Matrix Completion Discriminant Analysis

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Abstract

Matrix completion discriminant analysis (MCDA) is designed for semi-supervised learning where the rate of missingness is high and predictors vastly outnumber cases. MCDA operates by mapping class labels to the vertices of a regular simplex. With c classes, these vertices are arranged on the surface of the unit sphere in $c - 1$ dimensional Euclidean space. Because all pairs of vertices are equidistant, the classes are treated symmetrically. To assign unlabeled cases to classes, the data is entered into a large matrix (cases along rows and predictors along columns) that is augmented by vertex coordinates stored in the last $c - 1$ columns. Once the matrix is constructed, its missing entries can be filled in by matrix completion. To carry out matrix completion, one minimizes a sum of squares plus a nuclear norm penalty. The simplest solution invokes an MM algorithm and singular value decomposition. Choice of the penalty tuning constant can be achieved by cross validation on randomly withheld case labels. Once the matrix is completed, an unlabeled case is assigned to the class vertex closest to the point deposited in its last $c - 1$ columns. A variety of examples drawn from the statistical literature demonstrate that MCDA is competitive on traditional problems and outperforms alternatives on large-scale problems.

Key words: Classification; Missing observations; MM algorithm; Semi-supervised learning; Singular value decomposition

1 Introduction

Whenever large data sets are collected, missing responses and missing predictors occur. Missing data values are now classified as missing completely at random (MCAR), missing at random (MAR), and missing not at random (MNAR). Statisticians have devised a host of methods for coping with missing data, including: listwise deletion, pairwise deletion, hot deck imputation, mean substitution, regression substitution, and multiple imputation. In model fitting in general, and regression in particular, the modern tendency is to impute missing values by maximum likelihood estimates or posterior means under a Gaussian model (Little and Rubin 2002; Schafer 2010). Regardless of the method of imputation, the consensus among statisticians is that one should use all available information. Failures to impute data can increase bias and compromise inference.

For data presented in matrix form, a new imputation method is now available. Matrix completion aims to recover a full matrix – usually of low rank – from a subset of observed entries. During the past five years, the subject of matrix completion has captured the attention of researchers from a variety of backgrounds in statistics, applied mathematics, and computer science. Candès and Recht (2009) prove that a low-rank matrix can be almost perfectly recovered when the number of observed entries exceeds a certain level. Fortunately, their strong uniformity condition on sampled entries can be relaxed (Recht 2011). Matrix completion can be accomplished by several algorithms: subspace evolution and transfer (SET) (Dai and Milenkovic 2009), gradient algorithms applied to the primal and dual problems (Lin et al. 2009), singular value thresholding (SVT) (Cai et al. 2010; Hu et al. 2012), fixed point and Bregman iteration (Ma et al. 2011), the alternating

direction method (Chen et al. 2012; Yuan et al. 2009), modified fixed point continuation (Ma and Zhi 2011), and alternating minimization (Jain et al. 2012).

Methods for handling missing data in discriminant analysis have lagged methods for model fitting. Most research has focused on classification trees and the nature of missingness, for example, whether missingness occurs in the testing data (Saar-Tsechansky and Provost 2007), in the training data, or in a combination of both (Ding and Simonoff 2010). Other relevant distinctions include missing responses in both training and testing (Ding and Simonoff 2010) and MCAR (Feelders 1999; Kim and Yates 2003; Zhang et al. 2005) versus a combination of MCAR, MAR, and MNAR (Kalousis and Hilario 2000; Twala 2009). Farhangfar et al. (2008) evaluated a variety of imputation methods on classifiers for discrete data, while Sun et al. (2009) studied the impact of imputation on classification accuracy with DNA microarray data. A common theme among these and other papers (Acuna and Rodriguez 2004; Luengo et al. 2012; Garcia-Laencina et al. 2010) is the deterioration of classification accuracy as the rate of missingness increases. Standard imputation methods are ill equipped to handle high rates of missingness. Two existing papers advocate matrix completion to handle missing data in transductive learning (Cabral et al. 2011; Goldberg et al. 2010). However, these papers deal with multi-label classification rather than multi-category classification and employ a fixed point continuation algorithm rather than an MM algorithm.

Our new combination of matrix completion with Vertex Discriminant Analysis (VDA) (Lange and Wu 2008; Wu and Lange 2010; Wu and Wu 2012) extends VDA into the realm of semi-supervised learning. VDA is geometrically motivated and attuned to matrix representation. Missing ob-

servations are ubiquitous in practice, and discarding cases with missing predictors leads to less accurate classification. Instead of conducting imputation and classification sequentially, we believe that classification can inform imputation and advocate conducting them simultaneously. Our new method, which we call Matrix Completion Discriminant Analysis (MCDA), is specifically designed for data exhibiting high rates of missingness and an excess of features over cases. It is precisely in this setting of high-dimensional sparse data that matrix completion is expected to shine. Our cancer classification results validate this intuition and justify the inclusion of incomplete cases and the strategy of simultaneous imputation and classification.

2 Matrix Completion Discriminant Analysis

2.1 Vertex Discriminant Analysis

VDA is a novel supervised classification method (Lange and Wu 2008; Wu and Lange 2010; Wu and Wu 2012). In classification with c classes, it operates by mapping the classes to the c vertices of a regular simplex in the Euclidean space $\mathbb{R}^{c-1}$. For example in binary classification, the two classes correspond to the numbers -1 and 1 on the real line. In trinary classification, the three classes correspond to the three vertices of an equilateral triangle in the plane. The advantages of mapping categories to vertices include dimension reduction, simplification of computation, ease of interpretation, and enhancement of geometric intuition. It is impossible to situate more than c equidistant points in $\mathbb{R}^{c-1}$ (Lange and Wu 2008).

There are several versions of VDA: VDA_R (Lange and Wu 2008), VDA_{LE} (Wu and Lange 2010), and VDA_K (Wu and Wu 2012), where the subscripts stand for Ridge, Lasso and Euclidean, and Kernel, respectively. The first two are linear classifiers, and the third is a nonlinear classifier. The linear VDA

classifiers rely on the linear regression model $\mathbf{y}_i = \mathbf{A}\mathbf{x}_i + \mathbf{b}$, $i = 1, \dots, n$, to predict the vertex associated with case i . Here $\mathbf{x}_i$ is a p -dimensional predictor vector for case i , $\mathbf{A} = (a_{jk})$ is a $(c-1) \times p$ matrix of slopes, and $\mathbf{b} = (b_j)$ is a $c-1$ column vector of intercepts. The linear VDA classifiers minimized the objective function

$$R(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^n g(\mathbf{y}_i - \mathbf{A}\mathbf{x}_i - \mathbf{b}) + \lambda P(\mathbf{A}), \quad (1)$$

where $g(\mathbf{z}) = \|\mathbf{z}\|_{2,\epsilon} = \max\{\|\mathbf{z}\|_2 - \epsilon, 0\}$ denotes ϵ -insensitive Euclidean distance, $\boldsymbol{\theta}$ signifies the parameters $(\mathbf{A}, \mathbf{b})$, and $P(\mathbf{A})$ denotes the penalty imposed on $\mathbf{A}$. In VDA_R,

$$P(\mathbf{A}) = \sum_{j=1}^{c-1} \sum_{k=1}^p a_{jk}^2$$

is a ridge penalty, while in VDA_{LE},

$$P(\mathbf{A}) = \sum_{j=1}^{c-1} \sum_{k=1}^p |a_{jk}| + \sum_{j=1}^{c-1} \sqrt{\sum_{k=1}^p a_{jk}^2}$$

is a mixture of lasso and Euclidean penalties. Lasso and Euclidean penalties promote sparseness in the estimate of the slope matrix $\mathbf{A}$.

Nonlinear VDA_K exploits reproducing kernel Hilbert spaces (RKHS). Every such Hilbert space of functions $\mathcal{H}_K$ is generated by a kernel function $K(\cdot, \cdot)$. If we fix a point $\mathbf{y}$, then the function $\mathbf{x} \mapsto K(\mathbf{x}, \mathbf{y})$ belongs to $\mathcal{H}_K$. In the current setting $\mathbf{x}$ is the predictor vector that discriminates between the various classes. The inner product of two such functions $\mathbf{x} \mapsto K(\mathbf{x}, \mathbf{y})$ and $\mathbf{x} \mapsto K(\mathbf{x}, \mathbf{z})$ turns out to be $K(\mathbf{y}, \mathbf{z})$. In VDA_K we minimize the objective function

$$\frac{1}{n} \sum_{i=1}^n g[\mathbf{y}_i - f(\mathbf{x}_i)] + \lambda \sum_{j=1}^{c-1} \|h_j\|_{\mathcal{F}_K}^2,$$

where $f(\mathbf{x}_i)$ has j th component

$$f_j(\mathbf{x}) = h_j(\mathbf{x}) + b_j = \sum_{k=1}^n a_{jk} K(\mathbf{x}, \mathbf{x}_k) + b_j.$$

The parameters in the model are again the slopes a_{jk} and intercepts b_j . Given the bilinearity of the kernel, the objective function can be written as

$$\frac{1}{n} \sum_{i=1}^n g[\mathbf{y}_i - \mathbf{f}(\mathbf{x}_i)] + \lambda \text{tr}(\mathbf{A} \mathbf{K} \mathbf{A}^T),$$

where $\mathbf{K}$ is the $n \times n$ symmetric matrix $[K(\mathbf{x}_k, \mathbf{x}_l)]$ and $\mathbf{A}$ is the $(c-1) \times n$ matrix (a_{jk}) . An attractive feature of VDA_K is that optimization and estimation are performed on $O(n)$ parameters rather than $O(p)$ parameters, where n is the number of cases, and p is the number of features.

2.2 Matrix Completion

Matrix completion (Cai et al. 2010; Candès and Tao 2010; Chen et al. 2012; Mazumder et al. 2010) dispenses with linear regression and approximates a matrix $\mathbf{Y} = (y_{ij})$ with missing entries by a low-rank matrix $\mathbf{X} = (x_{ij})$ of the same dimensions. In matrix completion one minimizes the objective function

$$f(\mathbf{X}) = \frac{1}{2} \sum_{(i,j) \in \Delta} (y_{ij} - x_{ij})^2 + \lambda \sum_k \sigma_k, \quad (2)$$

where Δ collects the index pairs (i, j) of the observed entries of $\mathbf{Y}$ and σ_i is the i th singular value of $\mathbf{X}$. Recall that the singular value decomposition (SVD) $\mathbf{X} = \sum_i \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ of $\mathbf{X}$ involves orthonormal singular vectors $\mathbf{u}_i$ and $\mathbf{v}_i$ and nonnegative singular values σ_i presented in descending order. The penalty $\sum_k \sigma_k$ is the nuclear norm $\|\mathbf{X}\|_{\text{nuc}}$ of $\mathbf{X}$. It plays a role in low-rank matrix approximation similar to that played by the ℓ_1 norm $\|\mathbf{b}\|_1 = \sum_k |b_k|$

in sparse regression. The positive tuning constant λ controls the strength of the penalization. The objective function (2) can be rewritten as

$$\frac{1}{2}\|P_{\Delta}(\mathbf{Y}) - P_{\Delta}(\mathbf{X})\|_F^2 + \lambda\|\mathbf{X}\|_{\text{nuc}}, \quad (3)$$

using the Frobenius norm $\|\mathbf{X}\|_F = \sqrt{\text{tr}(\mathbf{X}\mathbf{X}^T)} = \sqrt{\sum_i \sum_j x_{ij}^2}$ and the projection operator $P_{\Delta}(\mathbf{Y})$ with components

$$P_{\Delta}(\mathbf{Y})_{ij} = \begin{cases} y_{ij} & \text{if } (i, j) \in \Delta \\ 0 & \text{if } (i, j) \notin \Delta. \end{cases}$$

To recover $\mathbf{Y}$, one simply replaces a missing entry y_{ij} by the corresponding entry x_{ij} of $\mathbf{X}$; observed entries are left untouched.

2.3 Matrix Completion Discriminant Analysis

Discriminant analysis (supervised learning) involves both labeled and unlabeled cases. The labeled cases constitute the training sample. In semi-supervised learning, the problem requires (a) imputing missing predictors, (b) building a classification rule from the training sample, and (c) classifying the unlabeled cases. The traditional solution takes these steps sequentially. A wide variety of imputation and supervised classification rules exist. In our numerical comparisons to MCDA, we try a few of the most promising combinations. In contrast, MCDA performs imputation and classification simultaneously. When we map class labels to vertices, we assume that all components of a vertex are present or all components are absent. Each case should have at least one predictor present; otherwise, it is non-informative for classification.

Suppose there are c classes, p predictors, n_1 labeled cases, and n_2 unlabeled cases, for a total of $n = n_1 + n_2$ cases. As with other VDA methods, we map the c classes to the c vertices of a regular simplex in $\mathbb{R}^{c-1}$. There

are an infinity of such simplices. One appealing simplex has vertices

$$\mathbf{v}_j = \begin{cases} (c-1)^{-1/2}\mathbf{1} & \text{if } j = 1 \\ r\mathbf{1} + s\mathbf{e}_{j-1} & \text{if } 2 \leq j \leq c, \end{cases} \quad (4)$$

where

$$r = -\frac{1 + \sqrt{c}}{(c-1)^{3/2}}, \quad s = \sqrt{\frac{c}{c-1}},$$

and $\mathbf{e}_j$ is the j th standard coordinate vector in $\mathbb{R}^{c-1}$. These choices place the vertices on the surface of the unit sphere in $\mathbb{R}^{c-1}$. Any rotation, dilation, or translation of these vectors preserves the equidistant property. This particular geometric encoding of classes has two virtues. First, it is parsimonious compared to mapping classes to the standard unit vectors in $\mathbb{R}^c$. Second, it puts the class vertices and standardized predictors on a common unit scale. For a more detailed discussion of the merits of VDA, we refer the reader to our previous VDA papers (Lange and Wu 2008; Wu and Lange 2010; Wu and Wu 2012).

Without loss of generality, in MCDA we insert the n cases row by row into two blocks of a big matrix $\mathbf{U}$, with labeled cases coming above unlabeled cases. The two blocks $\mathbf{X}_1$ and $\mathbf{X}_2$ have dimensions $n_1 \times p$ and $n_2 \times p$, respectively. To the right of these blocks we insert the vertex coordinates case by case into two blocks $\mathbf{V}_1$ and $\mathbf{V}_2$ with dimensions $n_1 \times (c-1)$ and $n_2 \times (c-1)$. All of the entries of $\mathbf{V}_1$ are present, and all of the entries of $\mathbf{V}_2$ are absent. Overall, the matrix $\mathbf{U}$ has the form

$$\mathbf{U} = \begin{pmatrix} \mathbf{X}_1 & \mathbf{V}_1 \\ \mathbf{X}_2 & \mathbf{V}_2 \end{pmatrix}.$$

We then complete the matrix $\mathbf{U}$ to the matrix $\mathbf{U}^*$ with blocks

$$\mathbf{U}^* = \begin{pmatrix} \mathbf{X}_1^* & \mathbf{V}_1^* \\ \mathbf{X}_2^* & \mathbf{V}_2^* \end{pmatrix},$$

where $\mathbf{V}_1^* = \mathbf{V}_1$. The class of an unlabeled case can be assigned by finding the closest vertex to the appropriate row of $\mathbf{V}_2^*$. Because of the shrinkage entailed by the nuclear norm penalty, it is a good idea to standardize all predictors prior to their entry into $\mathbf{X}_1$ and $\mathbf{X}_2$. The vertex entries are already scaled properly since class vertices are unit vectors. Because matrix completion is insensitive to row and column permutations of the data, it is simply a matter of convenience to append class vertices on the right of the predictor matrix and to arrange labeled and unlabeled samples in blocks.

2.4 An MM Algorithm for Matrix Completion

For the sake of simplicity in the current study, we used the MM algorithm for matrix completion (Mazumder et al. 2010; Lange et al. 2013). See the references (Lange 1995; Hunter and Lange 2004; Lange 2004) for an exposition of the MM principle and numerous specific MM algorithms. Construction of the current MM algorithm is guided by the observation that one can exactly minimize the objective function (2) by a soft-thresholded SVD algorithm when $\mathbf{X}$ is complete (Donoho et al. 1995; Mazumder et al. 2010). Suppose $\mathbf{U}^m$ is the current approximation to $\mathbf{U}^*$. To restore the symmetry of full data, we replace a missing value u_{ij} by the corresponding entry u_{ij}^m of $\mathbf{U}^m$ and add the term $(u_{ij}^m - u_{ij})^2/2$ to the objective. This creates a surrogate function that equals the objective at $\mathbf{U}^m$ and lies above it for all other values of $\mathbf{U}$.

One can formalize this construction by introducing the complementary projection $P_{\Delta^c}(\mathbf{U})$ satisfying $\mathbf{U} = P_{\Delta}(\mathbf{U}) + P_{\Delta^c}(\mathbf{U})$. Setting

$$\mathbf{V}^m = P_{\Delta}(\mathbf{U}) + P_{\Delta^c}(\mathbf{U}^m)$$

allows one to write the surrogate function as

$$\begin{aligned} g(\mathbf{U} \mid \mathbf{U}^m) &= \frac{1}{2} \|\mathbf{V}^m - \mathbf{U}\|_F^2 + \lambda \|\mathbf{U}\|_{\text{nuc}} \\ &= \frac{1}{2} \|\mathbf{V}^m\|_F^2 - \text{tr}(\mathbf{V}^m \mathbf{U}^T) + \frac{1}{2} \|\mathbf{U}\|_F^2 + \lambda \|\mathbf{U}\|_{\text{nuc}}. \end{aligned} \quad (5)$$

The third term in equation (5) reduces to $\|\mathbf{U}^*\|_F^2 = \sum_k \sigma_k^2$. The second term satisfies the von-Neumann-Fan inequality (Borwein and Lewis 2006)

$$\text{tr}(\mathbf{V}^m \mathbf{U}^T) \leq \sum_k w_k \sigma_k$$

based on the ordered singular values w_k of $\mathbf{V}^m$ and σ_k of $\mathbf{U}$. Equality is attained when the matrices $\mathbf{V}^m$ and $\mathbf{U}$ have ordered singular value decompositions sharing their left and right singular vectors. In this circumstance, we can rewrite the surrogate function (5) as

$$\begin{aligned} g(\mathbf{U}^* \mid \mathbf{U}^m) &= \frac{1}{2} \sum_k w_k^2 - \sum_k w_k \sigma_k + \frac{1}{2} \sum_k \sigma_k^2 + \lambda \sum_k \sigma_k \\ &= \frac{1}{2} \sum_k (w_k - \sigma_k)^2 + \lambda \sum_k \sigma_k. \end{aligned} \quad (6)$$

It is easy to see that the shrunk singular values $\sigma_k = \max\{w_k - \lambda, 0\}$ are optimal. In practice, one only needs to extract the singular values $w_k > \lambda$ and corresponding singular vectors to construct the next approximate $\mathbf{U}^{m+1}$. This MM algorithm, along with all MM algorithms, is a descent algorithm in the sense that it consistently drives the objective function downhill.

2.5 Choice of Tuning Constant λ

To determine a nearly optimal value for the tuning constant λ , we employed K -fold cross validation on the labeled cases. This involves dividing the data into K equal subsamples, leaving one subsample out per fold, training the classifier based on the remaining data, and computing the testing error on the

omitted sample. The average testing error $c(\lambda)$ across these K subsamples is recorded and approximately minimized. In principle, one can compute $c(\lambda)$ on a dense grid of points and identify the optimal λ on the grid. This approach can be computationally inefficient, so we recommend the simple search strategy of taking an initial λ_0 equal to the largest singular value of $P_\Delta(\mathbf{U})$ and working downward. One keeps reducing λ by multiplying it by a fixed factor $0 < r < 1$ until $c(\lambda_{k+1}) \geq c(\lambda_k)$. The optimal value is then set to λ_k .

2.6 Soft Classification

So far we have discussed hard classification based on assigning a case to its nearest class vertex. In contrast, soft classification operates by estimating class probabilities and presenting a range of possible classes (Wahba and Wahba 2002; Liu et al. 2011). Liu et al. (2011) have pointed out that hard classifiers tend to work better when the class signal is weak, while soft classifiers tend to work better in high-dimensional settings with $p \gg n$ or when the class signal is strong. In applications such as image and speech recognition or classification of cancer subtypes, soft classifiers are often preferred. Because matrix completion avoids probabilistic modeling, calculation of posterior assignment probabilities is not an option. As an alternative, we suggest computing the Euclidean distances $d_{ij} = \|\hat{\mathbf{v}}_i - \mathbf{v}_j\|$ between the imputed row $\hat{\mathbf{v}}_i$ of $\mathbf{V}_2^*$ corresponding to case i and the vertex $\mathbf{v}_j$ corresponding to class j . The indices $r_{ij} = 1/d_{ij}$ can then be used to rank the assignment choices for case i . In our numerical examples, we will employ hard classification unless noted to the contrary. Misclassification is fairly common in the cancer data sets when the missing rate is high. Fortunately, soft classification sets containing the two nearest class vertices almost invariably capture the correct

class vertex.

3 Numerical Studies

In the following numerical examples, we first created the missing data by randomly deleting both features and class labels at prescribed rates via the *create.missing* function in the *mi* package of R. Mapping of labels to vertices was performed after deletion. Hence, in the MCDA matrix the block $\mathbf{V}_1$ had no entries missing, and the block $\mathbf{V}_2$ had all entries missing. As a semi-supervised classifier, MCDA performs imputation and classification over all the samples simultaneously. The cases with deleted class labels were used as testing data.

For comparison to MCDA, we combined three method of imputation with four methods of classification. The imputation methods included *missForest* (Stekhoven and Buehlmann 2012), *mice* (van Buuren and Groothuis-Oudshoorn 2011), and *imputePCA* (Josse and Husson 2013). All three were employed in our first example; for the sake of brevity only *missForest* was employed in the remaining examples. In classification we used linear discriminant analysis (LDA), the k -nearest neighbor method (KNN) with fixed $k = 2$ or optimal k between 1 to 10, one-versus-rest binary support vector machines (OVR), and random forest prediction (RanFor). We conducted 3-fold cross-validation to determine the optimal tuning parameters for KNN and MCDA.

3.1 Zoo Data Analysis

Our first example compares the classification accuracies of MCDA and the two-step methods on the zoo data (Forsyth 1990) from the UCI machine learning repository (Murphy and Aha 1994). This animal classification prob-

lem consists of 101 cases spread over 7 categories (mammal, bird, fish, reptile, amphibian, insect, and invertebrate). Each case is classified on 16 features, 15 of which are binary and 1 of which (number of legs) is numeric. We randomly deleted both features and classes at missing rates of 30%, 50%, 70%, and 90%. To compare MCDA to competitors, we averaged across 100 different random deletion experiments at each rate.

Table 1 compares the average misclassification rates of MCDA to those of the two-step procedures. Standard errors appear in parentheses in the table, and boldface type emphasizes the lowest misclassification rates. When the missing rate is low to moderate, random forest has the lowest error rates. As the missing rate increases, MCDA’s accuracy improves relative to the other methods and displays the lowest error rates. The accuracy of the two-step approach is insensitive to which three imputation method is applied. Since *missForest* is the fastest, we used it alone to impute the data in step 1 of the subsequent examples.

3.2 Glass, Wine, and Lympho Data Analysis

We also compared the performance of MCDA to other classification methods on three other benchmark data sets from the UCI machine learning repository: glass, wine, and lympho. These data sets and the zoo data are overdetermined ($n > p$). Missing data were created in the same way as in the zoo example. Table 2 summarizes the misclassification rates of MCDA and the competing methods, including now the model-based semi-supervised classification *Upclass* method (Cribbin 2008). The triples beneath each data set give in order the number of categories c , the number of cases n , and the number of predictors p . On the glass and wine data, MCDA outperforms the other methods when the missing rate is high. At moderate missing rates, the

Table 1: Comparison of mean (standard error) misclassification rates of MCDA and various imputation-classification methods on the zoo data. Each mean is averaged over 100 replicates at each missing rate.

Imputation	Classification	Missing Rate			
		30%	50%	70%	90%
	MCDA	13.4 (0.71)	21.8 (0.47)	34.5 (0.58)	66.18 (0.94)
missForest	LDA	10.8 (0.55)	23.3 (0.61)	NA	NA
missForest	KNN(2)	13.5 (0.68)	25.8 (0.69)	47.7 (0.71)	73.59 (0.77)
missForest	KNN	11.8 (0.64)	24.5 (0.58)	45.4 (0.70)	71.54 (0.86)
missForest	OVR	13.5 (0.63)	NA	NA	NA
missForest	RanFor	10.4 (0.54)	20.9 (0.57)	42.6 (0.68)	70.40 (0.91)
mice	LDA	10.8 (0.55)	23.3 (0.61)	NA	NA
mice	KNN(2)	12.9 (0.60)	25.7 (0.68)	47.6 (0.74)	72.58 (0.82)
mice	KNN	12.3 (0.62)	24.5 (0.64)	45.0 (0.74)	71.52 (0.90)
mice	OVR	13.5 (0.63)	NA	NA	NA
mice	RanFor	10.5 (0.58)	21.0 (0.59)	42.7 (0.69)	70.34 (0.89)
imputePCA	LDA	10.8 (0.55)	23.3 (0.61)	NA	NA
imputePCA	KNN(2)	12.9 (0.62)	25.5 (0.62)	47.7 (0.71)	73.50 (0.78)
imputePCA	KNN	11.9 (0.59)	24.7 (0.65)	45.1 (0.72)	71.53 (0.88)
imputePCA	OVR	13.5 (0.63)	NA	NA	NA
imputePCA	RanFor	10.4 (0.59)	20.8 (0.59)	42.5 (0.70)	70.43 (0.92)

misclassification rates of MCDA are close to the best rates. For the lympho data, MCDA has the lowest misclassification rates at all three missing rates.

3.3 High-dimensional Cancer Subtype Classification

In contrast to the small benchmark UCI data sets, we now investigate a few high-dimensional cancer classification problems where $p \gg n$. The data sets colon (Alon et al. 1999), prostate (Singh et al. 2002), SRBCT (Khan et al. 2001), and brain (Pomeroy et al. 2000) allow one to classify the molecular subtypes of these cancers based on a patient’s microarray gene expression levels. We randomly deleted observations via *create.missing* in *mi* at missing rates 50%, 70%, and 90%. Table 3, which averages over 50 replicates, makes it clear that MCDA’s performance is uniformly best. Since matrix completion was designed to recover large-scale matrices, this is the edge we expected.

Because the misclassification rates for these data sets are high, we evaluated soft classification. For example, with the SRBCT data given 50% missing data, the misclassification rate was 11.7%. Almost all of the misclassified cases are covered by the soft classification set containing the two closest class vertices. Furthermore, the ratio r_{ij}/r_{ik} of the best reciprocal distance to the second best reciprocal distance is always close to 1 for misclassified cases and well in excess of 1 for correctly classified cases. Figure 1 displays a boxplot of this ratio for the correctly and incorrectly classified cases for the SRBCT and brain examples. It would be helpful to establish a cutoff level. For a ratio exceeding the cutoff, the closest-vertex rule would be deemed trustworthy. On the basis of just a handful of data sets, it is probably premature to set a rule of thumb.

Table 2: Comparison of mean (standard error) misclassification rates of MCDA and other classification methods on the glass, wine, and lympho data. Each mean is averaged over 100 replicates at the missing rates of 50%, 70%, and 90%. Missing entries were imputed by the *missForest* method. The triples beneath each data set give in order the number of categories c , the number of cases n , and the number of predictors p .

Missing	Classification	Glass (6, 214, 10)	Wine (3, 178, 13)	Lympho (4, 148, 18)
50%	MCDA	53.75 (0.36)	13.39 (0.30)	35.4 (0.59)
	LDA	48.0 (0.52)	10.8 (0.34)	NA
	KNN(2)	49.6 (0.49)	34.6 (0.55)	53.2 (2.15)
	KNN	45.6 (0.52)	31.7 (0.53)	51.4 (2.32)
	OVR	NA	10.2 (0.33)	NA
	RanFor	42.1 (0.50)	11.6 (0.37)	48.7 (2.84)
	Upclass	50.2 (0.61)	9.9 (0.34)	68.8 (2.68)
70%	MCDA	61.60 (0.36)	23.54 (0.33)	44.93 (0.44)
	LDA	58.8 (0.43)	25.9 (0.42)	NA
	KNN(2)	62.2 (0.47)	43.9 (0.49)	63.3 (1.78)
	KNN	58.7 (0.50)	40.2 (0.61)	62.4 (2.01)
	OVR	NA	24.1 (0.42)	NA
	RanFor	57.4 (0.44)	25.6 (0.46)	62.0 (2.36)
	Upclass	61.2 (0.49)	23.8 (0.46)	78.5 (1.21)
90%	MCDA	69.08 (0.32)	53.24 (0.35)	66.31 (0.48)
	LDA	NA	63.36 (0.51)	NA
	KNN(2)	70.66 (0.50)	61.97 (0.55)	69.15 (1.29)
	KNN	69.68 (0.50)	61.61 (0.56)	70.33 (1.44)
	OVR	NA	60.63 (0.57)	NA
	RanFor	69.74 (0.52)	59.71 (0.64)	69.99 (1.51)
	Upclass	73.9 (0.61)	62.0 (0.57)	NA

Figure 1: Boxplot of the ratio of the highest classification index r_{ij} to the second highest classification index r_{ik} for the SRBCT (upper panel) and brain (lower panel) data with 50% missing rate

Table 3: Comparison of mean (standard error) misclassification rates of MCDA and other classification methods on four benchmark cancer data sets. Each mean is averaged over 50 replicates at the missing rates of 50%, 70%, and 90%. Missing entries were imputed by the *missForest* method. The triples beneath each data set give in order the number of categories c , the number of cases n , and the number of predictors p .

Missing	Classification	Colon (2,62,2000)	Prostate (2,102,6033)	SRBCT (4,63,2308)	Brain (5,42,5597)
50%	MCDA	19.16 (0.65)	14.42 (1.34)	11.70 (0.86)	23.06 (1.25)
	LDA	19.69 (0.79)	16.90 (0.81)	20.26 (1.44)	NA
	KNN(2)	26.44 (0.97)	23.72 (0.57)	19.87 (1.33)	36.43 (1.12)
	KNN	25.11 (1.00)	20.63 (0.67)	21.35 (1.69)	30.48 (0.86)
	OVR	28.00 (1.47)	19.89 (0.90)	20.26 (1.30)	NA
	RanFor	21.98 (1.06)	17.83 (0.92)	18.97 (1.33)	39.76 (1.67)
70%	MCDA	22.85 (0.78)	21.09 (1.04)	19.26 (0.71)	25.45 (0.66)
	LDA	23.77 (0.85)	21.87 (1.04)	43.37 (1.11)	NA
	KNN(2)	31.12 (0.75)	33.06 (0.72)	38.22 (1.13)	44.53 (1.17)
	KNN	27.86 (0.85)	33.43 (0.88)	35.45 (1.98)	41.38 (1.64)
	OVR	31.54 (1.19)	29.13 (1.33)	49.09 (1.39)	NA
	RanFor	26.23 (1.08)	21.28 (1.20)	35.98 (1.17)	45.73 (1.27)
90%	MCDA	35.18 (0.98)	41.33 (1.01)	49.59 (0.77)	50.51 (1.08)
	LDA	50.39 (1.60)	45.22 (1.00)	68.58 (1.07)	NA
	KNN(2)	51.95 (1.29)	47.25 (1.11)	67.22 (0.94)	75.11 (1.44)
	KNN	44.94 (1.47)	47.97 (0.95)	68.49 (0.81)	72.40 (1.36)
	OVR	42.08 (1.33)	49.18 (0.72)	68.24 (0.91)	NA
	RanFor	49.87 (1.69)	46.59 (0.98)	66.92 (1.03)	76.53 (1.92)

3.4 Computational Speed

Besides better accuracy and easy one-step implementation, MCDA enjoys advantages in numerical stability and computational speed. Table 4 records the average computing times of MCDA and competing methods on some of the sample data sets. Times include imputation via *missForest* and identification of tuning constants, but not random deletion of entries. All runs were carried out on a 64-bit Windows 7 desktop computer. **MCDA is always faster than the competing methods, especially when conducted by the low-rank matrix fitting (LMAFit) algorithm (Wen et al. 2012; Shen et al. 2014).** Savings are more dramatic in underdetermined problems than overdetermined problems and when missing rates are lower. MCDA computing times are subject to further improvements if a faster SVD algorithm is swapped into the MM algorithm, or another matrix completion method is employed.

In general, the MM algorithm is fast, robust, and sure to converge. It is, however, by no means the fastest algorithm for matrix completion. To give the reader a feel for the speed of the MM algorithm versus competing algorithms, we randomly populated the entries of two matrices $\mathbf{A}$ and $\mathbf{B}$ of dimensions $n_1 \times r$ and $r \times n_2$ with standard normal deviates. We then computed the rank r product $\mathbf{M} = \mathbf{AB}$, added random deviates with standard deviation 0.001 to its entries, and randomly deleted a prescribed fraction of these perturbed entries. Table 5 displays the number of iterations until convergence and the total computing time for five methods: (a) the MM algorithm, (b) the singular value thresholding (SVT) algorithm in MATLAB (Cai et al. 2010), (c) the fixed point continuation (FPC) algorithm with approximate SVD in MATLAB (Ma et al. 2011), (d) the LMAFit algorithm in MATLAB (Wen et al. 2012; Shen et al. 2014), and (e) the iterative soft-thresholded svd (softImpute) algorithm in R (Hastie et al. 2014). FPC is

Table 4: Mean computing time (in seconds) for MCDA and other classification methods. Times include *missForest* imputations on the wine and glass data. Missing rates are 50% and 90%.

Missing	Classification	Wine	Glass	Colon	SRBCT
50%	MCDA	0.15	0.17	92.9	132.6
	MCDA+LMaFit	0.07	0.05	0.12	0.14
	missForest+LDA	2.41	2.15	3317.4	4159.4
	missForest+KNN(2)	2.40	2.14	3316.0	4157.8
	missForest+KNN	2.41	2.14	3316.1	4157.9
	missForest+OVR	2.43	NA	30431.5	3316.6
	missForest+RanFor	2.47	2.23	3316.8	4158.9
90%	MCDA	0.37	0.29	170.2	213.1
	MCDA+LMaFit	0.08	0.09	0.18	0.21
	missForest+LDA	0.45	NA	3895.0	5403.4
	missForest+KNN(2)	0.44	0.35	3894.0	5402.4
	missForest+KNN	0.45	0.35	3894.0	5402.4
	missForest+OVR	0.46	NA	3894.5	5181.9
	missForest+RanFor	0.46	0.66	3894.1	5181.2

less reliable compared to other algorithms and fails to converge if the standard deviation of the added noise exceeds 0.005. Examination of the table suggests that the MM algorithm is competitive if the tuning constant is well chosen.

Other contenders for fast matrix completion are mentioned in the literature. For example, the rank-one matrix update rule for SVD algorithms (Wang et al. 2014) and the ADMM algorithm for bi-linear decomposition (Glashoff and Bronstein 2012) could be more efficient than the algorithms tested here. From our vantage point, superior discrimination is more important than sheer speed.

Table 5: Computing time (in seconds) for the MM and other matrix completion algorithms

Size ($n_1 \times n_2$)	Rank r	Algorithm	# Iters	Time
150×300	10	MM	14	11.9
		SVT	500	30.6
		FPC	111	15.5
		LMaFit	28	0.06
		softImpute	128	0.89
150×300	50	MM	6	4.5
		SVT	500	47.1
		FPC	2230	330.9
		LMaFit	13	0.08
		softImpute	34	0.22
1000×1000	10	MM	2	1.78
		SVT	500	57.8
		FPC	323	1714.5
		LMaFit	41	0.48
		softImpute	243	35.99
1000×1000	100	MM	7	5.78
		SVT	59	92.2
		FPC	NA	NA
		LMaFit	8	0.57
		softImpute	71	8.86

4 Discussion

Our examples demonstrate the promise of MCDA in discriminant analysis with missing data. In ordinary discriminant analysis it would be hard to improve on established methods, and we make no claim to this effect. Given the ubiquity of missing data and the prevalence of big data in modern statistics, MCDA has the potential to improve inference. It is competitive on small data sets with low missing rates. Its edge in extreme circumstances likely stems from (a) combining the steps of imputation and classification, (b) encoding classes in a geometrically symmetric and parsimonious way, and (c) filling in missing entries by matrix completion. Matrix completion does entail shrinkage, but this should not distort classification much. The rule of assigning an unlabeled case to the closest class vertex works fine if shrinkage is spherically symmetric and keeps imputed points within the conical zones of assignment of the class vertices.

The rigorous assumptions under which matrix completion have been validated most likely can be relaxed. Our examples feature completely random deletion of predictors and case labels. Deletion of vertex coordinates is an all or nothing decision and obviously not completely random. We have applied matrix completion to SNP (single nucleotide polymorphism) imputation in genetics with considerable success despite highly nonrandom patterns of missingness (Chi et al. 2013). For example, individuals are often genotyped on different but overlapping SNP sets, creating a strongly structured missingness pattern in a study’s genotype matrix.

MCDA is fast and capable of handling large data sets. The MM algorithm is conceptually simple and numerically stable. Its speed can be improved by limiting its extraction of singular values and vectors to those

that enter the imputed matrix. Other algorithms may prove faster on large data sets, so we are inclined to keep an open mind about tweaking the computational engine. The biggest drawback of MCDA is that handling a new case requires rerunning the entire analysis. All unlabeled cases, including a new one, inform discrimination.

Establishing the theoretical correctness of MCDA will be a challenge. To our frustration we have not been able to prove Fisher consistency, the minimal theoretical requirement of a classification method. A loss function $L(\mathbf{y}, \mathbf{x})$ is said to be Fisher consistent if minimizing its average risk $E\{L[f(\mathbf{X}), \mathbf{Y}]\}$ under the assignment rule $f(\mathbf{x})$ leads to the optimal Bayes decision rule. Tackling the consistency of MCDA is difficult because it relies on a complicated penalty, cross validation, and murky rules for missing entries. In developing MCDA our intuitive reach has exceeded our rigorous grasp. We would be happy for help from other statisticians in resolving the thorny questions of theory.

Of greater urgency from our perspective is the development of new applications of MCDA. One potential application that comes to mind is medical diagnosis. Suppose we consider the 100 most common ailments. Patients are scored on many tests of blood chemistry, physiology, imaging, and family history. Given the expense of testing, most patients are scored on a small minority of the possible tests. Diagnostic data is highly structured, and unfortunately, missingness is hardly random. Yet good classification could point physicians in productive directions. Given the uncertainty of medical diagnosis, it probably would be a mistake to make hard class assignments. However, singling out a few of the closest class vertices could inform judgments about what further tests to order. Obviously, a fairly large database of patient histories would be necessary to carry out this research agenda.

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