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The Multiple Adaptations of Multiple Imputation

Jerome P. REITER and Trivellore E. RAGHUNATHAN

Multiple imputation was first conceived as a tool that statistical agencies could use to handle nonresponse in large-sample public use surveys. In the last two decades, the multiple-imputation framework has been adapted for other statistical contexts. For example, individual researchers use multiple imputation to handle missing data in small samples, statistical agencies disseminate multiply-imputed data sets for purposes of protecting data confidentiality, and survey methodologists and epidemiologists use multiple imputation to correct for measurement errors. In some of these settings, Rubin's original rules for combining the point and variance estimates from the multiply-imputed data sets are not appropriate, because what is known—and thus the conditional expectations and variances used to derive inferential methods—differs from that in the missing-data context. These applications require new combining rules and methods of inference. In fact, more than 10 combining rules exist in the published literature. This article describes some of the main adaptations of the multiple-imputation framework, including missing data in large and small samples, data confidentiality, and measurement error. It reviews the combining rules for each setting and explains why they differ. Finally, it highlights research topics in extending the multiple-imputation framework.

KEY WORDS: Confidentiality; Measurement error; Missing data; Synthetic.

1. INTRODUCTION

Multiple imputation (Rubin 1987) was first conceived as a tool that statistical agencies could use to handle nonresponse in large data sets that are disseminated to the public. The basic idea is for the statistical agency to simulate values for the missing data repeatedly by sampling from predictive distributions of the missing values. This creates multiple, completed data sets that are disseminated to the public. This has been done for, for example, public release files for the Fatality Analysis Reporting System (Heitjan and Little 1991), the Consumer Expenditures Survey (Raghunathan and Paulin 1998), the National Health and Nutrition Examination Survey (Schafer et al. 1998), the Survey of Consumer Finances (Kennickell 1998), and the National Health Interview Survey (Schenker et al. 2006). Rubin (1996) and Barnard and Meng (1999) have provided other examples of multiple imputation for missing data.

Multiple imputation is appealing for handling nonresponse in large data sets because it moves the missing-data burden from data analysts to data producers, who typically have greater resources than analysts. When the imputation models meet certain conditions (Rubin 1987, chap. 4) analysts of the completed data sets can obtain valid inferences using complete-data statistical methods and software. Specifically, the analyst computes point and variance estimates of interest with each data set and combines these estimates using simple formulas developed by Rubin (1987). These formulas serve to propagate the uncertainty introduced by imputation through the analyst's inferences, allowing the analyst to focus on modeling issues rather than on estimation technicalities.

In the last 2 decades, multiple imputation has evolved beyond the context of large-sample survey nonresponse. Individual researchers now routinely use multiple imputation for missing data in small samples, as evidenced by the development of multiple-imputation procedures for mainstream software such as SAS, Stata, and S–PLUS. Statistical agencies release multiply-imputed data sets to protect the confidentiality of survey respondents' identities or sensitive attributes in public-use files (Kennickell 1998; Abowd and Woodcock 2001). Survey methodologists and epidemiologists use multiple imputation to edit and correct for measurement errors (Ghosh-Dastidar and Schafer 2003; Winkler 2003; Cole, Chu, and Greenland 2006) or to recode variables due to changes in definitions (Clogg, Rubin, Schenker, Schultz, and Weidman 1991; Schenker 2003). In some of these settings, Rubin's (1987) rules for combining point and variance estimates are not applicable, yielding confidence intervals without nominal coverage rates or significance tests without nominal levels. The original rules fail because what is considered known by the analyst (and thus part of the conditional expectations and variances used to obtain the multiple-imputation inferences) in these settings differs from that in the missing-data setting. Consequentially, new adaptations of the multiple-imputation framework have necessitated the development of new multiple-imputation inferences. In fact, more than 10 multiple-imputation inference methods appear in the literature, many published in the last 5 years.

This article summarizes some of the main adaptations of the multiple-imputation framework and explains why different adaptations warrant different inferential methods. The rest of the article is organized as follows. Section 2 reviews multiple imputation for missing data, including recent modifications; Section 3 reviews multiple imputation for data confidentiality, also known as synthetic data; and Section 4 reviews multiple imputation for measurement error corrections, including a clarification of the appropriate combining rules in this context. In these sections we write primarily from the perspective of a statistical agency releasing data to the public. Of course, this is only one area of application for multiple imputation. Finally, Section 5 cites examples of applications in other areas and suggests new applications.

2. MULTIPLE IMPUTATION FOR MISSING DATA

We begin this review with its original purpose: handling missing data in large samples. After summarizing Rubin's (1987) original methods, we discuss several adaptations, including inference with small samples (Barnard and Rubin 1999), significance tests of multicomponent hypotheses (Li, Raghunathan, and Rubin 1991b; Meng and Rubin 1992), and nested imputation (Shen 2000; Harel and Schafer 2003; Rubin 2003b). We do not cover conditional mean imputation (Schafer and Schenker 2000), which is an approximation

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to multiple imputation. This section does not address practical issues, such as congeniality, specifying imputation models, and ignorability of the missing data. For excellent discussions of these issues, see Rubin (1987, 1996), Meng (1994), Schafer (1997), Little and Rubin (2002), Zhang (2003), Gelman, Van Mechelen, Verbeke, Heitjan, and Meulders (2005), and Reiter, Raghunathan, and Kinney (2006).

2.1 Standard Multiple Imputation

For a finite population of size N, let $I_j = 1$ if unit j is selected in the survey and $I_j = 0$ otherwise, where $j = 1, 2, \ldots, N$. Let $\mathbf{I} = (I_1, \ldots, I_N)$. Let $\mathbf{R}_j$ be a $p \times 1$ vector of response indicators, where $R_{jk} = 1$ if the response for unit j to survey item k is recorded and $R_{jk} = 0$ otherwise. Let $\mathbf{R} = (\mathbf{R}_1, \ldots, \mathbf{R}_N)$. Let $\mathbf{Y}_{\text{inc}} = (\mathbf{Y}_{\text{obs}}, \mathbf{Y}_{\text{mis}})$ be the $n \times p$ matrix of survey data for the n units with $I_j = 1$; $\mathbf{Y}_{\text{obs}}$ is the portion of $\mathbf{Y}_{\text{inc}}$ that is observed, and $\mathbf{Y}_{\text{mis}}$ is the portion of $\mathbf{Y}_{\text{inc}}$ that is missing due to nonresponse. Let $\mathbf{Y} = (\mathbf{Y}_{\text{inc}}, \mathbf{Y}_{\text{exc}})$ be the $N \times p$ matrix of survey data for all units in the population. Let $\mathbf{X}$ be the $N \times d$ matrix of design variables for all N units in the population, such as, stratum or cluster indicators or size measures. We assume that such design information is known for all population units, for example, from census records or the sampling frame(s). Missing values in $\mathbf{X}$ can be treated as part of $\mathbf{Y}_{\text{mis}}$. Finally, we write the observed data as $\mathbf{D} = (\mathbf{X}, \mathbf{Y}_{\text{obs}}, \mathbf{I}, \mathbf{R})$.

The agency fills in values for $\mathbf{Y}_{\text{mis}}$ with draws from the posterior predictive distribution of $(\mathbf{Y}_{\text{mis}} \mid \mathbf{D})$ or approximations of that distribution, such as the sequential regression approach of Raghunathan, Lepkowski, van Hoewyk, and Solenberger (2001). These draws are repeated independently m times to obtain m completed data sets, $\mathbf{D}^{(l)} = (\mathbf{D}, \mathbf{Y}_{\text{mis}}^{(l)})$, where $1 \le l \le m$, which are disseminated to the public. Multiple rather than single imputations are used so that analysts can estimate the variabilities due to imputing missing data.

2.1.1 Univariate Estimands: The Large-Sample Case. From these imputed data sets, the analyst seeks inferences about some estimand $Q = Q(\mathbf{X}, \mathbf{Y})$, for example, a population mean or regression coefficient, where the notation $Q(\mathbf{X}, \mathbf{Y})$ indicates a function of $\mathbf{X}$ and $\mathbf{Y}$. In each imputed data set, the analyst estimates Q with some estimator $\hat{Q}$ and the variance of $\hat{Q}$ with some estimator $\hat{U}$. It is assumed that the analyst specifies $\hat{Q}$ and $\hat{U}$ by acting as if each $\mathbf{D}^{(l)}$ was in fact data collected from a random sample of $(\mathbf{X}, \mathbf{Y})$ based on the original sampling design $\mathbf{I}$, that is, $\hat{Q}$ and $\hat{U}$ are complete-data estimators.

For $i = 1, \ldots, m$, let $Q^{(l)}$ and $U^{(l)}$ be the values of $\hat{Q}$ and $\hat{U}$ in the completed data set $\mathbf{D}^{(l)}$. Under assumptions described by Rubin (1987), the analyst can obtain valid inferences for scalar Q by combining the m replicates of $Q^{(l)}$ and $U^{(l)}$. Specifically, the following quantities typically arise in inferences:

$$\bar{Q}_m = \sum_{l=1}^{m} \frac{Q^{(l)}}{m} \tag{1}$$

$$B_m = \sum_{l=1}^{m} \frac{(Q^{(l)} - \bar{Q}_m)^2}{m-1}, \tag{2}$$

and

$$\bar{U}_m = \sum_{l=1}^{m} \frac{U^{(l)}}{m}. \tag{3}$$

The analyst uses $\bar{Q}_m$ to estimate Q and $T_m = (1 + 1/m)B_m + \bar{U}_m$ to estimate $\text{var}(Q|\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(m)})$. Here $\bar{U}_m$ estimates the variance if the data were complete, and $(1 + 1/m)B_m$ estimates the increase in variance because of the missing data.

When $m = \infty$, which is a useful case for motivating combining rules for other adaptations of multiple imputation, under the posited imputation model, $\text{var}(Q|\mathbf{D})$ equals $\text{var}(E(Q|\mathbf{D}, \mathbf{Y}_{\text{mis}})|\mathbf{D}) + E(\text{var}(Q|\mathbf{D}, \mathbf{Y}_{\text{mis}})|\mathbf{D}) = B_\infty + \bar{U}_\infty$. This is because each $Q^{(l)}$ and $U^{(l)}$ is a draw from the posterior distributions of $E(Q|\mathbf{D}, \mathbf{Y}_{\text{mis}})$ and $\text{var}(Q|\mathbf{D}, \mathbf{Y}_{\text{mis}})$, as discussed by Rubin (1987, chap. 3).

When n is large and m is modest, inferences for Q are based on the t distribution, $(\bar{Q}_m - Q) \sim t_{\nu_m}(0, T_m)$, with $\nu_m = (m-1)(1 + \bar{U}_m/((1 + 1/m)B_m))^2$ degrees of freedom. These degrees of freedom are derived by matching the first two moments of $T_m/\text{var}(Q|\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(m)}, B_\infty)$ to the first two moments of a chi-squared distribution.

It has been shown (Wang and Robins 1998; Robins and Wang 2000; Nielsen 2003; Kim, Brick, Fuller, and Kalton 2006) that T_m can be biased. This bias is usually positive. Whereas bias in T_m is clearly undesirable, Rubin (2003a) and others have argued that it typically is not substantial enough to outweigh the benefits of using T_m (which is simple to compute) and multiple imputation more generally. The properties of confidence intervals for Q in genuine samples are more important than the asymptotic properties of T_m. Indeed, the primary purpose of estimating T_m lies in constructing confidence intervals for Q. Empirical evidence from genuine applications of the approach suggests that for sensible complete-data inferences and imputation models, inferences based on T_m perform well for various Q's (Rubin 2003a).

2.1.2 Univariate Estimands: The Small-Sample Case. Rubin's (1987) derivations assume that complete-data inferences about Q can be based on normal distributions. But when n is small, t distributions are more appropriate. Barnard and Rubin (1999) developed inferential methods that account for this difference. Their methods still use $\bar{Q}_m$ and T_m as the point and variance estimates, but the degrees of freedom change from ν_m to $\nu_m^* = (\nu_m^{-1} + \hat{\nu}_{\text{obs}}^{-1})^{-1}$, where $\hat{\nu}_{\text{obs}} = \nu_{\text{com}}(\bar{U}_m/T_m)(\nu_{\text{com}} + 1)/(\nu_{\text{com}} + 3)$ and ν_{com} is the degrees of freedom if the data were complete. The quantity $\hat{\nu}_{\text{obs}}$ is ν_{com} downweighted by a multiplicative factor that equates the increase in variance due to missing data to a $(\bar{U}_m/T_m) \times 100\%$ reduction in effective sample size.

The quantity ν_m^* has several features that led Barnard and Rubin (1999) to recommend its general use, regardless of the size of n. First, $\nu_m^* \le \nu_{\text{com}}$, whereas ν_m can exceed ν_{com}. This property of ν_m^* is desirable, because the presence of missing data should decrease rather than increase the degrees of freedom. Second, $\nu_m^* < \nu_m$ with approximate equality when n is large, so that using ν_m^* instead of ν_m is slightly conservative in large samples. Third, ν_m^* is always between ν_{com} and ν_m, making it a compromise degrees of freedom.

2.1.3 Multicomponent Estimands: The Large-Sample Case. Using the m imputed data sets, the analyst seeks to test the null hypothesis $\mathbf{Q} = \mathbf{Q}_0$ for some k-component estimand $\mathbf{Q}$, for example, to test whatever k regression coefficients equal 0. Let $\bar{\mathbf{Q}}_m$, $\mathbf{B}_m$, and $\bar{\mathbf{U}}_m$ be the multivariate analogs of $\bar{Q}_m$, B_m, and

$\bar{U}_m$. These are computed using k-dimensional estimates $\mathbf{Q}^{(l)}$ and $k \times k$ covariance matrices $\mathbf{U}^{(l)}$, where $1 \le l \le m$, in (1)–(3). It may appear reasonable to use a Wald test with statistic $(\bar{\mathbf{Q}}_m - \mathbf{Q}_0)^T((1+1/m)\mathbf{B}_m + \bar{\mathbf{U}}_m)^{-1}(\bar{\mathbf{Q}}_m - \mathbf{Q}_0)$; however, this test is unreliable when $k > m$ and m is moderate, as is frequently the case, because $\mathbf{B}_m$ can have large variability (Rubin 1987; Li, Raghunathan, and Rubin 1991b). Estimating $\mathbf{B}_m$ in such cases is akin to estimating a covariance matrix using fewer observations than there are dimensions. This difficulty is avoided by making m large.

To mitigate the effects of variability when m is moderate, Rubin (1987) proposed taking $\mathbf{B}_\infty = r_\infty \bar{\mathbf{U}}_\infty$, where r_∞ is a scalar. Equivalently, the percentage increases in variance due to nonresponse are equal for all components of $\mathbf{Q}$. Under this restriction, only one additional parameter, r_∞, is needed to estimate $\mathbf{B}_\infty$. Each diagonal element of $\mathbf{B}_m$ (after rescaling) provides an estimate of r_∞. Thus, assuming that $\mathbf{B}_\infty$ is proportional to $\bar{\mathbf{U}}_\infty$ turns the problem of having $m-1$ degrees of freedom to estimate $k(k+1)/2$ (possibly $>m$) parameters into the problem of having $k(m-1)$ degrees of freedom to estimate one parameter.

Using Rubin's proposal, the test statistic is $S_m = (\bar{\mathbf{Q}}_m - \mathbf{Q}_0)^T \bar{\mathbf{U}}_m^{-1}(\bar{\mathbf{Q}}_m - \mathbf{Q}_0)/(k(1+r_m))$, where $r_m = (1+1/m)\,\mathrm{tr}(\mathbf{B}_m \bar{\mathbf{U}}_m^{-1})/k$. The reference distribution for S_m is an approximate F distribution, F_{k,v_w}, with $v_w = 4 + (t-4)(1+(1-2/t)/r_m)^2$ and $t = k(m-1) > 4$. When $t \le 4$, we set $v_w = (k+1)v_m/2$. The p value for testing $\mathbf{Q} = \mathbf{Q}_0$ is $\Pr(F_{k,v_w} > S_m)$. Simulations by Li et al. (1991b) suggest that for many practical situations with moderate m, this test has better properties than other tests.

The test statistic S_m has the familiar quadratic form of the Wald statistic but with a correction factor $k(1+r_m)$ in the denominator. The factor of k is needed for a good F approximation, which is derived by matching the first two moments of S_m. The factor of $1+r_m$ adjusts the quadratic form so that the test statistic is based on the appropriate estimate of variance rather than on $\bar{\mathbf{U}}_m$ alone. To see this, it is instructive to consider the case where Q is scalar, that is, $k = 1$. Then $(1+r_m) = T_m/\bar{U}_m$ estimates the percentage increase in the variance due to the missing data relative to the estimated complete-data variance, so that $(1+r_m)\bar{U}_m = T_m$ is the correct variance for the quadratic form. When $\mathbf{Q}$ is multivariate and proportionality holds, r_m estimates $(1+1/m)r_\infty$, so that $(1+r_m)$ can be interpreted as the average percentage increase in variance.

Working with $\bar{\mathbf{U}}_m$ may be cumbersome for large k. Meng and Rubin (1992) developed an alternative significance test based on the log-likelihood ratio test statistics from the m imputed data sets, which are easily computed for common models like those from exponential families. Their strategy is to (a) find a statistic asymptotically equivalent to S_m based only on values of the Wald statistics calculated in each imputed data set, (b) use the asymptotic equivalence of Wald and likelihood ratio test statistics to define the likelihood ratio test statistic, and (c) use a reference F distribution like that for the Wald tests. The key to this strategy is to approximate S_m and r_m without using $\bar{\mathbf{U}}_m$.

Let $\boldsymbol{\psi}$ be the vector of parameters in the analyst's model, and let $\boldsymbol{\psi}^{(l)}$ be the maximum likelihood estimate of $\boldsymbol{\psi}$ computed from $\mathbf{D}^{(l)}$, for $l = 1, \ldots, m$. Suppose that the analyst is interested in a k-dimensional function, $\mathbf{Q}(\boldsymbol{\psi})$, and forms the hypothesis that $\mathbf{Q}(\boldsymbol{\psi}) = \mathbf{Q}_0$. Let $\boldsymbol{\psi}_0^{(l)}$ be the maximum likelihood estimate of $\boldsymbol{\psi}$ obtained from $\mathbf{D}^{(l)}$ subject to $\mathbf{Q}(\boldsymbol{\psi}) = \mathbf{Q}_0$. The log-likelihood ratio test statistic associated with $\mathbf{D}^{(l)}$ is $L^{(l)} = 2\log f(\mathbf{D}^{(l)}|\boldsymbol{\psi}^{(l)}) - 2\log f(\mathbf{D}^{(l)}|\boldsymbol{\psi}_0^{(l)})$. Let $\bar{L} = \sum_{l=1}^m L^{(l)}/m$, $\bar{\boldsymbol{\psi}} = \sum_{l=1}^m \boldsymbol{\psi}^{(l)}/m$, and $\bar{\boldsymbol{\psi}}_0 = \sum_{l=1}^m \boldsymbol{\psi}_0^{(l)}/m$. Meng and Rubin (1992) also used the average of the log-likelihood ratio test statistics evaluated at $\bar{\boldsymbol{\psi}}$ and $\bar{\boldsymbol{\psi}}_0$, which we write as $\bar{L}_0 = (1/m)\sum_{l=1}^m (2\log f(\mathbf{D}^{(l)}|\bar{\boldsymbol{\psi}}) - 2\log f(\mathbf{D}^{(l)}|\bar{\boldsymbol{\psi}}_0))$.

The likelihood ratio test statistic is $\hat{S}_m = \bar{L}_0/(k(1+\hat{r}_m))$, where $\hat{r}_m = ((m+1)/t)(\bar{L} - \bar{L}_0)$ is asymptotically equivalent to r_m and $\bar{L}_0$ is asymptotically equivalent to $k(1+r_m)S_m$. The reference distribution for $\hat{S}_m$ is $F_{k,\hat{v}_w}$, where $\hat{v}_w$ is defined as v_w but using $\hat{r}_m$ in place of r_m.

Because the likelihood ratio test is an asymptotic equivalent of the Wald test, it has similar properties to the Wald test when n is sufficiently large. Research comparing the properties of the two procedures for modest n is sparse. It also is possible to obtain inferences by combining only the p values from Wald tests (Li, Raghunathan, Meng, and Rubin 1991a); however, the performance of this method is unsatisfactory compared with that of other approaches (Meng and Rubin 1992; Schafer 1997).

2.1.4 Multicomponent Estimands: The Small-Sample Case. Tests of $\mathbf{Q} = \mathbf{Q}_0$ in small samples use the test statistic S_m. However, the denominator degrees of freedom v_w is not appropriate for small n. It is derived assuming that the reference distribution for the complete-data test is a chi-squared distribution, whereas for small samples it is an F distribution. In fact, with small n, v_w can exceed v_{com}, possibly resulting in a larger proportion of p values below the desired significance levels than would be expected under the null hypothesis for a test with valid frequentist properties.

Reiter (2007b) presented an alternative denominator degrees of freedom derived using a second-order Taylor series expansion and moment matching in the spirit of Barnard and Rubin (1999). A simplified approximation to these degrees of freedom is

$$v_{\mathrm{fapp}} = 4 + \left(\frac{1}{v_{\mathrm{com}}^* - 4(1+a)} + \frac{1}{t-4}\left(\frac{a^2(v_{\mathrm{com}}^* - 2(1+a))}{(1+a)^2(v_{\mathrm{com}}^* - 4(1+a))} \right) \right)^{-1}, \quad (4)$$

where $v_{\mathrm{com}}^* = v_{\mathrm{com}}(v_{\mathrm{com}}+1)/(v_{\mathrm{com}}+3)$ and $a = r_m t/(t-2)$. A more complicated expression involving higher-order terms has been given by Reiter (2007b). Note that $v_{\mathrm{fapp}} \le v_{\mathrm{com}}$ with near equality for small fractions of missing information when t is large relative to v_{com}. Also, $v_{\mathrm{fapp}} = v_w$ for infinite sample sizes, because in that case $(1+a)^2/a^2 = (1+(1-2/t)/r_m)^2$.

2.2 Nested Multiple Imputation

In some situations, it may be advantageous to generate different numbers of imputations for different variables. For example, imputers may want to generate relatively few values for variables that are computationally expensive to impute and many values for variables that are computationally inexpensive to impute. This approach was taken in the National Medical Expenditure Survey (Rubin 2003b). As a related example, when imputers seek to limit the total number of imputations, they may want to release few values for variables with low fractions

of missing information—because the between-imputation variance may be small for analyses involving these variables—and many values for variables with high fractions of missing information.

Using different numbers of imputations per variable is called nested multiple imputation (Shen 2000), or two-stage multiple imputation (Harel and Schafer 2003). The nesting refers to the way in which imputations are generated; the data are not necessarily organized in a multilevel structure. To describe nested imputation, we use the setting of expensive and inexpensive imputations. Let $\mathbf{Y}_{\text{exp}}$ be the missing values that are expensive to impute, and let $\mathbf{Y}_{\text{inexp}}$ be the missing values that are inexpensive to impute. The imputer generates imputations in a two-step process. First, the imputer draws values of $\mathbf{Y}_{\text{exp}}^{(l)}$, for $l = 1, \ldots, m$, from the predictive distribution for $(\mathbf{Y}_{\text{exp}} \mid \mathbf{D})$, resulting in m partially completed data sets. Second, in each partially completed data set, the imputer generates $\mathbf{Y}_{\text{inexp}}^{(l,1)}, \mathbf{Y}_{\text{inexp}}^{(l,2)}, \ldots, \mathbf{Y}_{\text{inexp}}^{(l,r)}$ by drawing from the predictive distribution of $(\mathbf{Y}_{\text{inexp}} \mid \mathbf{D}, \mathbf{Y}_{\text{exp}}^{(l)})$. The result is $M = mr$ completed data sets, $\mathbf{D}^{(l,i)} = (\mathbf{D}, \mathbf{Y}_{\text{exp}}^{(l)}, \mathbf{Y}_{\text{inexp}}^{(l,i)})$, where $l = 1, \ldots, m$ and $i = 1, \ldots, r$. Each data set includes a label indicating its value of l, that is, an indicator for its nest.

2.2.1 Univariate Estimands: The Large-Sample Case. As shown by Shen (2000), analysts can obtain valid inferences from these released data sets by combining inferences from the individual data sets. As before, let $Q^{(l,i)}$ and $u^{(l,i)}$ be the values of $\hat{Q}$ and $\hat{U}$ in data set $\mathbf{D}^{(l,i)}$, where $1 \le l \le m$ and $1 \le i \le r$. Analogous to (1)–(3), we have

$$\bar{Q}_M = \sum_{l=1}^{m} \sum_{i=1}^{r} \frac{Q^{(l,i)}}{mr} = \sum_{l=1}^{m} \frac{\bar{Q}^{(l)}}{m}, \tag{5}$$

$$\bar{W}_m = \sum_{l=1}^{m} \sum_{i=1}^{r} \frac{(Q^{(l,i)} - \bar{Q}^{(l)})^2}{m(r-1)} = \sum_{l=1}^{m} \frac{W^{(l)}}{m}, \tag{6}$$

$$B_m = \sum_{l=1}^{m} \frac{(\bar{Q}^{(l)} - \bar{Q}_M)^2}{m-1}, \tag{7}$$

$$\bar{U}_M = \sum_{l=1}^{m} \sum_{i=1}^{r} \frac{U^{(l,i)}}{mr}. \tag{8}$$

Provided that the complete-data inferences are valid from a frequentist perspective and the imputations are proper, we can estimate Q with $\bar{Q}_M$. An estimate of $\text{var}(Q|\mathbf{D}^{(1,1)}, \ldots, \mathbf{D}^{(m,r)})$ is $T_M = (1 + 1/m)B_m + (1 - 1/r)\bar{W}_m + \bar{U}_M$. When n is large, inferences can be based on the t distribution $(Q - \bar{Q}_M) \sim t_{\nu_M}(0, T_M)$, with degrees of freedom

$$\nu_M = \left(\frac{((1 + 1/m)B_m)^2}{(m-1)T_M^2} + \frac{((1 - 1/r)\bar{W}_m)^2}{m(r-1)T_M^2} \right)^{-1}. \tag{9}$$

To derive ν_M, match the first two moments of $T_M / \text{var}(Q|\mathbf{D}^{(1,1)}, \ldots, \mathbf{D}^{(m,r)}, B_\infty, \bar{W}_\infty)$ to those of a chi-squared distribution. Adjusted degrees of freedom for small n have not been developed for nested multiple imputation, although nested imputation is not particularly useful for small n because imputations are not computationally expensive.

The variance formula for T_M differs structurally from that for T_m, because data sets within any nest l use the common set of imputed values $\mathbf{Y}_{\text{exp}}^{(l)}$. To illustrate the difference, assume that $m = r = \infty$. Then $\bar{U}_\infty$ has the same interpretation as in standard multiple imputation: It estimates the complete-data variance associated with $Q(\mathbf{X}, \mathbf{Y}_{\text{inc}})$. But B_∞ has a different interpretation: It estimates the variance due to nonresponse in $\mathbf{Y}_{\text{exp}}$ and part of the variance due to nonresponse in $\mathbf{Y}_{\text{inexp}}$. This latter component is the variability of the $\bar{Q}^{(l)}$s across nests, that is, the variance of the within-nest expected values of the $Q^{(l,i)}$'s. The variability of the $Q^{(l,i)}$'s around their within-nest expected values is estimated by $\bar{W}_\infty$. Adding all sources together for $m = r = \infty$ gives

$$\begin{aligned} \text{var}(Q|\mathbf{D}) &= \text{var}\big(E\big(E(Q|\mathbf{D}, \mathbf{Y}_{\text{exp}}, \mathbf{Y}_{\text{inexp}})|\mathbf{D}, \mathbf{Y}_{\text{exp}}\big)|\mathbf{D}\big) \\ &\quad + E\big(\text{var}\big(E(Q|\mathbf{D}, \mathbf{Y}_{\text{exp}}, \mathbf{Y}_{\text{inexp}})|\mathbf{D}, \mathbf{Y}_{\text{exp}}\big)|\mathbf{D}\big) \\ &\quad + E\big(E\big(\text{var}(Q|\mathbf{D}, \mathbf{Y}_{\text{exp}}, \mathbf{Y}_{\text{inexp}})|\mathbf{D}, \mathbf{Y}_{\text{exp}}\big)|\mathbf{D}\big) \\ &= B_\infty + \bar{W}_\infty + \bar{U}_\infty. \end{aligned} \tag{10}$$

For the more realistic setting of moderate m and r, we need to adjust for using only a finite number of imputations at each stage. In standard multiple imputation, we add B_m/m, which is the between-imputation variance divided by the number of imputed data sets. For nested imputation, we follow a similar strategy, but there are m imputed sets of $\mathbf{Y}_{\text{exp}}$ and $M = mr$ sets of $\mathbf{Y}_{\text{inexp}}$. Roughly speaking, the between-imputation variance associated with $\mathbf{Y}_{\text{exp}}$ should be divided by m, and the between-imputation variance associated with $\mathbf{Y}_{\text{inexp}}$ should be divided by M.

Given B_∞ and $\bar{W}_\infty$, for finite M, the $\text{var}(Q|\mathbf{D}^{(1,1)}, \ldots, \mathbf{D}^{(m,r)})$ is $(1 + 1/m)B_\infty + (1 + 1/M)\bar{W}_\infty + \bar{U}_\infty$ (Shen 2000). We estimate B_∞ and $\bar{W}_\infty$ using an ANOVA decomposition. Here, B_m approximates $B_\infty + \bar{W}_\infty/r$, because each $\bar{Q}^{(l)}$ has between-nest (B_∞) and within-nest ($\bar{W}_\infty/r$) components of variance, and $\bar{W}_m$ approximates $\bar{W}_\infty$. Plugging in the implied point estimates for B_∞ and $\bar{W}_\infty$ provides T_M.

2.2.2 Multicomponent Estimands: Large-Sample Case. Shen (2000) developed significance tests of k-dimensional multicomponent hypotheses using strategies akin to those outlined in Section 2.1.3, with one key distinction: Because there are two missing-data variance components, the tests require two assumptions of proportionality.

Let $\bar{\mathbf{Q}}_M, \bar{\mathbf{W}}_M, \mathbf{B}_M$, and $\bar{\mathbf{U}}_M$ be the multivariate analogs of the quantities in (5)–(8). To deal with high-variability problems when m and r are modest relative to k, we assume that $\bar{\mathbf{W}}_\infty = r_\infty^{(w)}\bar{\mathbf{U}}_\infty$ and $\mathbf{B}_\infty = r_\infty^{(b)}\bar{\mathbf{U}}_\infty$. Equivalently, the fractions of missing information due to the missing $\mathbf{Y}_{\text{exp}}$ are the same for all components of $\mathbf{Q}$, as is also the case—with a possibly different fraction—for $\mathbf{Y}_{\text{inexp}}$.

Under these assumptions, the Wald statistic is $S_M = (\bar{\mathbf{Q}}_M - \mathbf{Q}_0)^T\bar{\mathbf{U}}_M^{-1}(\bar{\mathbf{Q}}_M - \mathbf{Q}_0)/(k(1 + r_M^{(b)} + r_M^{(w)}))$, where $r_M^{(b)} = (1 + 1/m)\,\text{tr}(\mathbf{B}_M\bar{\mathbf{U}}_M^{-1})/k$ and $r_M^{(w)} = (1 - 1/r)\,\text{tr}(\bar{\mathbf{W}}_M\bar{\mathbf{U}}_M^{-1})/k$. The quantity $(1 + r_M^{(b)} + r_M^{(w)})$ adjusts the quadratic form so that it is based on a correct estimate of variance. The reference distribution for S_M derived by Shen (2000) is an approximate F distribution, $F_{k,k\hat{\nu}_M}$, with

$$\hat{\nu}_M = \left(\frac{(r_M^{(b)})^2}{(m-1)(1 + r_M^{(b)} + r_M^{(w)})^2} + \frac{(r_M^{(w)})^2}{m(r-1)(1 + r_M^{(b)} + r_M^{(w)})^2} \right)^{-1}. \tag{11}$$

The denominator degrees of freedom is based on (9) with $(1 + 1/m)\mathbf{B}_m$, $(1 - 1/r)\bar{\mathbf{W}}_m$, and $\mathbf{T}_M$ replaced by their estimates under the foregoing proportionality assumptions.

Shen's (2000) degrees of freedom were not derived by matching moments to an F distribution, as was done for v_w in one-stage multiple imputation. For one-stage multiple imputation, Li et al. (1991b) found that tests based on v_w degrees of freedom performed better than tests based on $k\hat{v}_m$ degrees of freedom, where $\hat{v}_m = (m-1)(1 + r_m^{-1})^2$. For nested multiple imputation, Shen's (2000) degrees of freedom have not been compared with those based on the approach of Li et al. (1991b).

Shen (2000) derived a likelihood ratio test following the strategy outlined in Section 2.1.3. For each $\mathbf{D}^{(l,i)}$, let $\boldsymbol{\psi}_0^{(l,i)}$ and $\boldsymbol{\psi}^{(l,i)}$ be the maximum likelihood estimates of $\mathbf{Q}$ under the null and alternative hypotheses. Let $L^{(l,i)} = 2\log f(\mathbf{D}^{(l,i)}|\boldsymbol{\psi}^{(l,i)}) - 2\log f(\mathbf{D}^{(l,i)}|\boldsymbol{\psi}_0^{(l,i)})$ and $\bar{L}_M = \sum_{l=1}^m \sum_{i=1}^r L^{(l,i)}/(mr)$. Let $\bar{\boldsymbol{\psi}}^{(l)} = \sum_{i=1}^r \boldsymbol{\psi}^{(l,i)}/r$, $\bar{\boldsymbol{\psi}}_0^{(l)} = \sum_{i=1}^r \boldsymbol{\psi}_0^{(l,i)}/r$, and $\bar{L}^{(l)} = (1/m)\sum_{i=1}^r (2\log f(\mathbf{D}^{(l,i)}|\bar{\boldsymbol{\psi}}^{(l)}) - 2\log f(\mathbf{D}^{(l,i)}|\bar{\boldsymbol{\psi}}_0^{(l)}))$. Shen (2000) also used the average of the log-likelihood ratio test statistics evaluated at $\bar{\boldsymbol{\psi}}_M = \sum_{l=1}^m \boldsymbol{\psi}^{(l)}/m$ and $\bar{\boldsymbol{\psi}}_{0M} = \sum_{l=1}^m \boldsymbol{\psi}_0^{(l)}/m$, which we write as $\bar{L}_{0M} = (1/M)\sum_{l=1}^m \sum_{i=1}^r (2\log f(\mathbf{D}^{(l,i)}|\bar{\boldsymbol{\psi}}_M) - 2\log f(\mathbf{D}^{(l,i)}|\bar{\boldsymbol{\psi}}_{0M}))$.

The likelihood ratio test statistic is $\hat{S}_M = \bar{L}_{0M}/(k(1 + \hat{r}_M^{(b)} + \hat{r}_M^{(w)}))$, where $\hat{r}_M^{(b)} = ((m+1)/t)(\sum_{l=1}^m \bar{L}^{(l)}/m - \bar{L}_{0M})$ and $\hat{r}_M^{(w)} = (1/k)(\bar{L}_M - \sum_{l=1}^m \bar{L}^{(l)}/m)$. The reference distribution for $\hat{S}_m$ is $F_{k,k\tilde{v}_M}$, where $\tilde{v}_M$ is defined like $\hat{v}_M$: Use $\hat{r}_M^{(b)}$ and $\hat{r}_M^{(w)}$ in place of $r_M^{(b)}$ and $r_M^{(w)}$.

3. MULTIPLE IMPUTATION FOR CONFIDENTIAL PUBLIC–USE DATA

Many national statistical agencies, survey organizations, and researchers disseminate data to the public. Wide dissemination greatly benefits society, allowing broad subsets of the research community to access and analyze the collected data. But, often data disseminators cannot release data in their collected form, because doing so would reveal some survey respondents' identities or values of sensitive attributes. Failure to protect confidentiality can have serious repercussions for data disseminators. They may be in violation of laws passed to protect confidentiality, such as the recently enacted Health Insurance and Portability Act and the Confidential Information Protection and Statistical Efficiency Act in the United States. Moreover, they may lose the trust of the public, so that potential respondents are less willing to give accurate answers or even participate in future surveys.

Data disseminators protect confidentiality by stripping unique identifiers like names, social security numbers, and addresses. But these actions alone may not eliminate the risk of disclosure when quasi-identifiers (e.g., age, sex, race, marital status) are released. These variables can be used to match units in the released data to other databases. Thus many data disseminators alter values of quasi-identifiers, and possibly values of sensitive variables, before releasing the data. Common strategies include recoding variables (e.g., releasing ages or geographical variables in aggregated categories), reporting exact values only above or below certain thresholds (e.g., reporting all incomes above 100,000 as "100,000 or more"), swapping data values for selected records (e.g., switching the sexes of some men and women to discourage users from matching), and adding noise to numerical data values to reduce the possibility of exact matching or to distort the values of sensitive variables.

These methods can be applied to various degrees. Generally, increasing the amount of alteration decreases the risks of disclosure, but it also decreases the accuracy of inferences obtainable from the released data, because these methods distort relationships among the variables. Unfortunately, it is difficult—and for some analyses, impossible—for data users to determine how much their particular estimation has been compromised by the data alteration, because disseminators rarely release detailed information about the disclosure limitation strategy. Even when such information is available, adjusting for the data alteration may be beyond some users' statistical capabilities. For example, to properly analyze data that include additive random noise, users should apply measurement error models or the likelihood-based approach of Little (1993), which are difficult to use for nonstandard estimands.

Because of the inadequacies of standard disclosure limitation techniques, several statistical agencies have decided to use, or are considering using, multiple-imputation procedures to limit the risk of disclosing respondents' identities or sensitive attributes in public use data files. This idea, now called synthetic data, was first proposed by Rubin (1993). In his original approach, the data disseminator (a) randomly and independently samples units from the sampling frame to comprise each synthetic data set, (b) imputes the unknown data values for units in the synthetic samples using models fit with the original survey data, and (c) releases multiple versions of these data sets to the public. These are called fully synthetic data sets. Some agencies use or are considering using a variant of Rubin's approach: Release multiply-imputed data sets composing the units originally surveyed with only some collected values, such as sensitive values at high risk of disclosure or values of quasi-identifiers, replaced with multiple imputations. These are called partially synthetic data sets.

Releasing synthetic data can preserve confidentiality, because identifying of units and their sensitive data can be difficult when some or all of the released data are not actual, collected values. Furthermore, using appropriate data generation and estimation methods based on the concepts of multiple imputation, analysts can make valid inferences for various estimands using standard, complete-data statistical methods and software, at least for inferences congenial to the model used to generate the data. Provided that the imputer releases some description of this model, analysts can determine whether or not their questions can be answered using the synthetic data. There are other benefits to using synthetic data, as well as limitations, most of which we do not describe here. For more descriptions of fully synthetic data, see Rubin (1993), Raghunathan, Reiter, and Rubin (2003), Raghunathan (2003), and Reiter (2002, 2005a). For partially synthetic data, see Little (1993), Kennickell (1997), Abowd and Woodcock (2001, 2004), Liu and Little (2002), Reiter (2003, 2004, 2005c), and Mitra and Reiter (2006).

As when imputing missing data, multiple copies of the synthetic data sets must be generated, to allow analysts to estimate variances correctly. However, and perhaps surprisingly at first glance, the Rubin (1987) rules for combining the point and variance estimates do not work in the synthetic data contexts; in fact, they can result in severely biased estimates of variances.

New combining rules are needed for each synthetic data strategy. In this section we review these combining rules and explain why they differ across the different applications of multiple imputation.

3.1 Fully Synthetic Data

To construct fully synthetic data, the imputer follows a two-part process. First, the imputer imputes values of $\mathbf{Y}_{\text{exc}}$ to obtain a complete-data population, $(\mathbf{X}, \mathbf{Y}_{\text{com}}^{(l)})$. Imputations are generated from the predictive distribution of $(\mathbf{Y}|\mathbf{D})$ or some approximation to it. Second, the imputer takes a simple random sample of n_{syn} units from $(\mathbf{X}, \mathbf{Y}_{\text{com}}^{(l)})$, producing the synthetic data set $\mathbf{d}^{(l)} = (\mathbf{X}, \mathbf{Y}_{\text{syn}}^{(l)})$. The lower-case $\mathbf{d}$ distinguishes the use of imputed values as synthetic data from the use of imputed values to fill in missing data. The process is repeated independently m times to generate m different synthetic data sets, which are then released to the public. The imputer also could simulate $\mathbf{Y}$ for all N units, thereby avoiding releasing actual values of $\mathbf{Y}$.

In practice, it is not necessary to generate completed-data populations for constructing $\mathbf{Y}_{\text{syn}}^{(l)}$; the imputer need generate only values of $\mathbf{Y}$ for units in the synthetic samples. The formulation of completing the population and then sampling from it, aids in deriving the combining rules.

3.1.1 Univariate Estimands. The analyst specifies $\hat{Q}$ and $\hat{U}$ acting as if the synthetic data were in fact a simple random sample of $(\mathbf{X}, \mathbf{Y})$. The analyst need not worry about the original complex sampling design, which is one benefit of the fully synthetic data approach, because the design information is accounted for in the imputation stage (e.g., imputation models condition on stratum and cluster effects). As before, the analyst can use $\bar{Q}_m$ from (1) to estimate Q and $T_f = (1 + 1/m)B_m - \bar{U}_m$ to estimate $\text{var}(Q|\mathbf{d}^{(1)}, \ldots, \mathbf{d}^{(m)})$, where B_m and $\bar{U}_m$ are as defined in (2) and (3). Although it is possible that $T_f < 0$, negative values can be avoided by making m and n_{syn} large. A more complicated variance estimator that is always positive has been described by Raghunathan et al. (2003). When $T_f > 0$, and n and n_{syn} are large, inferences for scalar Q can be based on a t distribution with $\nu_f = (m-1)(1 - m\bar{U}_m/((m+1)B_m))^2$ degrees of freedom. A degrees of freedom for small n has not been derived, although the typical application for fully synthetic data is dissemination of survey data with large n.

Obviously, $T_f \neq T_m$: $\bar{U}_m$ is subtracted, not added. This seemingly minor difference in T_f and T_m hides fundamental differences in the sources of variability estimated by B_m and $\bar{U}_m$. To illustrate these differences, we first take the case where $m = \infty$ and $n_{\text{syn}} = N$, so that each $\mathbf{d}^{(l)}$ is a completed population. In this case, each $U^{(l)} = 0$ because entire populations of values are released, so that $T_f = B_\infty$. The process of repeatedly completing populations and estimating Q is equivalent to simulating the posterior distribution of Q. Thus when $n_{\text{syn}} = N$, B_∞ estimates $\text{var}(Q|\mathbf{D})$. This differs greatly from the standard missing-data case, where B_∞ estimates the increase in variance due to nonresponse and $B_\infty + \bar{U}_\infty$ estimates $\text{var}(Q|\mathbf{D})$.

Now consider the case where $m = \infty$ and $n_{\text{syn}} < N$ to motivate the subtraction in T_f. Each $Q^{(l)}$ is affected by two sources of variance: the variance due to imputing $\mathbf{Y}_{\text{exc}}$, which causes the values of $Q_{\text{com}}^{(l)} = Q(\mathbf{X}, \mathbf{Y}_{\text{com}}^{(l)})$ to differ across completed populations, and the variance due to sampling n_{syn} records from $(\mathbf{X}, \mathbf{Y}_{\text{com}}^{(l)})$. The first source is $\text{var}(Q|\mathbf{D})$, because the infinite collection of $Q^{(l)}$s simulates the posterior distribution of Q. The second source is $\bar{U}_\infty$. Thus $B_\infty = \text{var}(Q|\mathbf{D}) + \bar{U}_\infty$ and $\text{var}(Q|\mathbf{D}) = B_\infty - \bar{U}_\infty$. Because $\bar{Q}_\infty = Q_{\text{obs}}$, we have $\text{var}(Q|\mathbf{d}^{(1)}, \ldots, \mathbf{d}^{(\infty)}) = \text{var}(Q|\mathbf{D})$.

For moderate m, we replace B_∞ with B_m and U_∞ with $\bar{U}_m$, and add B_m/m to adjust for using only a finite number of synthetic data sets.

3.1.2 Multicomponent Estimands. Significance tests for multicomponent estimands are derived using the logic described in Section 2.1.3 (Reiter 2005b). To minimize the impact of high variability in $\mathbf{B}_m$, the test statistics are derived under the assumption of equal fractions of missing information across all components of Q, that is, $\mathbf{B}_\infty = r_\infty \mathbf{U}_\infty$. This assumption is generally reasonable in fully synthetic data, because all variables are imputed.

The Wald statistic is $S_f = (\bar{\mathbf{Q}}_m - \mathbf{Q}_0)^T \bar{\mathbf{U}}_m^{-1} (\bar{\mathbf{Q}}_m - \mathbf{Q}_0)/(k(r_f - 1))$, where $r_f = (1 + 1/m)\,\text{tr}(\mathbf{B}_m \bar{\mathbf{U}}_m^{-1})/k$. The reference distribution for S_f is an F distribution, F_{k,v_f}, with $v_f = 4 + (t-4)(1 - (1-2/t)/r_f)^2$. The likelihood ratio test statistic is $\hat{S}_f = \bar{L}_0/(k(\hat{r}_f - 1))$, where $\hat{r}_f = ((m+1)/t)(\bar{L} - \bar{L}_0)$. The reference distribution for $\hat{S}_f$ is $F_{k,\hat{v}_f}$, where the $\hat{v}_f$ is defined as for v_f using $\hat{r}_f$.

The correction factor $r_f - 1$ serves a purpose akin to $1 + r_m$ in the missing-data setting—it adjusts the quadratic form so that the test statistic is based on an appropriate estimate of the variance of $\bar{\mathbf{Q}}_m$. This is most easily seen with a scalar Q. Here $r_f - 1 = T_f/\bar{U}_m$, so that adding $r_f - 1$ appropriately adjusts the quadratic form to be based on T_f. The quantity $\bar{L}_0$ is an asymptotically equivalent replacement for the quadratic form in the Wald statistic for S_f, and $\hat{r}_f$ replaces r_f.

3.2 Partially Synthetic Data

Partially synthetic data sets look like data sets with multiple imputations for missing data. But synthetic data imputations are replacements rather than completions, which leads to variance formulas that differ from T_m. We first describe partially synthetic data assuming no missing data (i.e., $\mathbf{Y}_{\text{inc}} = \mathbf{Y}_{\text{obs}}$), then broaden our discussion to the case where there are missing data.

To generate partially synthetic data sets when $\mathbf{Y}_{\text{inc}} = \mathbf{Y}_{\text{obs}}$, the imputer replaces selected values from the observed data with imputations. Let $Z_j = 1$ if unit j has any of its observed data replaced with synthetic values and $Z_j = 0$ for those units with all data left unchanged. Let $\mathbf{Z} = (Z_1, \ldots, Z_n)$. Let $\mathbf{Y}_{\text{rep}}^{(l)}$ be all of the imputed (replaced) values in the lth synthetic data set, and let $\mathbf{Y}_{\text{nrep}}$ be all unchanged (unreplaced) values of $\mathbf{Y}_{\text{obs}}$. The $\mathbf{Y}_{\text{rep}}^{(l)}$ are assumed to be generated from the predictive distribution of $(\mathbf{Y}_{\text{rep}} \mid \mathbf{D}, \mathbf{Z})$, or a close approximation of it. Each synthetic data set, $\mathbf{d}^{(l)}$, comprises $(\mathbf{X}, \mathbf{Y}_{\text{rep}}^{(l)}, \mathbf{Y}_{\text{nrep}}, \mathbf{I}, \mathbf{Z})$. Imputations are made independently m times to yield m different partially synthetic data sets, which are released to the public.

3.2.1 Univariate Estimands. Inferences from partially synthetic data sets are based on quantities defined in (1)–(3). The analyst specifies $\hat{Q}$ and $\hat{U}$, acting as if each $\mathbf{d}^{(l)}$ is a random sample of $(\mathbf{X}, \mathbf{Y})$ collected with the original sampling design $\mathbf{I}$. As was shown by Reiter (2003), the analyst uses $\bar{Q}_m$ to estimate Q and $T_p = B_m/m + \bar{U}_m$ to estimate $\text{var}(Q|\mathbf{d}^{(1)}, \ldots, \mathbf{d}^{(m)})$. Inferences are based on t distributions with $\nu_p = (m-1)(1 +$

$\bar{U}_m/(B_m/m))^2$ degrees of freedom. As for fully synthetic data, there are no adjusted degrees of freedom for small n, nor are any likely to be useful.

The formula for T_m includes $(1 + 1/m)B_m$, whereas the formula for T_p includes just B_m/m. This difference is explained by letting $m = \infty$. In the partially synthetic data context, $\bar{U}_\infty$ estimates the variance of the completed data, as is the case in standard multiple imputation. But when $\mathbf{Y}_{\text{inc}} = \mathbf{Y}_{\text{obs}}$, the completed and observed data are identical, so that $\bar{U}_\infty$ by itself estimates var$(Q|\mathbf{D})$. Adding B_∞, as is done in the missing-data case, is not necessary. For finite m, we replace $\bar{U}_\infty$ with $\bar{U}_m$ and add B_m/m for the additional variance due to the use of a finite number of imputations.

3.2.2 Multicomponent Estimands. The logic for significance tests for multicomponent estimands again parallels that summarized in Section 2.1.3 (Reiter 2005b). The derivations of the test statistics use the assumption of equal fractions of missing information across all variables.

The Wald statistic for partially synthetic data is $S_p = (\bar{\mathbf{Q}}_m - \mathbf{Q}_0)^T \bar{\mathbf{U}}_m^{-1} (\bar{\mathbf{Q}}_m - \mathbf{Q}_0)/(k(1 + r_p))$, where $r_p = (1/m)\,\text{tr}(\mathbf{B}_m \times \bar{\mathbf{U}}_m^{-1})/k$. The reference distribution for S_p is an F distribution, F_{k,w_p}, with $\nu_p = 4 + (t - 4)(1 + (1 - 2/t)/r_p)^2$, where $t = k(m - 1)$. The likelihood ratio test statistic is $\hat{S}_p = \bar{L}_0/(k(1 + \hat{r}_p))$, where $\hat{r}_p = (1/t)(\bar{L} - \bar{L}_0)$. The reference distribution for $\hat{S}_p$ is $F_{k,\hat{\nu}_p}$, where $\hat{\nu}_p$ is defined akin to ν_p using $\hat{r}_p$.

In this setting, $1 + r_p$ can be interpreted as the average relative increase in variance across the components of $\mathbf{Q}$ from the partial synthesis. It adjusts the quadratic form so that the test statistic is based on an appropriate estimate of variance.

3.2.3 Imputation of Missing Data and Partially Synthetic Data. When some data are missing, it is logical to impute the missing and partially synthetic data simultaneously, possibly from different distributions, because the replacement imputations should condition on $\mathbf{Z}$. Imputing $\mathbf{Y}_{\text{mis}}$ and $\mathbf{Y}_{\text{rep}}$ simultaneously generates two sources of variability in addition to the sampling variability in $\mathbf{D}$, which the analyst must account for to obtain valid inferences. Neither T_m nor T_p correctly estimates the total variation introduced by the dual use of multiple imputation. The bias of each can be illustrated with two simple examples. Suppose that only one value needs to be replaced but that there are hundreds of missing values to be imputed. Intuitively, the variance of the point estimator of Q should be well approximated by T_m, and T_p should underestimate the variance, because it is missing a B_m. On the other hand, suppose that only one value is missing but there are hundreds of values to be replaced. Then the variance should be well approximated by T_p, and T_m should overestimate the variance, because it includes an extra B_m.

To allow analysts to estimate the total variability correctly, imputers can use a three-step procedure for generating imputations (Reiter 2004, 2007a). First, the imputer fills in $\mathbf{Y}_{\text{mis}}$ with draws from the predictive distribution for $(\mathbf{Y}_{\text{mis}} \mid \mathbf{D})$, resulting in m completed data sets, $\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(m)}$. Second, in each $\mathbf{D}^{(l)}$, the imputer selects the units whose values are to be replaced, that is, those with $Z_j = 1$. Third, in each $\mathbf{D}^{(l)}$, the imputer imputes values $\mathbf{Y}_{\text{rep}}^{(l,i)}$ for those units with $Z_j = 1$, using the predictive distribution for $(\mathbf{Y}_{\text{rep}} \mid \mathbf{D}^{(l)}, \mathbf{Z})$. This is repeated independently r times for $l = 1, \ldots, m$, so that a total of $M = mr$ data sets are generated. Each data set, $\mathbf{d}^{(l,i)} = (\mathbf{X}, \mathbf{Y}_{\text{nrep}}, \mathbf{Y}_{\text{mis}}^{(l)}, \mathbf{Y}_{\text{rep}}^{(l,i)}, \mathbf{I}, \mathbf{R}, \mathbf{Z})$, includes a label indicating the l of the $\mathbf{D}^{(l)}$ from which it was drawn. These M data sets are released to the public.

This procedure is closely related to nested multiple imputation, and the methods for obtaining inferences use the quantities from Section 2.2.1. As described by Reiter (2004), the analyst can use $\bar{Q}_M$ to estimate Q, where $\bar{Q}_M$ is defined as in (5). An estimate of var$(Q|\mathbf{d}^{(1,1)}, \ldots, \mathbf{d}^{(m,r)})$ is $T_{\text{MP}} = (1 + 1/m)B_m - \bar{W}_m/r + \bar{U}_M$, where B_m, $\bar{W}_m$, and $\bar{U}_M$ are as defined in (6)–(8). When n is large, inferences can be based on the t distribution, $(Q - \bar{Q}_M) \sim t_{\nu_{\text{MP}}}(0, T_{\text{MP}})$, with degrees of freedom

$$\nu_{\text{MP}} = \left(\frac{((1 + 1/m)B_m)^2}{(m - 1)T_{\text{MP}}^2} + \frac{(\bar{W}_m/r)^2}{m(r - 1)T_{\text{MP}}^2} \right)^{-1}. \quad (12)$$

Significance tests for multicomponent hypotheses have not yet been developed for this setting.

The behavior of T_{MP} and ν_{MP} in special cases is instructive. When r is large, $T_{\text{MP}} \approx T_m$. This is because each $\bar{Q}^{(l)} \approx Q^{(l)}$, which is the point estimate of Q based on $\mathbf{D}^{(l)}$, so that we obtain the results from analyzing $\mathbf{D}^{(l)}$. When the fraction of replaced values is small relative to the fraction of missing values, $\bar{W}_m$ is small relative to B_m, so that once again, $T_{\text{MP}} \approx T_m$. In both of these cases, ν_{MP} approximately equals ν_m, which is Rubin's (1987) degrees of freedom when imputing missing data only. When the fraction of missing values is small relative to the fraction of replaced values, $B_m \approx \bar{W}_m/r$, so that T_{MP} is approximately equal to T_p with M released data sets.

The distinction between T_M from Section 2.2.1 and T_{MP} mirrors the distinction between T_m and T_p: There is an extra $\bar{W}_m$ in T_M that is not present in T_{MP}. With T_M, the varying imputations within each nest fill in the inexpensive missing values, whereas with T_{MP}, the varying imputations within each nest replace existing values. This distinction results in the different formulas. To illustrate, consider the case with $m = r = \infty$, so that $T_M = B_\infty + \bar{W}_\infty + \bar{U}_\infty$ and $T_{\text{MP}} = B_\infty + \bar{U}_\infty$. In this case T_M estimates var$(Q|\mathbf{D})$, as explained in Section 2.2.1. T_{MP} also estimates var$(Q|\mathbf{D})$, because when $r = \infty$, the setting is equivalent to multiple imputation for missing data. The extra $\bar{W}_\infty$ is not needed in T_{MP}, because the data associated with the replacements were observed, much like an extra B_∞ is not needed in T_p.

Given B_∞ and $\bar{W}_\infty$, for finite m and r, var$(Q|\mathbf{d}^{(1,1)}, \ldots, \mathbf{d}^{(m,r)}) = (1 + 1/m)B_\infty + \bar{W}_\infty/M + \bar{U}_\infty$ (Reiter 2004). As with nested imputation, B_m approximates $B_\infty + \bar{W}_\infty/r$. Plugging in the implied point estimates for B_∞ and $\bar{W}_\infty$ produces T_{MP}.

4. MULTIPLE IMPUTATION FOR MEASUREMENT ERROR/DATA EDITING

Many surveys contain nonsampling errors from sources other than nonresponse bias; for example, respondents can misunderstand questions or provide incorrect information, interviewers can affect respondents' answers, and the recording process can generate errors. Statistical agencies routinely edit collected data, fixing obvious mistakes and inconsistencies. But for some errors there is no deterministic fix, and thus the measurement error is treated as stochastic. Stochastic measurement error can be handled directly using measurement error models or Bayesian posterior simulation approaches. Similar issues plague observational data in many fields; for example, in medical studies, good

measures of exposure may be available only for some records in the file, whereas other records have poorly measured exposures.

Agencies disseminating data to the public generally have more resources and knowledge to correct measurement errors than individual researchers. Thus it is prudent for the agency to make corrections for analysts before dissemination. The multiple-imputation framework is well suited for this task; the agency replaces values with stochastic measurement errors with draws from probability distributions designed to correct the errors, creating "ideal" data sets. Analysts of these data sets can use standard methods rather than measurement error techniques, because the adjustments for measurement error are automatically included in the ideal data sets. Releasing multiply-imputed ideal data sets allows analysts to incorporate the uncertainty due to simulation. For examples of the multiple imputation approach to data editing, see Winkler (2003) and Ghosh-Dastidar and Schafer (2003), who used multiple imputation to handle missing data and measurement error simultaneously. Individual researchers can follow similar strategies for measurement error correction, as was done in medical contexts by Raghunathan and Siscovick (1998), Yucel and Zaslavsky (2005), Cole et al. (2006), and Raghunathan (2006).

As with all applications of multiple imputation, the analyst estimates the parameters of interest and their associated measures of uncertainty in each ideal data set. But how to combine the point and variance estimates is not obvious; does Rubin's (1987) variance estimator T_m apply, or is a different combining rule needed? The answer depends on what distribution is used for imputations and what data are used for analyses, as we now illustrate.

For simplicity, suppose that the observed data compose one variable $\mathbf{X}$ without measurement error and one variable $\mathbf{E}$ subject to measurement error. Let $\mathbf{Y}$ be the unknown, true values associated with $\mathbf{E}$. The observed data are $\mathbf{D} = (\mathbf{X}, \mathbf{E}, \mathbf{I})$. Assume that there are no missing values in $\mathbf{D}$. Measurement error corrections use information about the relationship between $\mathbf{Y}$ and $\mathbf{E}$, for example, from a validation sample of records on which both the true and with-error values are measured. The validation sample could comprise records from an external file or records from $\mathbf{D}$.

Suppose that the validation sample is an external file, $\mathbf{D}_{\text{val}} = (\mathbf{X}_{\text{val}}, \mathbf{Y}_{\text{val}}, \mathbf{E}_{\text{val}})$. The imputer simulates values of $\mathbf{Y}$ in $\mathbf{D}$ by drawing from $f(\mathbf{Y}|\mathbf{D}, \mathbf{D}_{\text{val}})$ to obtain the ideal data sets $\mathbf{D}^{(l)} = (\mathbf{X}, \mathbf{Y}^{(l)}, \mathbf{E})$, for $l = 1, \ldots, m$. One approach to analyzing these data is to append $\mathbf{D}_{\text{val}}$ to each $\mathbf{D}^{(l)}$ without distinction, so that the analyses are based on $\mathbf{D}^{(*l)} = (\mathbf{D}^{(l)}, \mathbf{D}_{\text{val}})$, for $l = 1, \ldots, m$. This essentially treats the measurement error imputations as completions of missing values of $\mathbf{Y}$ in $(\mathbf{D}, \mathbf{D}_{\text{val}})$, so that Rubin's (1987) theory can apply (after adjustment of any original survey weights) and T_m is the appropriate variance estimator. In the public-use context, data producers can release each $\mathbf{D}^{(*l)}$ without $\mathbf{E}$, because analyses should be based on $\mathbf{Y}$. By similar logic, analyses with internal validation samples also use T_m.

On the other hand, suppose that $\mathbf{D}_{\text{val}}$ cannot be released to the public and is used solely for correcting measurement error; that is, analysis must be based on $\mathbf{D}^{(l)}$ for $l = 1, \ldots, m$. This does not fit cleanly into the missing-data setup, which calls the use of T_m into question. This is evident in the work of Rubin and Schenker (1987) and Clogg et al. (1991), who used multiple imputation to recode occupations in an example that fits this context and found find that T_m overestimates variances. In a way, releasing only the $\mathbf{D}^{(l)}$s is akin to synthesizing replacement values for $\mathbf{Y}$, as is done in the context of disclosure limitation. But the parameter values of the imputation model are estimated from $\mathbf{D}_{\text{val}}$ rather than from $\mathbf{D}$, which differs from partial synthesis. This suggests that inferential techniques other than those based on Rubin's (1987) rules or Reiter's (2003) rules are appropriate in this setting. As of this writing, the proper combining rules for this context have not yet been developed.

As suggested by Harel and Schafer (2003), versions of nested multiple imputation might be used to handle missing data and editing simultaneously. The results of Section 2 suggest that T_M should be appropriate when the completed data include both the original and validation samples. It is not clear what variance is appropriate when the completed data include only the original sample.

5. OTHER APPLICATIONS AND OPEN RESEARCH TOPICS

The previous sections have described adaptations of multiple imputation within the context of an organization releasing survey data. By no means is multiple imputation limited to this context, however. Many problems fit into the incomplete-data framework. Among its numerous applications, multiple imputation has been used to analyze data in coarse categories, as occurs with age heaping (Heitjan and Rubin 1990) or interval censored data (Pan 2000); to estimate the distribution of times from human immunodeficiency virus seroconversion to AIDS (Taylor et al. 1990); to handle missing covariates in case-control studies involving cardiac arrest (Raghunathan and Siscovick 1996); to integrate data from different sources into one file (Gelman, King, and Liu 1998; Rassler 2003); to estimate latent abilities in educational testing (Mislevy, Beaton, Kaplan, and Sheehan 1992); to reduce respondent burden by asking subsets of questions to different respondents (Thomas, Raghunathan, Schenker, Katzoff, and Johnson 2006); to impute missing outcomes in causal studies, for example, to handle noncompliance in anthrax vaccine studies (Rubin 2004); and to select models in the presence of missing values (Yang, Belin, and Boscardin 2005; Ibrahim, Chen, Lipsitz, and Herring 2005).

All multiple-imputation analyses require combining the point and variance estimates from the imputed data sets, but the rules for combining them depend on what is known in the conditioning, which in turn determines what the various multiple imputation quantities estimate. Using the proper conditioning results in variance formulas for the data confidentiality contexts that differ from the missing-data context.

Many open research topics remain. These include (a) further investigating reference distributions for large-sample significance tests of multicomponent hypotheses for nested multiple imputation, (b) developing large-sample significance tests of multicomponent significance tests for the version of nested multiple imputation presented in Section 3.2.3, (c) developing small-sample degrees of freedom for the t distributions used in inferences for nested multiple imputation and for multiple imputation for data confidentiality (although these techniques are most likely to be applied in large samples), and (d) developing the proper combining rules for measurement error settings

when only the original data are available for analysis. In addition, it would be profitable to extend the two-stage procedure in nested multiple imputation to more than two stages. This could enable data disseminators to handle nonresponse, editing, and data confidentiality simultaneously in a principled manner.

As these research topics and existing applications indicate, even 20 years after Rubin's seminal book on multiple imputation, we can expect continued adaptation of multiple imputation to handle challenging statistical problems.

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