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3 **Partitioning error components for accuracy-assessment of near-**
4 **neighbor methods of imputation.**
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17 **Acknowledgement**

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22 that the result is much improved, but any remaining deficiencies are certainly our
23 responsibility.

24 **Abstract:** Imputation is applied for two quite different purposes: to supply missing data to complete a
25 data set for subsequent modeling analyses, or to estimate sub-population totals. Error properties of the
26 imputed values have different effects in these two contexts. We partition errors of imputation derived from
27 similar observation units as arising from three sources: observation error, the distribution of observation
28 units with respect to their similarity and pure error given a particular choice of variables known for all
29 observation units. Two new statistics based on this partitioning measure the accuracy of the imputations,
30 facilitating comparison of imputation to alternative methods of estimation such as regression and
31 comparison of alternative methods of imputation generally. Knowing the relative magnitude of the errors
32 arising from these partitions can also guide efficient investment in obtaining additional data. We illustrate
33 this partitioning using three extensive data sets from western North America. Application of this
34 partitioning to compare near-neighbor imputation is illustrated for Mahalanobis- and two canonical
35 correlation-based measures of similarity.

36 **Keywords:** Most-similar-neighbor, *k*-nn inference, missing data, landscape modeling.

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38 **Introduction**

39 Imputation methods are important tools for completing data sets in which some observation units
40 lack observed values for a portion of their attributes. The objective is to impute a value as close to “truth”
41 for each missing value in the observation unit as if it were examined in great detail for all attributes.
42 Criteria for imputations to support this objective are essentially different from criteria for estimates of
43 population totals. The difference is that pure error, rather than being a nuisance, is of real value for
44 subsequent resource analyses and displays. These analyses are often non-linear optimizations or
45 simulations. For them to be realistic, the structure of the variances and covariances among attributes
46 inherent in the population should be preserved in the data set. Even for display purposes, omission of pure
47 error will cause the range of the displayed values to be contracted. Unfortunately, these inherently useful
48 variances may be combined with variances attributable to the methodology used in the sampling and
49 imputation processes. This mixture complicates choice among analytical methods for imputation. In this
50 report we provide statistics based on a partitioning of the error components which facilitate finding a closer

51 approximation of “truth”. We partition imputation errors independently for each variable in the data set
 52 although the joint distribution of their error components would be of interest for some applications.

53 Imputation uses values of variables measured for all observation units (X 's) to guide the
 54 imputation of values of Y 's that are measured only for a sample subset of the observation units (the
 55 *Reference* set) to those units for which the Y 's are missing (the *Target* set). Both X_i and Y_i may be vectors
 56 of attributes for the i^{th} observation unit. Near-neighbor imputation selects units from the reference set to
 57 serve as surrogates for members of the target set using a measure of similarity based on the X 's. Choice of
 58 a particular measure of similarity, in turn, may depend on the relation of the Y 's to the X 's. Elements of Y_i
 59 and X_i , y_i and x_i , will be subscripted only to identify the i^{th} observation unit. T and R will be used as
 60 additional subscripts when it is relevant to indicate that a Reference observation unit is being used as if it
 61 were a Target unit (hence a “pseudo-target”). Unit identifying subscripts (i or j) will be omitted when the
 62 variables are referred to collectively. $\text{Var}(\cdot)$ capitalized will be used for expected values, lower case $\text{var}(\cdot)$
 63 for statistics calculated from the data.

64 Imputation from near-neighbor observations is often used for classification. However, when the
 65 “classes” are arbitrary intervals on scales of essentially continuous variables, we argue that the imputation
 66 should be based directly on the scales of the underlying continuous variables. If classes are needed for
 67 display purposes, the classification algorithm should use the imputed data. We will not consider in this
 68 paper errors in classification in which the classes are inherently discrete, requiring the concept of
 69 “membership”. For discrete classes, other methods for classification such as using a discriminant function
 70 may be more appropriate than near-neighbor. For example, classification by a discriminant function may
 71 assign different classes to members of a target/reference pair of near neighbors because the discriminating
 72 boundary passes between them whereas near-neighbor imputation would assign the target to the same class
 73 as the reference member of the pair. However, there is a parallel process of partitioning the error sources in
 74 imputation of discrete variables that is beyond the scope of this paper. .

75 Error properties of estimates derived from imputation differ from those of regression-based
 76 estimates because the two methods include a different mix of error components. For example, the
 77 reference-set data may not be beyond reproach because of measurement error. These error properties
 78 influence how we evaluate quality of the imputations, compare alternative methods for imputation and

79 invest in data collection. Commonly computed statistics that compare imputed values to those of a
80 presumably similar observation unit mask methodological differences in this cloud of variation. We
81 address this problem by partitioning the variation into components that can be estimated from the reference
82 set. Then, new statistics based on this partitioning are presented for assessing the accuracy of imputation
83 methods.

84 Several questions may be answered using these error components:

- 85 1) How does the accuracy of imputed Y 's compare to accuracy of estimates from regression, stratum
86 means or other model-based estimates?
- 87 2) How large is the error caused by imputing values to a target unit from reference units where there is
88 substantial difference in their X 's? Is there room for improvement by obtaining additional
89 reference observations to fill gaps in their distribution? How is this error component affected by
90 the choice of a particular measure of similarity?
- 91 3) How is the accuracy of imputation affected by the choice of variables and their transformations?
- 92 4) What is the effect on imputed values of pooling k reference observations?
- 93 5) How do the measurement accuracies compare to components of variation from other sources?
- 94 6) Would investments in additional data be more efficient if used to obtain information on variables to be
95 added to the target set (new X 's), to refine the estimates of the X 's already included, or to obtain
96 data on additional units for the reference set?

97 Resolution of these questions requires quantitative estimates of the sources of imputation error.
98 These estimates can be obtained from the information in the n observation units in the reference data. In
99 analysis of data in the reference-set data, although we will use some of the data as if they were targets,
100 there is no difference in their approximation of "truth", no intrinsic differences between "observed" and
101 "predicted". We are simply describing the properties of differences between members of pairs of
102 observations. When the value to be imputed is a weighted average of k near neighbors, then its error
103 properties are derived from the error properties of the k separate pairs and the weights defined by the
104 particular k -nn procedure.

105 Bootstrap and cross-validation methods for answering some of these questions have been
106 developed for imputation methods other than near-neighbor (Shao and Sitter 1996) or for classification

107 with k -nn (Mullin and Sukthankar 2000). Neither of these papers has addressed the problem of partitioning
108 the errors as to sources. Moeur and Stage (1995) used data-splitting and jackknife methods to evaluate
109 capability of Most Similar Neighbor (MSN) to reproduce the variance and covariance structure of the
110 reference data and to compare error rates to those obtained by stratified sampling and regression. Their
111 analyses of errors also included variation in the coefficients in the measure of similarity caused by
112 sequentially omitting 1.7% of their data as well as the difference between the observed and imputed Y
113 values for the pair selected by the calculated similarity measure.

114 Splitting data into “calibration” and “validation” subsets, which was intended to reduce bias in
115 error estimates, introduces a different bias into estimates of imputation errors. The withheld reference
116 observations in sparsely-represented parts of X -space could have supplied imputations for nearby target
117 observations. In the analysis of imputation error, however, those targets will be paired with a more remote
118 reference observation, thereby increasing the **estimated** error. A further disadvantage of the jackknife
119 procedure is that it may increase the estimate of error by increasing the mean-square bias. Targets in the
120 midst of a cloud of reference observations may be paired with an observation from any direction. Targets
121 at the edge of a cloud, however, will likely be paired with a more central point. If there is a trend in the Y 's
122 with distance from the center of the cloud, then the asymmetry of direction to the reference introduces bias
123 in the imputed value. Withholding data increases this bias unnecessarily. The jackknife procedure using
124 a single reference observation as if a target minimizes this bias by using the full range of data (except for
125 the single reference unit). Other methods to reduce this bias in k -nn imputation have been evaluated by
126 Malinen (2003).

127 A statistic commonly used to evaluate imputation error estimates the root-mean-square differences
128 between reference and target observations by withholding each observation unit in the reference set while
129 searching for its similar neighbor in the remainder of the reference set. The term RMSE (root-mean-square
130 error) used for this statistic is unfortunate (e.g. Moeur and Stage 1995, Crookston et al. 2002). The term as
131 used in imputation includes different components of error than the same term used in a regression or
132 sampling context. Therefore, we use the term Mean Squared Difference (MSD) for the statistic describing
133 squared differences in a pair of similar observations. Thus, our partitioning is applicable for evaluating any
134 of the near-neighbor methods of imputation that are judged on the basis of sums of squared errors.

135 We use the term “distance” for the value produced by the function measuring dissimilarity
 136 between the i^{th} and j^{th} pair of observation units. Although Podani (2000) cites more than 60 distance
 137 functions, those most widely used for imputation are of the quadratic form:

$$138 \quad d_{ij}^2 = (\mathbf{X}_i - \mathbf{X}_j) \mathbf{W} (\mathbf{X}_i - \mathbf{X}_j)' \quad (1)$$

139 where:

140 \mathbf{X}_i is the $(1 \times p)$ vector of \mathbf{X} -variables for the i^{th} target observation unit,

141 \mathbf{X}_j is the $(1 \times p)$ vector of \mathbf{X} -variables for the j^{th} reference observation unit, and

142 \mathbf{W} is a $(p \times p)$ symmetric matrix of weights.

143 If the weight matrix, \mathbf{W} , is the diagonal identity matrix, then we have a simple Euclidean distance
 144 (squared). As a variation of Euclidean distance, some analysts empirically vary the diagonal elements to
 145 improve the imputation. If correlations among the variates are to be considered, then the inverse of their
 146 correlation matrix is used for \mathbf{W} to produce a Mahalanobis distance—a distance function that plays a key
 147 role in estimating the error components. MSN distances are of the same form with \mathbf{W} derived from
 148 analyses of canonical correlation (Moeur and Stage 1995), canonical regression (Stage and Crookston
 149 2002) or of canonical correspondence (Ohmann and Gregory 2002). With a simple transformation of the
 150 \mathbf{X} 's to $x_i / \sqrt{\sum_{i=1}^p x_{il}^2}$ the quadratic form with identity matrix for \mathbf{W} also includes spectral analysis
 151 imputation as used by Sohn et al. (1999).

152 Our following presentation is in four sections: 1) defining error sources in the process of imputation, 2)
 153 partitioning MSD into components arising from these sources, 3) presenting some new statistics based on
 154 the partitioning relevant to the key questions stated above, and 4) applying these statistics to three extensive
 155 data sets.

156 **Components of Error**

157 Variation in imputed values arises from both natural variability of attributes of the ecosystem, and
 158 from the measurement and analytical procedures used to describe the ecosystem. While natural variability
 159 is useful in analyses requiring the completed data set, variation introduced by measurement and analytical
 160 procedures is a nuisance to be reduced.

161 Imputation error arises from four sources for a given set of \mathbf{X} and \mathbf{Y} variables:

162 1) Measurement errors of the Y 's in the reference set. These errors are defined as:

$$163 \quad \varepsilon_{Yj} = y_j - y_j^* \quad (2)$$

164 in which the starred variables represent the true, but unknown, values. The ε_{Yj} are not properties
 165 of the ecosystem being described, but rather, properties of the accidents of how we observed it.
 166 The measurement errors may arise from using a sample-based estimate as if it were a complete
 167 census within the j^{th} unit, from changes during elapsed time since observation, from lack of
 168 standardization among different observers or their instruments, or any combination of such causes.
 169 These errors often are assumed to be zero (e.g. Moeur and Stage 1995). We now relax that
 170 assumption because in some applications, errors from this source have been quite large relative to
 171 total error. We assume that the measurement errors can be rendered unbiased and are independent
 172 of the true y_j^* and of the observed X 's.

173 2) Pure error. That there exists a relation between the Y 's and the X 's is a key premise of near-neighbor
 174 inference. For a given set of X 's the departure of an element of Y_j^* from the underlying true, but
 175 unknown, model is termed pure error.

$$176 \quad \varepsilon_{Pj} = y_j^* - g(X_j) \quad (3)$$

177 Magnitude of the pure error (ε_{Pj}) depends on the particular choice of Y - and X -variables. By
 178 definition, pure error, which arises from effects not associated with the X 's is independent of the
 179 X 's and has zero expectation. Examples of omitted factors are myriad, but would include
 180 predicting species composition (the Y 's) from Landsat spectra (the X 's), but omitting elevation as
 181 an additional X -variable that might improve the imputation.

182 Not so obvious as a source of pure error would be the effect of lack of accurate
 183 registration between the Y -variable observation units located on the ground and the paired X -
 184 variable observation units from a remote sensing platform. In effect, the observed values of X_j
 185 from a complete census from the erroneous position are just a differently defined variable for
 186 imputation than the X_j 's from a properly registered observation unit. Therefore, variation from
 187 lack of registration would contribute to pure error that might be reduced by improving registration.

188 From [2] and [3]

$$189 \quad y_j = g(X_j) + \varepsilon_{Pj} + \varepsilon_{Yj} \quad (4)$$

190 in which the error components include measurement error (ε_{Yj}), and pure error (ε_{Pj}). Pure error
 191 and measurement error are inseparable in many data sets. To estimate pure error alone requires an
 192 external estimate of the measurement error. For example, if the observation unit is a spatial
 193 polygon represented by the mean of each of the attributes over a number of plots within the
 194 polygon, then the estimated variance-of-the-mean would provide the sampling portion of
 195 measurement variance to be subtracted to leave pure error.

196 3) Factors affecting the availability and similarity of reference observation units to serve as surrogates for
 197 the target units. This component depends on both the choice of a distance function and on the
 198 distribution of observation units in the space spanned by the X -variables. Ideally, all the target data
 199 should be within the span of the reference data. The denser the data, the shorter will be the average
 200 distance between a target unit and its nearest surrogate in the reference set. And shorter distances
 201 usually imply greater similarity. The magnitude of this effect can be appreciated by comparing the
 202 distribution of distances to nearest neighbors among the reference data to the distribution of
 203 distances from each target observation to its nearest neighbor in the reference set. The distances
 204 between the real targets and their near neighbors in the reference set usually would be, on average,
 205 shorter than the distances among members of the reference set. Thus, estimated errors based only
 206 on the reference set will be biased upward. Effects of the density and range of the data apply to all
 207 methods of imputation and are determined by the inventory design.

208 4) And, finally, the choice of k , the number of reference observations and their relative weights in k -nn
 209 methods of estimating Y 's as a weighted average of k near neighbors.

210 Error analyses we propose are based upon the data in the reference set. Inferences about the error
 211 properties of the estimates for the entire population based on these analyses depend on the extent to which
 212 the reference set represents the target set. As with inferences about any population parameter, appropriate
 213 randomization is a prerequisite to the assumption that the partitioning of error based on the reference set
 214 will apply to imputations for the real target set.

215 **Imputation Error Statistics Based on the Reference Set**

216 In the imputation context $\sum_i (y_{Ti} - y_{Ri})^2 / n$ is the statistic commonly reported as "squared error" based
 217 on the n observation units in the reference set. We use the term Mean Square Difference (MSD) for it to

218 emphasize that it is not an “error”—rather it is simply a function of the difference between two co-equal
 219 observations, neither of which is any more “true” than the other. In this and the expressions to follow, the
 220 subscript j identifies the reference observation to be imputed to the i^{th} pseudo-target observation unit. For
 221 each observation unit i , the value of j is determined by the minimum of d_{ij}^2 in (1). In k -nn imputation y_{Rj} is
 222 replaced by an average of k values of y_m using a weighting rule for the particular flavor of k -nn inference,
 223 where m is from the set of indices of the k observations selected as near-neighbors. We will develop the
 224 partitioning of error components for $k = 1$ because the notation is much more compact. However, the
 225 extension to $k > 1$ introduces no new concepts and will be treated when we discuss the choice of k as an
 226 error source.

227 Each member of the pairs being averaged in MSD includes stochastic components which do not
 228 change whether the observation unit is playing the role of target or reference. Each pair also includes a
 229 component determined by the distribution of the X 's within the reference set. Thus, the statistics we
 230 compute are conditional on distribution of X 's in the reference set—and may be used to guide decisions on
 231 how or whether to augment that reference set. The stochastic components, pure error and measurement
 232 error, are assumed to be drawn from distributions having zero mean and zero covariance. Therefore, for
 233 both stochastic error sources:

$$234 \quad E[\varepsilon_{pj}] = E[\varepsilon_{yj}] = 0; \text{Var}(\varepsilon_p) = E[\sum_j \varepsilon_{pj}^2/n]; \text{Var}(\varepsilon_y) = E[\sum_j \varepsilon_{yj}^2/n]; E[\varepsilon_{yj}\varepsilon_{pj}] = 0. \quad (5)$$

235 We will define the estimated variances of the stochastic error terms $\text{var}(\varepsilon_p)$ and $\text{var}(\varepsilon_{yj})$ as the
 236 average over the reference set, dividing by n rather than $(n-p)$ because the error terms are defined relative to
 237 true values rather than from a computed mean.

238 We first introduce the measurement error from (2) into an addend of MSD:

$$239 \quad (y_{Ti} - y_{Rj})^2 = (y_{Ti}^* + \varepsilon_{yi} - y_{Rj}^* - \varepsilon_{yj})^2 \quad (6)$$

240 Expanding (6) on the starred terms from (3) we have:

$$241 \quad (y_{Ti} - y_{Rj})^2 = [g(\mathbf{X}_{Ti}) + \varepsilon_{pi} + \varepsilon_{yi} - g(\mathbf{X}_{Rj}) - \varepsilon_{pj} - \varepsilon_{yj}]^2 \quad (7)$$

242 Averaging over the n pseudo target units (y_{Ti}) in (7) assuming ε_{pj} and ε_{yj} are independent of each other and
 243 using (6), the expectation of MSD becomes:

$$244 \quad E[\text{MSD}] = E[\sum_i (y_{Ti} - y_{Rj})^2/n] = \sum_i [g(\mathbf{X}_{Ti}) - g(\mathbf{X}_{Rj})]^2/n + 2 \text{Var}(\varepsilon_y) + 2 \text{Var}(\varepsilon_p) \quad (8)$$

245 The term: $\sum_i [g(X_{Ti}) - g(X_{Rj})]^2/n$ in (8) is, therefore, the error component arising from the distance between
 246 a pseudo-target point and its selected surrogate reference point. Note that in addition to the distance error
 247 component, the other error variances are included twice in MSD.

248 *Estimating pure error and measurement error*

249 In a regression context, sums of squares for pure error plus measurement error can be estimated
 250 from differences between the y 's for observations having the same X 's. The corresponding concept in
 251 imputation is for observations separated by zero Mahalanobis distance. Mahalanobis distances are
 252 calculated in the space spanned by the normalized, but uncorrelated X -variables. The Mahalanobis distance
 253 was selected because other distance functions may transform the X 's such that the dimension of the space
 254 spanned by the transformed X 's is of lower dimension than the original X -space. Zero distances in the
 255 space of reduced dimension would not necessarily indicate that X_{Ti} for a target unit is identical to the X_{Rj}
 256 for the selected reference unit. We argue that an estimate of the twice the sum of variances of pure error
 257 and measurement error can be obtained by averaging the squared differences for some fraction of the units
 258 with short Mahalanobis distances. We call this estimate MMSD(0), adding an initial M and the (0) to
 259 suggest it is derived from pairs of units with Mahalanobis distances of close to zero. Using (8),

$$260 \quad E[\text{MMSD}(0)] = 2 \text{Var}(\varepsilon_P) + 2 \text{Var}(\varepsilon_Y) + \text{bias} \quad (9)$$

261 where the bias equals the amount by which the mean of the squared distance component (as in (8) but
 262 averaged over only the observation units with close-to-zero distances) differs from zero. Note that whereas
 263 MSD may be derived from any of the many distance functions, MMSD(0) always uses Mahalanobis
 264 distance.

265 The estimate is biased by the average of $[g(X_{Ti}) - g(X_{Rj})]^2$ in MMSD(0). The bias might be
 266 reduced by regressing the values of $(y_{Ti} - y_{Rj})^2$ on their distances where the near-neighbor pairings are
 267 determined using a Mahalanobis distance function. The intercept of this regression may provide an
 268 improved estimate of MMSD(0) by extrapolation to zero distance. However, for some obstreperous Y -
 269 variables, the squared deviations decline with increasing distance so that the intercept is above the mean.
 270 This circumstance indicates that the X 's do not measure similarity for those elements of Y or that their
 271 stochastic components are heteroskedastic.

272 *Estimating distance component*

273 The distance component depends only on the range and density of the X 's and on the measure of
 274 similarity used to select the near neighbor(s). Equation (8) showed that $E[\text{MSD}]$ is comprised of the
 275 distance component, $\sum_i [g(\mathbf{X}_{Ti}) - g(\mathbf{X}_{Rj})]^2/n$ plus two times the sum of variances of pure error and
 276 measurement error. Therefore, the distance component of MSD can be estimated by subtracting twice the
 277 components of pure error and measurement error estimated by (9) in the previous section:

$$278 \quad \sum_i [g(\mathbf{X}_{Ti}) - g(\mathbf{X}_{Rj})]^2/n \approx \text{MSD} - \text{MMSD}(0). \quad (10)$$

279 This error component does not depend on the specific functional form of the relations of the Y 's to the X 's
 280 so any model lack-of-fit is not involved. Therefore, it applies equally to near-neighbor pairing of units
 281 without regard for the distance function. Unfortunately, $\text{MSD} - \text{MMSD}(0)$ is not constrained to be positive
 282 if $[g(\mathbf{X}_{Ti}) - g(\mathbf{X}_{Rj})]^2$ decreases with increasing distance.

283 Using the partitioning to illuminate key questions

284 We now revisit key questions posed in the introduction, developing some new statistics based on
 285 the partitioning to provide answers.

286 *Accuracy of imputed values*

287 The fundamental variance statistic in sampling inference compares an estimate with its true value.
 288 In our notation that comparison is $y_{Rj} - g(\mathbf{X}_i)$ for k equal to one. Therefore, we propose that the efficacy of
 289 the imputation process should be based on a statistic we term the Standard Error of Imputation (SEI).

$$290 \quad \text{SEI}^2 = \sum_i [y_{Rj} - g(\mathbf{X}_{Ti})]^2 / n \quad i = 1, \dots, n \text{ and } j \text{ minimizes } d_{ij}^2 \quad (11)$$

291 Unfortunately, the addends in the bracket of SEI cannot be computed directly from the data in the reference
 292 set because the true value, $g(\mathbf{X}_{Ti})$, is not directly observable. The proposed aggregate statistic (11),
 293 however, can be obtained by replacing the "estimate" y_{Rj} in (11) with (4) evaluated for the j^{th} reference unit.

$$294 \quad \text{SEI}^2 = \sum_i [g(\mathbf{X}_{Rj}) + \varepsilon_{pj} + \varepsilon_{Yj} - g(\mathbf{X}_{Ti})]^2 / n \quad (12)$$

295 Then averaging with the same assumptions of error independence used in deriving (8).

$$296 \quad E[\text{SEI}^2] = E[\sum_i [y_{Rj} - g(\mathbf{X}_{Ti})]^2 / n] = \sum_i [g(\mathbf{X}_{Rj}) - g(\mathbf{X}_{Ti})]^2 / n + \text{Var}(\varepsilon_p) + \text{Var}(\varepsilon_Y) \quad (13)$$

297 which differs from MSD (8) by omitting the terms for the variances of pure error and sampling error arising
 298 from the target members of (11). If the distance component of $\text{MMSD}(0)$ can be assumed to be trivially
 299 small when (8) is averaged over only the shorter distances, then:

$$300 \quad E[\text{SEI}^2] = E[y_{Rj} - g(\mathbf{X}_{Ti})]^2 \approx \text{MSD} - \text{MMSD}(0)/2. \quad (14)$$

301 *Imputation compared to estimates using $f(X)$*

302 The regression model is: $y_j^* = f(X_j) + \varepsilon_j$ where the ε_j includes pure error, and the lack of fit of the
 303 assumed model. The regression model could be, but is not limited to the familiar linear parameterization
 304 $f(X_j) = \mathbf{B}\mathbf{X}'$. Alternatively it could be a nonlinear or nonparametric regression model or a collection of
 305 means for strata defined by the \mathbf{X} 's. The true model $y_j^* = g(X_j) + \varepsilon_{pj}$ differs from the regression model by
 306 the lack-of-fit of the regression model:

$$307 \quad \varepsilon_{L(X_j)} = g(X_j) - f(X_j). \quad (15)$$

308 The error statistic commonly calculated for a regression is the Standard Error of Estimate (SEE) (ignoring
 309 the reduction of the divisor by the number of estimated parameters):

$$310 \quad \text{SEE}^2 = \sum_j (y_j - f(X_j))^2 / n. \quad (16)$$

311 We assume that the lack-of-fit will sum to zero for the particular \mathbf{X} 's (certain if $f(\mathbf{X})$ is fit by least-squares
 312 and includes an intercept) in the Reference set.

313 Then, from (2), (3) and (15):

$$314 \quad (y_j - f(X_j))^2 = (\varepsilon_{pj} + \varepsilon_{Y_j} + \varepsilon_{L(X_j)})^2 \quad (17)$$

315 The terms for the model lack-of-fit were assumed to be independent of the \mathbf{X} 's and of ε_{pj} and ε_{Y_j} so $E(\text{SEE}^2)$
 316 is the sum of these three sources:

$$317 \quad E[\text{SEE}^2] = E[\sum_j (y_j - f(X_j))^2 / n] = \text{Var}(\varepsilon_p) + \text{Var}(\varepsilon_Y) + \sum_j [\varepsilon_{L(X_j)}^2] / n \quad (18)$$

318 Comparison of $E[\text{SEI}^2]$ in (13) with $E[\text{SEE}^2]$ in (18) shows that they differ only by the substitution of the
 319 distance component, $\sum_i [g(\mathbf{X}_{R_i}) - g(\mathbf{X}_{T_i})]^2 / n$, in imputation error variance for lack of fit, $\sum_j (\varepsilon_{L(X_j)})^2 / n$, in
 320 regression estimation error variance.

321 Rearranging (18) and substituting (9):

$$322 \quad \sum_j [\varepsilon_{L(X_j)}^2] / n = E[\text{SEE}^2] - E[\text{MMSD}(0)/2] \quad (19)$$

323 The ideal contents for a data set for subsequent analysis would be \mathbf{Y}_j^* which would have variance
 324 about $g(\mathbf{X}_j)$ of $\text{Var}(\varepsilon_p)$. Unfortunately, the best imputation can do for a given data set is \mathbf{Y}_{T_j} which differs
 325 from the ideal by inclusion of measurement error variance plus the distance component. Alternatively,
 326 regression estimation could supply as estimates $f(\mathbf{X}_j)$ plus a random element drawn from a distribution with

327 variance $\text{Var}(\varepsilon_p)$. Using (4) and (15) and the independence of pure error relative to the model lack-of-fit,
 328 these estimates would have variance about $g(X_j)$ given by:

$$329 \quad E[\Sigma_j [f(X_j) + \varepsilon_{pj} - g(X_j)]^2/n] = \Sigma_j (\varepsilon_{L(X_j)})^2/n + \text{Var}(\varepsilon_p) = E[\text{SEE}^2] - \text{Var}(\varepsilon_Y) \quad (20)$$

330 which can be estimated by:

$$331 \quad \Sigma_j [f(X_j) + \varepsilon_{pj} - g(X_j)]^2/n = \text{SEE}^2 - \text{MMSD}(0)/2 + \text{var}(\varepsilon_p) = \text{SEE}^2 - \text{var}(\varepsilon_Y) \quad (21)$$

332 Subtracting (21) from (14) the comparison of SEI^2 to (21) becomes:

$$333 \quad E[y_{Rj} - g(X_{Ti})]^2 - E[\Sigma_j [f(X_j) + \varepsilon_{pj} - g(X_j)]^2/n] \approx \text{SEI}^2 - [\text{SEE}^2 - \text{var}(\varepsilon_Y)] \quad (22)$$

334 which is the same as (13)–(18) plus pure error variance:

$$335 \quad \Sigma_i [g(X_{Rj}) - g(X_{Ti})]^2/n - [\Sigma_j (\varepsilon_{L(X_j)})^2/n + \text{var}(\varepsilon_p)] \quad (23)$$

336 Thus, the variance of the imputed values would be greater than regression estimated values for each y if
 337 (22) or equivalently if (23) is greater than zero. However, the regression alternative would not guarantee
 338 that the true correlation among the estimated y 's within each observation unit would be retained.

339 *Effects of distribution of X's*

340 The second key question concerning distributions of the X 's and alternative measures of similarity
 341 is addressed by considering the distance component of MSD: $\Sigma_i [g(X_{Ti}) - g(X_{Rj})]^2/n$. This error component
 342 should be made as small as possible either by adding new members to the reference set to reduce average
 343 distance between target units and their similar reference unit(s) or by adopting a better measure of
 344 similarity or both.

345 An important consideration in accuracy assessment based only on the reference observation units
 346 is the relation between the distribution of the X 's in the target set in relation to that distribution in the
 347 reference set. Ideally, the reference set would completely cover the ranges of X -variables of the target set
 348 and have an approximately uniform distribution over the range of the combined sets. The distance function
 349 being invoked may weight variation of some of the X 's heavier than others, thereby stretching and rotating
 350 the space spanned by the X 's. Therefore, the overall effect the distributions should be compared in terms
 351 of the distances between reference unit and the pseudo-target unit of the reference pairs of near neighbors
 352 and the distances between the paired reference unit and the real target for which imputations are required.

353 A statistic sensitive to the merits of alternative distance functions would reduce the influence of
 354 pure error and sampling error to focus on $\sum_i [g(\mathbf{X}_{Ti}) - g(\mathbf{X}_{Rj})]^2$. At short distances, the values of $(y_{Ti} - y_{Rj})^2$
 355 are dominated by the pure error plus sampling error. Therefore, a better alternative to MSD calculated as
 356 the average over all references is to average only using pairs separated by the longer distances.

357 *Choice of X's and their transformations*

358 How these decisions affect MSD for a particular variable y depends on the choice of the weight
 359 matrix \mathbf{W} in (1). If \mathbf{W} gives little or no weight to a particular x , then that x is effectively omitted.
 360 Conversely an x may be heavily weighted because of its contribution to $g(\mathbf{X})$ for other y 's. Then, even
 361 though a subset of the x 's may effectively predict the y under consideration, their contribution will be
 362 diluted by differences in the extraneous x 's and MSD for that element, y of \mathbf{Y} will be dominated by pure
 363 error and measurement error to such an extent that $[g(\mathbf{X}_{Ti}) - g(\mathbf{X}_{Rj})]^2$ may decrease with distance. If it does
 364 decrease, then the distance component and model lack-of-fit will be under-estimated.

365 Transformations in variables are typically invoked to simplify a model such as $y=f(\mathbf{X})$ and to
 366 render errors more homogeneous. Consideration of (8) and (10) and (17) as estimates of sources of
 367 imputation errors from the three sources shows that transformations of the \mathbf{X} -variables, while modifying the
 368 fit of the regression model $y=f(\mathbf{X})$, affect MSD only through the distance component, $\sum_i [g(\mathbf{X}_{Ti}) - g(\mathbf{X}_{Rj})]^2/n$,
 369 and homogeneity of the pure error component. Transformations affect the distance component through the
 370 selection of surrogates, which in turn depend on the choice of the weight matrix \mathbf{W} . In dense regions of the
 371 space spanned by the \mathbf{X}_j 's of the reference set, the distance component in MSD is small relative to pure
 372 error plus measurement error for any choice of near neighbor. On the other hand, where the \mathbf{X}_{Ti} are not
 373 closely spaced (sparse), their imputations to the \mathbf{X}_{Tj} will be few in number, so their effect on MSD will be
 374 small. This ambiguity explains a puzzling property of near-neighbor imputation: that it has not appeared to
 375 be very sensitive to monotonic transformations of the variables. However, for imputation methods that base
 376 \mathbf{W} on the relations of the \mathbf{Y} 's to the \mathbf{X}_j 's in distance calculations (e.g. MSN), the non-linear components
 377 represented by lack-of-fit would change the selection of "near neighbors". The extent of the change would
 378 be greatest in pairs of observation units in which model lack-of-fits were of opposite sign.

379 *Choice of k*

380 The partitioning of error provides useful insight concerning the choice of k for imputation using a
 381 weighted average of k near neighbors. The obvious effect is that larger k , by averaging over the errors of
 382 more reference observations, would seem to reduce the error of the imputed value. However, it is not that
 383 simple. Following the same assumptions used in deriving (8) MSD becomes:

$$384 \quad E[\Sigma_i [y_{Ti} - \Sigma_m w_{im} y_{Rm}]^2 / n] = \Sigma_i [g(\mathbf{X}_{Ti}) - \Sigma_m w_{im} g(\mathbf{X}_{Rm})]^2 / n + (1 + \Sigma_i \Sigma_m w_{im}^2 / n) [\text{Var}(\varepsilon_Y) + \text{Var}(\varepsilon_P)] \quad (24)$$

385 In k -nn imputation y_{Rj} of (8) is replaced by an average of k values of y_m using a weighting rule for the
 386 particular flavor of k -nn inference, where m is from the set of indices of the k observations selected as near-
 387 neighbors to the i^{th} target and $\Sigma_m w_{im} = 1$. When $w_{im} = 1/k$, the multiplier of the variances in (24) becomes
 388 $(1 + 1/k)$. To the extent that it is pure error being reduced, increasing k is counter-productive for the
 389 subsequent analysis. Offsetting this effect, measurement error will also be reduced in the same proportion.
 390 Hence there is a tradeoff, either lose valuable pure error or reduce undesirable measurement error. The net
 391 effect of changing k also depends on the change in $\Sigma_i [g(\mathbf{X}_{Ti}) - \Sigma_m w_{im} g(\mathbf{X}_{Rm})]^2 / n$. Whether this component
 392 increases or decreases the total error depends on the change of $[g(\mathbf{X}_{Ti}) - \Sigma_m w_{im} g(\mathbf{X}_{Rm})]^2$ for the reference
 393 observation being added or omitted by changing k .

394 **Application to Example Data Sets**

395 Three data sets will be used to illustrate the estimation of error components and application of
 396 these estimates in evaluating alternative weight matrices. All three use suites of remotely sensed data and
 397 data from digital terrain models to impute data from ground-based observations. As examples of real
 398 imputation analyses, they illustrate the behavior of the statistics we propose. We do not purport to second-
 399 guess the analysis of these data sets, so the definitions of the 69 specific variables in these three data sets
 400 are mostly irrelevant to our purposes. Where we do discuss behavior of the partitioning as a consequence
 401 of the biological situation, we will define those variables explicitly in the text. Otherwise, readers desiring
 402 more detail are directed to the original sources.

403 The first example uses data used by Moisen and Frescino (2002) obtained by the USDA Forest
 404 Service, Rocky Mountain Experiment Station Forest Inventory and Analysis Unit (FIA). The ground-based
 405 data (Y -variables) are from routine FIA observations for Utah, USA. The X -variables were obtained from
 406 LANDSAT and digital terrain data.

407 The other two data-sets use ground data from inventories of stands defined as polygons. One,
 408 from the Deschutes National Forest in Oregon, USA has been used in previously reported analyses by
 409 Moeur (2000) and is the example in the MSN User's Guide (Crookston et al. 2002). The third data set is
 410 from Tally Lake area in the Helena National Forest in Montana, USA. For these comparisons, the Y -
 411 variables will be limited to those measured on continuous scales. These analyses differ from those reported
 412 by Stage and Crookston (2002) in that all discrete and a few redundant y 's have been omitted to achieve
 413 approximately equal numbers of y 's in the three examples, and additional x 's (transformations of the
 414 original variables) have been added. Table 1 summarizes numbers of variables and sample sizes for the
 415 three data-sets. Of the three data sets, Users Guide has remarkably fewer observations in relation to the
 416 number of unique coefficients in the weight matrix being estimated (last line, Table 1).

417 The Utah data set differs from the other two in that it contains a notable portion of locations in
 418 non-forest although the continuous Y -variables describe forest stand parameters. By contrast, y -values of
 419 zero in the other two data sets indicate lack of stocking in otherwise forested polygons. Proportion of
 420 zeroes in the three data sets are indicated in figure 2.

421 Table 2 summarizes the structure of the correlations between the canonical vectors for the three
 422 data sets. Multivariate regression R^2 of y on X are listed in col. B of table 2. Correlations between the Y 's
 423 and the X 's were lowest in the Utah data because the measurement errors of the Y 's from the FIA plot
 424 clusters were larger than in the two data sets based on inventories of stand polygons.

425 *Components of Variance*

426 Data for partitioning variance for the three example data sets are displayed in table 3. Columns A-
 427 C contain statistics for each y -variable considered independently of the remaining elements of Y . Columns
 428 D-F contains statistics for each y -variable, but for pairs of near neighbors selected using a multivariate
 429 Mahalanobis distance measure.

430 *Accuracy of imputed values*

431 Standard error of imputation squared (SEI^2) (as a fraction of variance of each variable) of values
 432 imputed using a Mahalanobis distance function are shown in figure 3. The error component arising from
 433 distance between target and reference: $\sum_i [(g(\mathbf{X}_{Ti}) - g(\mathbf{X}_{Rj}))^2]/n$ as estimated by (10) is shown in figure 3 by

434 the shaded portions of the bars for each y -variable. This figure also shows the combined components of
 435 pure error and measurement error as estimated by (9).

436 *Imputation compared to linear regression*

437 Figure 4 compares the distance component of imputations (plotted as its negative) with the model-
 438 lack-of-fit computed as $SEE^2 - \text{Min}(\text{MMSD}(0)/2, SEE^2)$ for $f(\mathbf{X}) = \beta\mathbf{X}'$. As a corollary of the differences
 439 between imputation distance component and regression lack of fit, SEE^2 is almost always less than SEI^2 .
 440 The exceptions to the inequality are Crown Cover (CCover) and logarithm of Pinus ponderosa volume
 441 (Vlg'PP) in the Tally Lake data set. We conjecture that the linear regression is just not a very effective
 442 model for crown cover, and that the large proportion of zero data for Pinus ponderosa preclude effective
 443 prediction of volume. Also, there would be two anomalies leading to negative estimates of lack-of-fit if the
 444 minimum of $\text{MMSD}(0)$ and SEE^2 were not used: logarithm of Engelmann spruce volume (Vlg'ES) in the
 445 Tally Lake data and net growth in cubic feet (NGRWCF) in the Utah data. The larger values of $\text{MMSD}(0)$
 446 for these variables are the consequence of squared differences between y_{Ti} and y_{Rj} that decrease with
 447 increasing differences in the \mathbf{X} -variables. As a result, $\text{MMSD}(0)$ is larger than SEE^2 . We attribute this
 448 anomaly to unequal pure error in different regions of the \mathbf{X} -space. Engelmann spruce in the Tally Lake
 449 area occurs bi-modally with elevation—either very common at high elevations, or as sparse stringers in
 450 valley bottoms. However, the density in the \mathbf{X} -space of the observations representing valley bottoms and
 451 stands at similar elevations is higher than the density of data representing high elevations. Thus
 452 observation pairs with near-zero distances tend to come from low elevations where the sporadic presence of
 453 spruce gives large squared differences whereas at high elevations, spruce is more ubiquitous giving smaller
 454 differences in volume even at larger separations in \mathbf{X} -space.

455 That SEE is almost always less the SEI is not surprising because whereas SEE is a least squares
 456 minimization of the model prediction, SEI is not the result of an explicit minimization and includes the
 457 pure error and measurement error components. When pure error should be included in estimates for
 458 subsequent analyses, the proportion of pure error that might be added to regression lack of fit that would
 459 just make (23) equal zero is indicated by the white bars in figure 4. Unfortunately, we lack a direct
 460 estimate of measurement error that should be subtracted from SEI , so we can only show the margin from
 461 which it would be subtracted.

462 *Effect of distances between X's*

463 The three data sets show differences in the proportions of variance attributable to the Mahalanobis
464 distances between target and reference (figure 3, shaded bar). The low ratio of number of observations
465 compared to number of coefficients to be estimated and large linear model lack-of-fit of the User's Guide
466 data produces a relatively large distance component compared to the Tally Lake data. Utah data show an
467 intermediate level because the effect of the larger number of data relative to the number of coefficients to
468 be estimated is offset by the low correlations between the Y's and the X's (table 3) caused by the inclusion
469 of non-forest observations (figure 2).

470 In the Tally Lake application, average distances from reference observation units to actual target
471 observation units is 2.04 times the average distance from each reference observation unit to its nearest
472 neighbor also in the reference set. Nearly one-third of the targets are farther from their nearest reference
473 than the ninth percentile of the distribution of distances among the references. The significance of this
474 extrapolation might be determined by modeling squared differences for each element of Y as a function of
475 distance. Such analysis is beyond the scope of this report.

476 *Comparison of alternative distance functions*

477 The difficulty of using MSD to compare alternative distance functions can be appreciated by
478 considering that the influence of pure error plus sampling error would be double that shown in figure 3.
479 Although the absolute value of differences in MSD arising from different distance functions would not
480 change, the relative importance of the differences among the alternative distance functions would be under-
481 estimated.

482 Figure 5 a,b,c compares three alternative distance functions, the Mahalanobis distance used
483 heretofore in this report, the original canonical-correlation-based distance (CC) of Moeur and Stage (1995),
484 and the newer canonical-regression-based distance (CR) introduced by Stage and Crookston (2002). The
485 panels present both estimated means of $[g(\mathbf{X}_{Ti}) - g(\mathbf{X}_{Rj})]^2$ based on all data for comparison to means for the
486 50% of the data separated by the longer distances. Only the Utah data show the alternative similarity
487 measures to rank differently in the full data set than in the reduced data set containing only the 50% longer
488 distances. Also, the Utah data set was the only one to show a distinct advantage to using one or the other of
489 the canonical-based distances over the Mahalanobis distances. And the differences would be even greater

490 if the non-forest data were masked because the Mahalanobis distances did slightly better at matching the
491 zero data. The result seems anomalous because the Utah data had the lowest canonical correlations
492 between Y 's and X 's. However, one of the merits of the canonical approach lies in its capability to ignore
493 X 's that are irrelevant. Moisen and Frescino (2002) found that several of the x 's were superfluous. The
494 Mahalanobis distance would have given these variables weights equal to the weights of the useful
495 variables. The other two data sets were obtained after extensive analysis by others that probably had
496 already screened the X 's for utility.

497 **Conclusions**

498 This report concerns the error properties of imputation processes used to fill in a data set by
499 imputing values from a sample of intensively measured observation units to interspersed, less completely
500 measured units. The error statistics for the imputed, continuous-valued variables presented in this report
501 are based on partitioning of the error components into measurement error, error inherent in the particular
502 imputation method and the pure error not associated with the variables measured on all observation units.
503 These statistics can assist in the design of inventories and their analysis with near-neighbor imputation
504 methods. It is now possible to consider the relative gains from reducing measurement error versus
505 increasing the density of the sampled observation units. They also clarify comparisons to other inference
506 methods such as regression or stratum-mean based estimators, and help to choose among alternative weight
507 matrices in similarity measures.

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535

Table Captions

536

537 Table 1. Statistics for three data sets used as examples. Number of coefficients to be estimated in relation
538 to number of samples.

539 Table 2. Comparison between three example data sets of first four squared canonical correlations between
540 Y 's and X 's.

541 Table 3. Table 3. Components of variance for three example data sets. Columns C – F are standardized by
542 division by variance in column A. Column B and C are for a linear model used as $y=f(X)$. Columns D-F
543 are obtained with a Mahalanobis distance function.

544

545 Table 1. Statistics for three data sets used as examples. Number of coefficients to be estimated in relation
 546 to number of samples.

	Tally Lake	Users Guide	Utah
Number of Y variables	8	6	10
Number of X's (p)	21	12	12
Number of reference obs. (n)	847	197	1076
Significant canonical pairs (s)	7	5	4
$n/(s+p*s)$	5.50	3.03	16.55

547

548 Table 2. Comparison between three example data sets of first four squared canonical correlations between
 549 Y 's and X 's.
 550

<i>Canonical</i>	<i>Tally</i>	<i>User's</i>	
<i>Pair</i>	<i>Lake</i>	<i>Guide</i>	<i>Utah</i>
<i>(m)</i>			
1	0.697	0.686	0.450
2	0.477	0.456	0.153
3	0.325	0.376	0.109
4	0.292	0.244	0.034

551

552 Table 3. Components of variance for three example data sets. Columns C – F are standardized by division
 553 by variance in column A Column B and C are for a linear model used as $y=f(X)$. Columns D-F are
 554 obtained with a Mahalanobis distance function.

Y-Variable	Total variance of Y-variable in reference set	Multivariate regression R^2	Squared error about regression of single Y SEE^2 1.-B	Mean square between target and nearest reference for all pairs in MSD	Mean square between target and nearest reference for 1/8 of shorter distances (MMSD(0))	Calculated Distance component D –E
	(A)	(B)	(C)	(D)	(E)	(F)
Tally Lake						
Top height	566.669	0.6713	0.3287	0.6990	0.2837	0.4153
Vlg'AF	8.69601	0.4716	0.5284	1.0380	0.8461	0.1919
Vlg'ES	9.01080	0.4322	0.5678	1.2098	1.4075	-0.1977
Vlg'DF	7.03682	0.3696	0.6304	1.0064	0.6292	0.3772
CCover	222.797	0.2999	0.7001	1.1628	1.0061	0.1567
Vlg'L	6.66466	0.2556	0.7444	1.3189	0.9271	0.3918
Vlg'LP	8.18933	0.1956	0.8044	1.4893	1.0475	0.4418
Vlg'PP	0.71893	0.1076	0.8924	1.1779	0.6486	0.5294
Users Guide						
TotBA	2822.19	0.5917	0.4083	0.7695	0.735	0.0345
LN-FIR	4.43945	0.5440	0.4560	0.8217	0.087	0.7347
TopHT	292.968	0.4839	0.5161	0.9453	0.287	0.6583
LN_PINE	7.0639	0.3858	0.6142	1.0768	0.087	0.9898
LN-BADF	1.85368	0.3548	0.6452	0.9557	0	0.9557
LN-BALP	3.55926	0.3225	0.6775	1.2927	0.6712	0.6215
Utah						
MAICF	684.346	0.3567	0.6433	1.1259	0.3334	0.7925
NVOLTOT	2064882.	0.3142	0.6858	1.3522	0.7868	0.5654
NVOLMER	1546287.	0.2976	0.7024	1.3472	0.8143	0.5329
BA	4211.15	0.2736	.07264	1.3271	0.7525	0.5746
CRCOV	779.175	0.2621	0.7379	1.4426	0.8551	0.5876
STAGECL	3746.17	0.2528	0.7472	1.3367	1.0754	0.2613
NGRWCF	905.920	0.2434	0.7566	1.4868	2.1123	-0.6255
BIOTOT	636.018	0.2390	.07610	1.4758	0.5886	0.8872
NGRWBA	0.75238	0.2280	0.7720	1.5302	1.0740	0.4562
QMDALL	19.5868	0.1711	0.8289	1.6427	0.6462	0.9965

555

Figure Captions

556

557 Figure 1. Error components for imputing y_{Rj} (e.g. species volume) to a target observation at x_{Ti} from one of
 558 two reference observations in a one dimensional space of X (e.g. elevation). Pure error (ε_{pi}) is the vertical
 559 distance from y_i^* to the dashed line $g(x)$. Measurement error (ε_{yi}) is the vertical distance between y_i^* and y_i .
 560 Model lack-of-fit ($\varepsilon_{L(Xj)}$) is the vertical separation between the dashed $g(X)$ and solid $f(X)$ lines.

561

562 Figure 2. Proportion of zero values in example data sets.

563

564 Figure 3. Partitioning of relative variance of imputed values (SEI equation (13)) for Mahalanobis distance
 565 function. Variables within a data set are ordered from left to right by increasing SEE. Values standardized
 566 by division by attribute variance.

567

568 Figure 4. Distance error component of imputation (plotted as its negative) compared to lack of fit of a linear
 569 regression, and pure error plus measurement error. Clear portion of the bar is amount of error that would
 570 be added to lack of fit to make expression (23) equal zero. Stippled bar is remaining portion of pure error
 571 plus measurement error. Variables within a data set are ordered from left to right by increasing SEE for a
 572 linear regression model. Values standardized by division by attribute variance.

573

574 Figure 5a. Tally Lake Comparison of distance components (10) for two canonical-correlation-based
 575 distance functions with Mahalanobis distance function. Variables within a data set are ordered from left to
 576 right by increasing SEE.

577

578 Figure 5b. Users Guide. Comparison of distance components (10) for two canonical-correlation-based
 579 distance functions with Mahalanobis distance function. Variables within a data set are ordered from left to
 580 right by increasing SEE.

581

582 Figure 5c. Utah. Comparison of distance components (10) for two canonical-correlation-based distance
583 functions with Mahalanobis distance function. Variables within a data set are ordered from left to right by
584 increasing SEE.

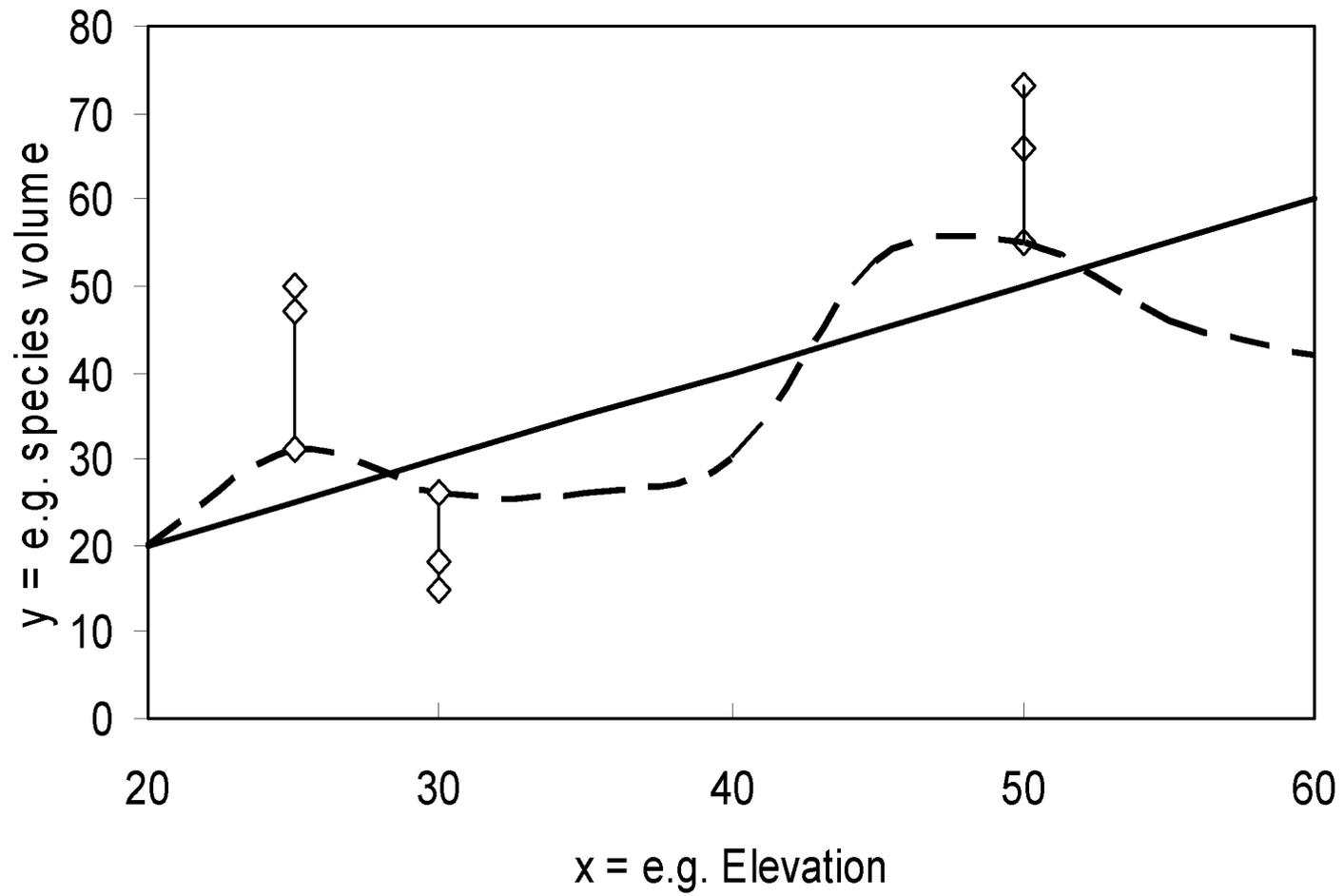


Fig. 1

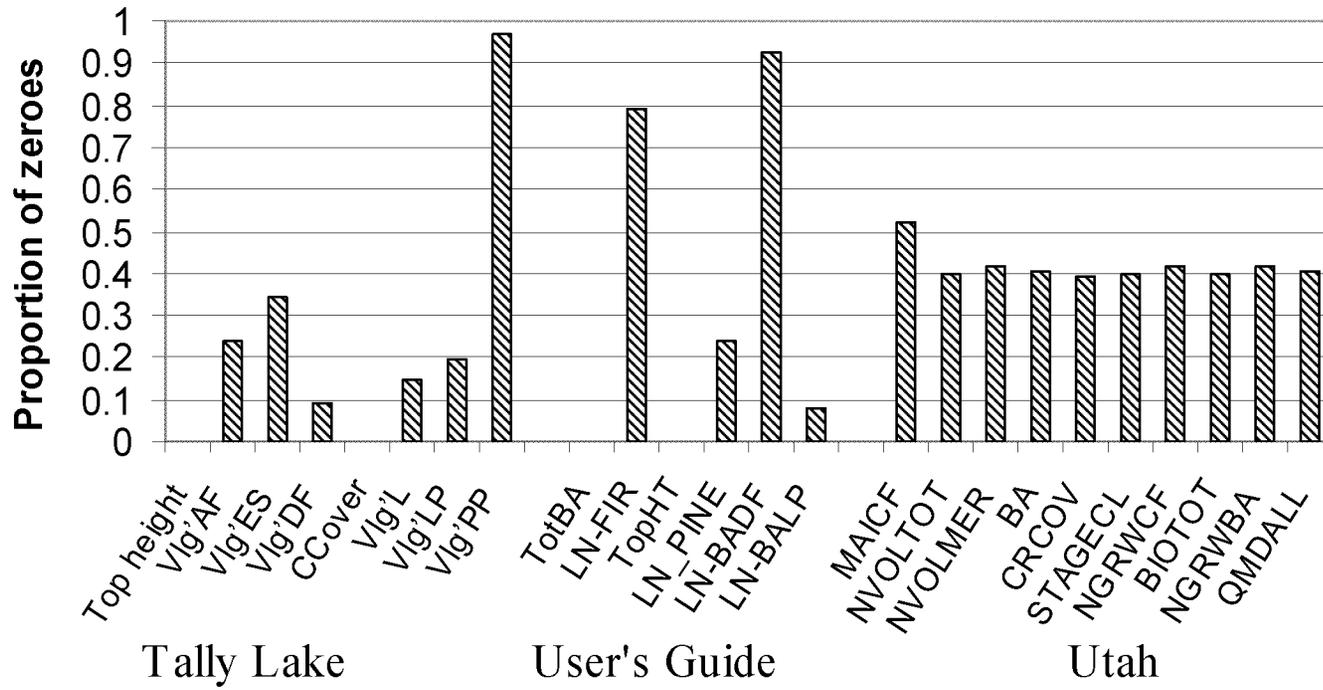


Fig. 2

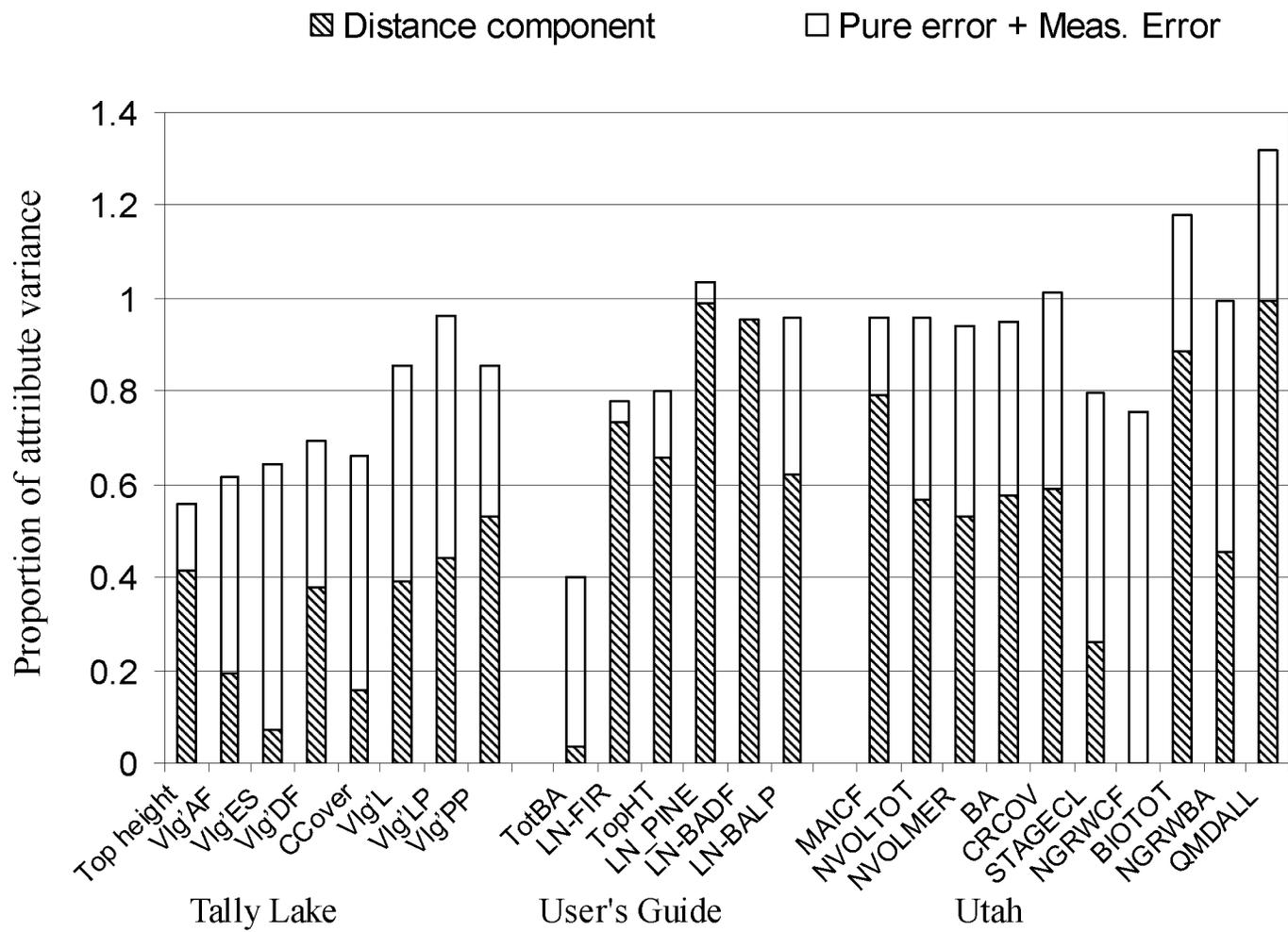


Fig 3

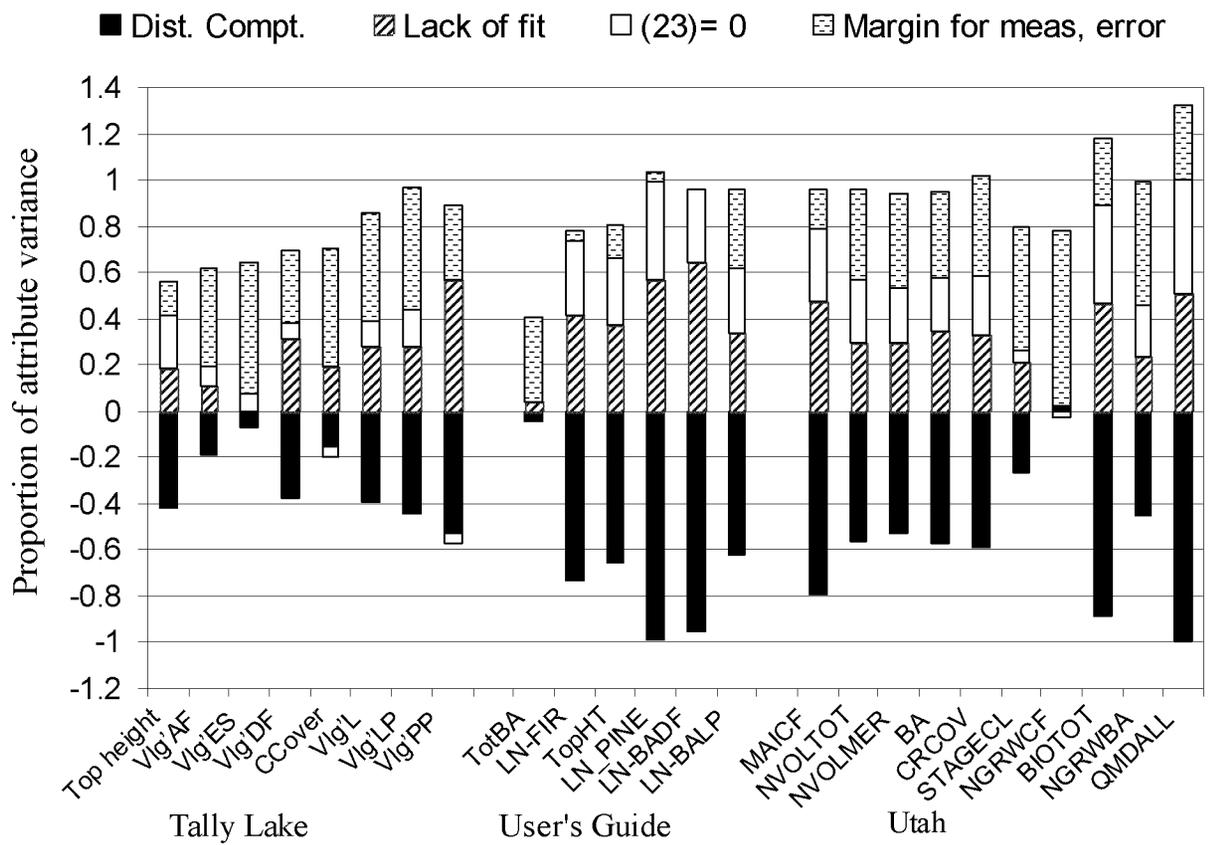


Fig. 4

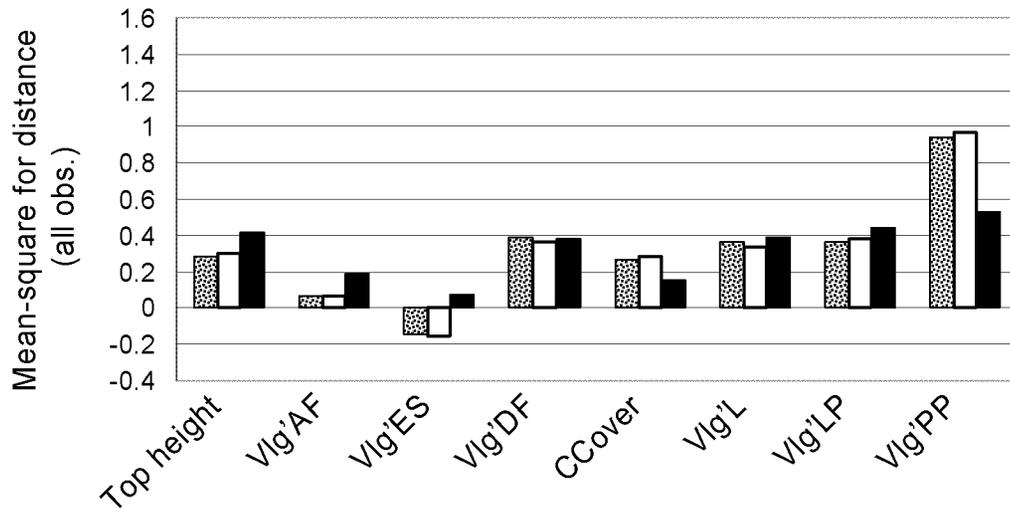
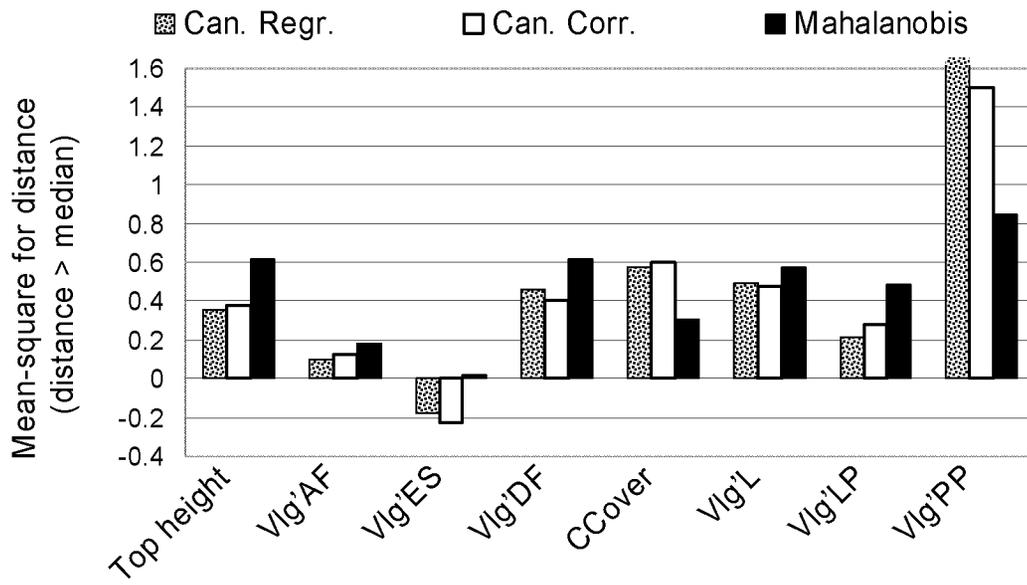


Fig 5a

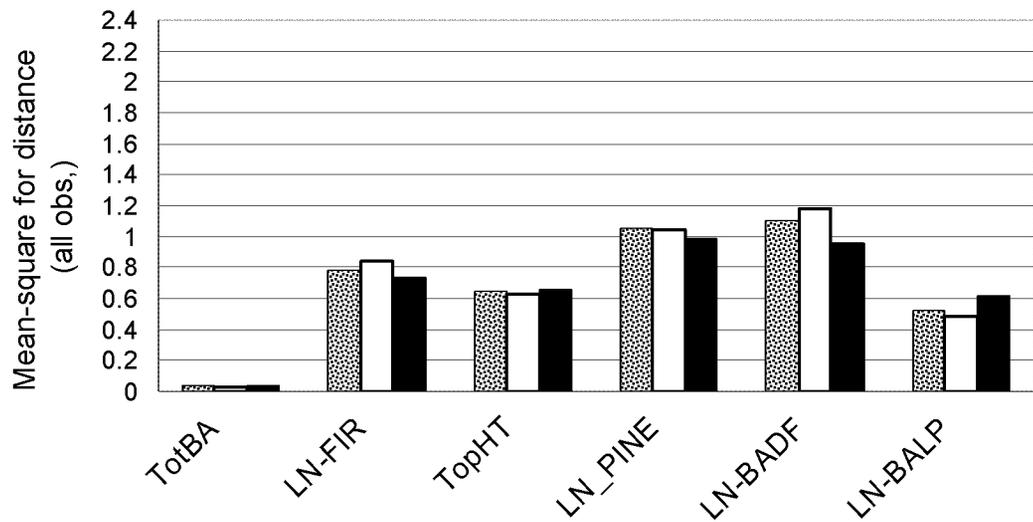
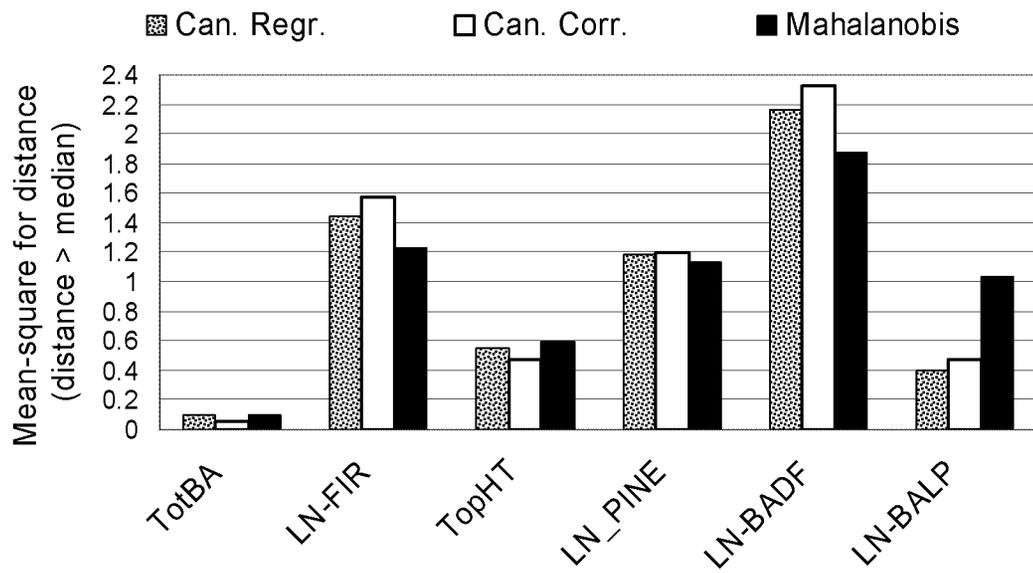


Fig 5b

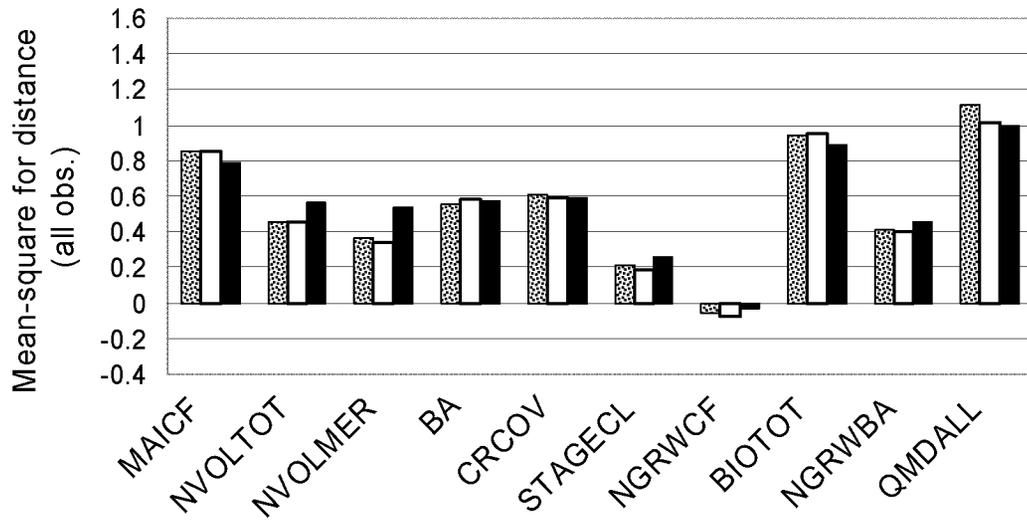
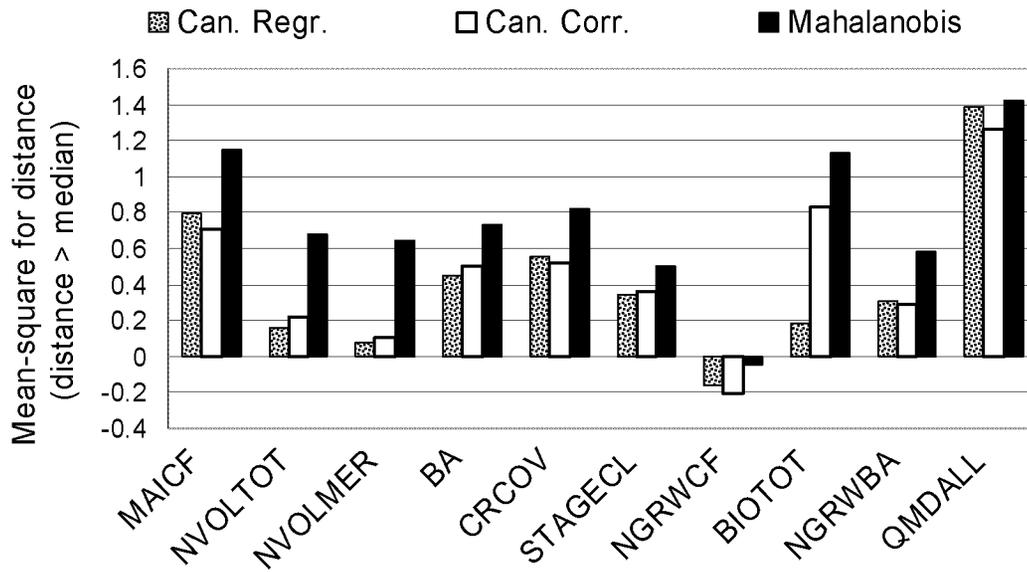


Fig 5c