbuckle, 1995) and Mx (Neale, 1995). The FIML approach was originally outlined by Finkelstein (1979) for use with factor analysis and is similar to the multiple group method, except that a likelihood function is calculated at the individual, rather than the group, level. For this reason, the FIML approach has been referred to as raw maximum likelihood estimation (Duncan, Duncan, & Li, 1998; Graham, Hofer, & MacKinnon, 1996).

Like the multiple-group approach, the FIML algorithm is conceptually analogous to PD (although mathematically unrelated) in the sense that all available data is used for parameter estimation. An examination of the individual level likelihood function illustrates this point. Assuming multivariate normality, the case wise likelihood of the observed data is obtained by maximizing the function

$$\log L_i = K_i - 1/2 \log |\Sigma_i| - 1/2 \log(x_i - \mu_i)' \Sigma_i^{-1} (x_i - \mu_i)$$

where x_i is the vector of completed data for case i , μ_i contains the corresponding mean estimates derived from the entire sample, and K_i is a constant that depends on the number of completed data points for case i . Like μ_i , the determinant and inverse of Σ_i are based only on the

se variables that are observed for case i . The overall discrepancy function value is obtained by summing the n case wise likelihood functions as follows:

$$\log L(\mu, \Sigma) = \sum_{i=1}^n \log L_i$$

To illustrate, suppose ML parameter estimates are sought for a model comprised of three observed variables: X_1 , X_2 , and X_3 . The parameters of interest are

$$\mu = [\mu_1, \mu_2, \mu_3] \text{ and } \Sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}$$

The likelihood value for an observation with X_2 missing would be a function of the two complete observations as well as the parameter estimates that involved X_1 and X_3 . The relevant parameters are shown in the following.

$$\mu = [\mu_1, 0, \mu_3] \text{ and } \Sigma = \begin{bmatrix} \sigma_{11} & 0 & \sigma_{13} \\ 0 & 0 & 0 \\ \sigma_{31} & 0 & \sigma_{33} \end{bmatrix}$$

Based on the previous examples, the mathematical similarities between the multiple group and FIML algorithms should be apparent; the primary difference is that FIML fitting function is the sum of n case wise likelihood values, whereas the multiple group function is the sum of G group wise likelihood values. Several points should be made about the FIML algorithm. First, like the multiple group approach, one of the advantages of the FIML algorithm is its applicability to both just-identified and over-identified models. In the latter case, the likelihood equation in Equation 3 is extended such that the first and second order moments (μ and Σ , respectively) are expressed as functions of some parameter vector, γ (Arbuckle, 1996). As such, the method is quite general and can be applied to a wide variety of analyses, including the estimation of means, covariance matrices, multiple regression, and SEM. Second, when used in SEM applications, FIML yields a chi-square test of model fit. However, the chi-square statistic generated by FIML does not take the usual form $F(N - 1)$, where F is the value of the fitting function. Clearly, the chi-square test cannot be calculated in the normal fashion, as there is no single value of N that is applicable to the entire sample. Also, unlike the usual SEM fitting functions, there is no minimum value associated with the FIML log-likelihood function, although the value of this statistic will increase as model fit worsens. Instead, a chi-square test for model fit is calculated as the difference in log likelihood functions between the unrestricted (H_0) and restricted (H_1) models with degrees of freedom equal to the difference in the number of estimated parameters between the two models. Third, although many popular fit

indexes can be computed under FIML, the specification of a means structure (required for estimation) renders certain fit indexes undefined (e.g., GFI). Fourth, similar to PD, indefinite covariance matrices are a potential byproduct of the FIML approach. However, Wothke (2000) suggested that indefiniteness problems are less pervasive with FIML than with PD. Fifth, unlike the EM algorithm (discussed in the following), standard error estimates are obtained directly from the analysis, and bootstrapping is not necessary. Finally, it is important to note that the FIML algorithm does not impute missing values; only model parameters are estimated.

IV. EM ALGORITHM

At least three packages currently implement the EM algorithm: SPSS Missing Values, EMCOV (Graham & Hofer, 1993), and NORM (Schafer, 1998). An early work by Orchard and Woodbury (1972) explicated the underlying method, which they called the "missing information principle." Dempster et al. (1977) provided an extensive generalization and illustration of the method and named it the EM algorithm. The EM algorithm uses a two-step iterative procedure where missing observations are filled in, or imputed, and unknown parameters are subsequently estimated. In the first step (the E step), missing values are replaced with the conditional expectation of the missing data given the observed data and an initial estimate of the covariance matrix. That is, missing values are replaced by the predicted scores from a series of regression equations where each missing variable is regressed on the remaining observed variables for a case i . Using the observed and imputed values, the sums and sums of squares and cross products are recalculated. To illustrate, suppose a mean vector and covariance matrix, $\theta = (\mu, \Sigma)$, is sought for an $n \times K$ data matrix, Y , that contains sets of observed and missing values (Y_{obs} and Y_{mis} , respectively). Using the observed values (Y_{obs}) and current parameter estimates ($\theta^{(t)}$), the calculations for the sufficient statistics at the t th iteration of the E step are

$$\sum_{i=1}^n y_{ij} | y_{obs} \theta^{(+)} = \sum_{i=0}^n y_{ij}^{(t)} \quad j=1, \dots, k$$

$$\sum_{i=1}^n y_{ij} y_{ik} | y_{obs} \theta^{(+)} = \sum_{i=0}^n y_{ij}^{(t)} y_{ik}^{(t)} c_{jkt}^{(t)}, k=1, \dots, k$$

where

$$y_{ij}^{(t)} = \begin{cases} y_{ij}, \Sigma(y_{ij} | y_{obs}, \theta^{(t)}), & \text{if } y_{ij} \text{ is observed} \\ & \text{if } y_{ij} \text{ is missing} \end{cases}$$

and

$$c_{ikj}^{(t)} = \begin{cases} y_{ij}, y_{ik} & \text{if } y_{ij} \text{ or } y_{ik} \text{ is observed,} \\ y_{obs} & \text{if } y_{ij} \text{ and } y_{ik} \text{ are missing} \end{cases} \theta^{(t)}$$

Thus, missing values of y_{ij} are replaced with conditional means and covariance's given the observed data and the current set of parameter estimates.² It should be noted that the preceding formulas can be found in Little and Rubin (1987). In the second step (the *M* step), ML estimates of the mean vector and covariance matrix are obtained just as if there were no missing data using the sufficient statistics calculated at the previous *E* step. Thus, the *M* step is simply a complete-data ML estimation problem. The resulting covariance matrix and regression coefficients from the *M* step are then used to derive new estimates of the missing values. As pointed out by Little and Rubin (1987), missing values are not necessarily replaced with actual data points, but are replaced by the conditional functions of the missing values in the complete-data log-likelihood. At the next *E* step, and the process begins again. The algorithm repeatedly cycles through these two steps until the difference between covariance matrices in subsequent *M* steps falls below some specified convergence criterion. Readers are encouraged to consult Little and Rubin (1987) for further technical details. Several points should be noted concerning the EM algorithm. First, unlike the multiple-group and FIML approaches, the EM algorithm cannot be used to obtain direct estimates of linear model parameters (e.g., regression, SEM); as currently implemented, the EM algorithm can only be used to obtain ML estimates of a mean vector and covariance matrix. Obviously, this matrix can be used for input in subsequent linear model analyses. Additionally, the covariance matrix can be used to estimate, or impute, missing data points at the final iteration. The latter approach may, at first glance, be appealing due to the illusion of a complete data set, but there is a notable drawback associated with this practice. Although the imputed values are optimal statistical estimates of the missing observations, they lack the residual variability present in the hypothetically complete data set; the imputed values fall directly on a regression line and are thus imputed without a random error component. As a result, standard errors from subsequent analyses will be negatively biased to some extent, and bootstrap (Efron, 1981) procedures must be employed to obtain correct estimates. Alternatively, multiple imputation procedures designed to recover residual variability are available in the EMCOV (Graham & Hofer, 1993) and NORM (Schafer, 1998) packages and are discussed next. However, it is important to note that a correction factor is added to the conditional expectation of the missing data at each *E* step to correct for this negative bias in the output covariance matrix; this is seen in the c_{ijk} Equation 5. Although no studies have compared the impact of these two EM methods in

the context of SEM, it seems reasonable to run analyses using the output covariance matrix rather than the singly imputed dataset. Despite the difficulties previously noted, the EM algorithm may be preferred in situations where the missing data mechanism (i.e., the variables are assumed to influence missingness) is not included in the linear model being tested. This is because the MAR assumption discussed previously is defined relative to the analyzed variables in a given dataset. For example, if the missing values on a variable *Y* are dependent on the values of another variable *X*, the MAR assumption no longer holds if *X* is not included in the ultimate analysis. This is clearly problematic for the two direct estimational algorithms, as *X* must be incorporated in the substantive model for MAR to be tenable. However, this is not the case with the EM algorithm, as the input covariance matrix used to estimate substantive model parameters may be a subset of a larger covariance matrix produced from an EM analysis. In this case, the EM mean vector and covariance matrix are estimated using the full set of observed variables, and the elements that are of substantive interest are extracted for future analyses. Of course, the application of the EM algorithm in this scenario assumes that the researcher has explicit knowledge of the missing-data mechanism, which may not likely be the case in practice. Nevertheless, the use of the EM algorithm in the manner described previously may make the MAR assumption more plausible in certain circumstances.

V. MULTIPLE IMPUTATION

The primary problem associated with EM algorithm is that the variability in the hypothetically completed dataset is not fully captured during the imputation process. Multiple imputation, as outlined by Rubin (1987), creates $m > 1$ imputed datasets that are analyzed using standard completed data methods. The *m* set of parameter estimates are subsequently pooled into a single set of estimates using formulas provided by Rubin. The logic of multiple imputation is based on the notion that two sources of variability are lost during the EM imputation process. As described previously, the first occurs due to regression imputation; imputed values fall directly on the regression line and thus lack residual variability. The second source of lost variability is due to the fact that the regression equations are derived from a covariance matrix that is, itself, estimated with error due to the missing data. That is, the covariance matrix used to impute values is one of many plausible covariance matrices. The multiple imputation process attempts to restore the lost variability from both of these sources. Currently, there are at least two widely available multiple imputation programs based on the EM algorithm: EMCOV (Graham & Hofer, 1993) and NORM (Schafer, 1998).³ Although conceptually similar, the multiple imputation algorithms are quite different: EMCOV generates *m* imputed datasets using the bootstrap technique, whereas NORM does so using Bayesian simulation. Following an initial EM analysis,

EMCOV (Graham & Hofer, 1993) restores residual variability by adding a randomly sampled (with replacement) residual term to each of the imputed data points. For every nonmissing-data point in the original dataset, a vector of residuals for each variable is calculated as the difference between the actual and predicted values from the regression equations (all other variables serving as predictors) used to impute missing values. Next, m datasets are created by repeatedly imputing missing values to the original datasets such that m imputations are based on new estimates of the covariance matrix. In the first step, a bootstrap is performed on the original data, yielding a new data matrix of the same dimensions as the original. Next, the bootstrapped data are analyzed using the EM algorithm, and a new estimate of the covariance matrix is obtained. Finally, missing values in the original dataset are imputed using regression equations generated from the new covariance matrix. This bootstrap process is repeated m times (the imputed data matrix from the original EM analysis serves as the first of the m data sets), and residual variation is restored to the m set of imputed data points using randomly sampled residual terms, as described previously. In contrast, NORM (Schafer, 1998) uses iterative Bayesian simulation to generate m imputed datasets. Like the EM algorithm, the NORM algorithm repeatedly cycles through two steps: Missing observations are imputed (the imputation, or I step) and unknown parameters are estimated (the posterior, or P step). However, unlike EM, the data augmentation (DA) algorithm implemented in NORM uses a stochastic rather than a deterministic process. In the first step, missing data points are replaced by randomly drawn values from the conditional distribution of the missing data given the observed data and a current estimate of the parameter vector θ ; parameter estimates from an EM analysis provide start values for the first iteration. Next, new parameter estimates are randomly drawn from a Bayesian posterior distribution conditioned on the observed and imputed values from the first step. These new parameter values are used to impute values in the subsequent I step, and the process begins again. This two-step procedure is iterated until convergence occurs, at which point the first of m imputed data matrices is created from a final I step. Additional imputed datasets are obtained by repeating the DA process $m-1$ times. Finally, it should be noted that the stochastic nature of the DA process requires a different convergence criterion than the EM algorithm. Because DA parameter estimates are drawn randomly from a posterior probability distribution, values will naturally vary between successive iterations, even after convergence occurs. Thus, the DA algorithm converges when the *distribution* of the parameter estimates no longer changes between contiguous iterations. Readers are encouraged to consult Schafer (1997) and Schafer and Olsen (1998) for further details. After implementing EMCOV or NORM, complete-data analyses are performed on each of the m imputed data sets, and the parameter estimates from these analyses are

stored in a new file. Using rules provided by Rubin (1987), a single set of point estimates and standard error values can be obtained; both EMCOV and NORM include routines that will perform the necessary calculations. Two final points should be made regarding multiple imputation. First, Schafer (1997) suggested that adequate results could be obtained using as few as five imputed data sets. Second, a straightforward method of obtaining SEM goodness-of-fit tests is not currently available, although work on the topic is on-going (Schafer & Olsen, 1998).

VI. SUMMARY

Recent software advances have provided applied researchers with powerful options for analyzing data with missing observations. Specifically, three ML algorithms (multiple group analysis, FIML, and the EM algorithm) are widely available in existing software packages. However, the wide array of data analytic options has resulted in some confusion over the differences among the three algorithms. As such, the goal of this article was to provide a brief overview of ML algorithms in hopes that applied researchers can make informed decisions regarding the use of ML algorithms in various data analytic settings. The EM algorithm may be preferable when the missing-data mechanism does not appear in the substantive model.

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