An Investigation of Methods for Handling Missing Data with Penalized Regression

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Abstract: We investigate methods for penalized regression in the presence of missing observations. This paper introduces a method for estimating the parameters which compensates for the missing observations. We first, derive an unbiased estimator of the objective function with respect to the missing data and then, modify the criterion to ensure convexity. Finally, we extend our approach to a family of models that embraces the mean imputation method. These approaches are compared to the mean imputation method, one of the simplest methods for dealing with missing observations problem, via simulations. We also investigate the problem of making predictions when there are missing values in the test set.

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1 Introduction

Incomplete data is often found in real world statistical applications. As most statistical methods are developed on an assumption of complete data, it is unclear how to apply a statistical method to a data set with missing values. Various approaches have been developed to deal with this problem[8]. In this paper, we focus on the missing observation problem in penalized regression.

First, we introduce an approach using a modified minimization criterion of penalized regression[6]. Reviewing the elastic net approach, given a data matrix $X \in \mathbb{R}^{N \times p}$ and a
Y. Choi and R. Tibshirani

response vector $Y \in \mathbb{R}^N$, the objective function is as follows:

$$
\min_{\beta \in \mathbb{R}^p} \left[ \frac{1}{2N} ||Y - X\beta||^2 + \lambda_1 ||\beta||_1 + \lambda_2 ||\beta||_2^2 \right].
$$

(1)

The objective function involves the data matrix $X$, so when there are missing values in $X$, it is difficult to construct a criterion for estimating $\beta$ in the first place. For our approach, assuming the observations are missing at random, we utilize an unbiased estimator of (1). Unlike the objective function, the unbiased estimator is not necessarily convex. In this case, we modify the unbiased estimator by adding an appropriate amount of $\ell_2$ regularization to make it convex. In this way, the computation is simple compared to other imputation methods, especially when there are numerous missing values. Thus, estimation using this approach, which in this paper we refer to as non-negative definite covariance approach, are mainly compared to the mean imputation method since it is one of the simplest. We compare the MSE of each approach via simulated data.

Additionally, we extend our approach to combine the non-negative definite covariance and the mean imputation methods by introducing a balancing parameter between these two approaches. As the combined method is a generalized method including the non-negative definite covariance approach and mean imputation methods, it can sometimes yield better results than either one. The role of the balancing parameter is investigated by simulated examples.

Along with the coefficient parameter estimation, we investigate practical issues in handling missing observations in a test set. Appropriate ways of running cross validation and predicting from an incomplete test set are discussed with examples.

2 Review of Penalized Regression

Penalized regression is a generalized version of ordinary linear regression. By adding a penalty term to an objective function of linear regression, the resulting estimators have useful properties such as variable selection and applicability to singular design matrices. Let $X \in \mathbb{R}^{N \times p}$ be a data matrix and $Y \in \mathbb{R}^N$ be a response vector following the model $E(Y|X = x) = \beta_0 + \beta^T x$. The minimization criterion of penalized regression is as follows:

$$
\min_{(\beta_0, \beta) \in \mathbb{R}^{p+1}} \left[ \frac{1}{2N} \sum_{i=1}^N \left( y_i - \beta_0 - x_i^T \beta \right)^2 + \lambda P_\alpha(\beta) \right]
$$

(2)

where

$$
P_\alpha(\beta) = (1 - \alpha) \frac{1}{2} ||\beta||_2^2 + \alpha ||\beta||_1 \quad \text{or} \quad P_\alpha(\beta) = \sum_{j=1}^p \left[ \frac{1}{2}(1 - \alpha) \beta_j^2 + \alpha |\beta_j| \right].
$$
By solving the subgradient equations of (2) with respect to $\beta_j$, we have
\[
\tilde{\beta}_j \leftarrow S \left( \frac{1}{N} \sum_{i=1}^{N} x_{ij} (y_i - \tilde{y}_i^{(j)}), \lambda \alpha \right)
\]
\[
\frac{1}{N} \sum_{i=1}^{N} x_{ij}^2 + \lambda (1 - \alpha)
\]
(3)

Here, we used $\tilde{y}_i^{(j)} := \tilde{\beta}_0 + \sum_{l \neq j} \tilde{\beta}_l x_{il}$, the fitted value ignoring the role of $j^{th}$ variable and $S(z, \gamma) := \text{sign}(z)(|z| - \gamma)_+$, a soft-thresholding operator. $\beta$ can be estimated by the cyclic coordinate descent update using the formula (3).

Here, note that $\tilde{y}_i^{(j)} = \hat{y}_i - \tilde{\beta}_j x_{ij}$ where $\hat{y}_i$ is a fitted value using the full model. Thus,

\[
\sum_{i=1}^{N} x_{ij} (y_i - \tilde{y}_i^{(j)}) = \sum_{i=1}^{N} x_{ij} (y_i - \hat{y}_i) + \sum_{i=1}^{N} x_{ij}^2 \tilde{\beta}_j
\]

\[
= \langle X^{(j)}, Y \rangle - \langle X^{(j)}, \hat{Y} \rangle + \tilde{\beta}_j \langle X^{(j)}, X^{(j)} \rangle
\]

\[
= \langle X^{(j)}, Y \rangle - \sum_{|\tilde{\beta}_k| > 0} \tilde{\beta}_k \langle X^{(j)}, X^{(k)} \rangle + \tilde{\beta}_j ||X^{(j)}||_2^2.
\]

where $X^{(j)}$ denotes the $j^{th}$ column of the data matrix $X$. Now, rewriting (3) in a covariance sense, it becomes

\[
\tilde{\beta}_j \leftarrow S \left( \frac{1}{N} \langle X^{(j)}, Y \rangle - \sum_{|\tilde{\beta}_k| > 0} \tilde{\beta}_k \langle X^{(j)}, X^{(k)} \rangle + \tilde{\beta}_j ||X^{(j)}||_2^2, \lambda \alpha \right)
\]

\[
\frac{1}{N} ||X^{(j)}||_2^2 + \lambda (1 - \alpha)
\]

3 Penalized Regression with Missing Observations

3.1 Existing Methods

There are several existing methods for handling the missing values problem not only for the penalized regression but for general statistical analysis. Complete case analysis, mean imputation, likelihood-based methods and low rank matrix completion are popular methods to deal the missing values and each method has its motivations and merits\[8\]\[2\]. We also discuss an approach in Loh and Wainwright\[9\] which also is motivated from an unbiased estimator of an objective function for estimating parameters like the non-negative definite covariance approach.

Complete case analysis is one of the most basic ways to confront the missing value problem. This approach ignores all the data points containing any missing feature and uses only complete data points as its inputs\[8\]. This method is solid in a sense that it does not use any contaminated data, but also has the drawback of wasting potentially meaningful information.

Along with complete case analysis, mean imputation is popular for its simplicity. It imputes the mean of all available cases of a feature for the missing observations for that feature\[8\].
The Likelihood-based approach, like the mean imputation method, imputes the missing values in some manner. Assuming some distribution for the features, in the likelihood-based approach missing values are imputed using the EM algorithm. Multiple items can be imputed simultaneously in a systematic manner and sometimes this can be computationally expensive depending on the model assumptions [8].

Instead of imputing missing entries, the low rank matrix completion method approximates a data matrix based on the singular value decomposition [2]. This method is appropriate when the positions of missing entries are not too informative and an original matrix is amenable to low rank approximation.

Loh and Wainwright [9] suggest using an unbiased estimator of an objective function to estimate coefficients $\beta$ in regression when data is partially observed or noisy. This approach provides statistical error bounds of estimated $\hat{\beta}$ and also shows polynomial convergence time to global minimum when the gradient descent algorithm is implemented.

3.2 Non-negative Definite Covariance Approach

Our approach uses an unbiased estimator of (2) for estimating a true parameter $\beta$, where unbiasedness is with respect to a missing pattern of observations. Under common assumptions of missing features, such as uniform distribution and independence within and between features, calculation of the unbiased estimator is straightforward. The unbiased estimator, however, can be non-convex without extra conditions on $\beta$ and thus inconvenient as an optimization criterion. We avoid this problem by coercing the estimator of covariance matrix $\frac{1}{N}X'X$ to be non-negative definite. Using a non-negative definite covariance matrix estimator, the objective function becomes convex and thus is more attractive for optimization.

3.2.1 Unbiased Estimator of the Minimization Criterion

In this paper, we adopt three basic assumptions of the missing pattern in our data matrix: the existence of missing observations is independent in both within a column and between feature spaces and is uniformly random within each feature space. To be specific, we define $O \in \mathbb{R}^{N \times p}$ to be an indicator matrix of observations where $N$ and $p$ represent a number of data points and a dimension of feature space respectively:

$$O_{ij} := I\{x_{ij} \text{ non-missing}\},$$

$$O_{ij} \sim \text{Uniform and i.i.d for fixed } j, \text{ and for } i = 1, ..., N,$$

$$O_{ij} \text{ and } O_{ik} \text{ are independent for fixed } i \text{ and for } j \neq k \in \{1, ..., p\}.$$  

Construction of an unbiased estimator of (2) is simple under these assumptions. Given a fully-observed standardized data matrix $X$ and a response vector $Y$ as in the previous section, we define $Z \in \mathbb{R}^{N \times p}$ as an observed data matrix, $N_j$ as a number of observed data points in the $j^{th}$ feature and $N_{jk}$ as a number of observed data points in both $j^{th}$
and $k^{th}$ features. We rewrite these as follows:

$$Z_{ij} := O_{ij} \cdot X_{ij}, \quad N_j := \sum_{i=1}^{N} O_{ij} \quad \text{and} \quad N_{jk} := \sum_{i=1}^{N} O_{ij} \cdot O_{ik}. $$

Then the unbiased estimator of (2) with respect to the random variable $O$ is as follows:

$$\frac{1}{2} \left( \beta^t C_{ZZ} \beta - 2 C_{YZ} \beta + ||Y||_2^2 \right) + \lambda P_\alpha(\beta) \tag{4}$$

where $C_{ZZ} \in \mathbb{R}^{p+1 \times p+1}$ and $C_{YZ} \in \mathbb{R}^{1 \times p}$ such that

$$[C_{ZZ}]_{ij} = \begin{cases} 
\langle Z^{(i)}, Z^{(j)} \rangle / N_{ij} & \text{if } i \neq j \\
||Z||_2 / N_j & \text{if } i = j
\end{cases} \quad \text{and} \quad [C_{YZ}]_j = \langle Y, Z^{(j)} \rangle / N_j. \tag{5}$$

### 3.2.2 Modification for convexity

Noting that $C_{ZZ}$ is not necessarily non-negative definite, (4) can be non-ideal for optimization without constraining the range of $\beta$. We make $C_{ZZ}$ non-negative definite by adding an additional term, converting (4) to be tractable by the second order condition of convexity. Specifically, when $C_{ZZ}$ is negative definite, it is replaced by $C_{ZZ} + \gamma I_p$ for $\gamma > \Lambda_{min}$ where $\Lambda_{min}$ is the smallest eigen value of $C_{ZZ}$. The modified objective function is:

$$\frac{1}{2} \left( \beta^t (C_{ZZ} + \gamma I_p) \beta - 2 C_{YZ} \beta + ||Y||_2^2 \right) + \lambda P_\alpha(\beta) \quad \text{for } \gamma > |\Lambda_{min}| I_{\{\Lambda_{min} < 0\}}. \tag{6}$$

After reparameterization, it can be rewritten as

$$\frac{1}{2} \left( \beta^t C_{ZZ} \beta - 2 C_{YZ} \beta + ||Y||_2^2 \right) + \lambda_1 ||\beta||_{l_1} + \lambda_2 ||\beta||_{l_2} \tag{6}$$

where $\lambda_2 > \frac{1}{2} |\Lambda_{min}| I_{\{\Lambda_{min} < 0\}}$, or equivalently,

$$\frac{1}{2} \left( \beta^t C_{ZZ} \beta - 2 C_{YZ} \beta + ||Y||_2^2 \right) + \lambda \left( \alpha ||\beta||_{l_1} + \frac{1}{2} (1 - \alpha) ||\beta||_{l_2}^2 \right) \tag{7}$$

with $\lambda (1 - \alpha) > |\Lambda_{min}| I_{\{\Lambda_{min} < 0\}}$, $\lambda \leftarrow \lambda + |\gamma|$ and $\alpha \leftarrow \frac{\lambda}{\lambda + |\gamma|}$. One remarkable thing is that this effort to compensate non-convexity in (6), has resulted in optimization criterion of penalized function again as in (6) or (7). A change from the original criterion (2) is the range of regularization parameters. Now, $\beta$ can be estimated by minimizing (7) using cyclic coordinate descent as in section 2 [5, 3]:

$$\tilde{\beta}_j \leftarrow S(\frac{1}{N_j} \langle Z^{(j)}, Y \rangle - \sum_{i=1}^{N} \beta_k > 0 \frac{\beta_k}{N_j} (Z^{(j)} Z^{(k)}) \lambda_0), \frac{1}{N_j} ||Z^{(j)}||_{l_2}^2 + \lambda (1 - \alpha) \right) . \tag{8}$$
Note that the meaningful upper bound for $\lambda$ would be $\lambda < \frac{1}{\alpha} \max_{j \in \{1, 2, \ldots, p\}} \left| \frac{\langle Z(j), Y \rangle}{N} \right|$ since beyond this threshold, the estimated $\hat{\beta}$ is estimated to be 0. Combining this with the bound from (7), the valid range of $\lambda$ and $\alpha$ are as follow:

$$\lambda \alpha \in \left[ 0, \max_{j \in \{1, \ldots, p\}} \left| [C_{YZ}]_j \right| \right]$$

and $\alpha \in \left[ 0, \max_{j \in \{1, \ldots, p\}} \left| [C_{YZ}]_j \right| \right]$. 

### 3.2.3 Test Set Prediction and Cross Validation

When there are missing observations in a test set, it is unclear how to make a prediction on the set. For the same reason, applying cross validation is problematic. Here we impute the incomplete test observations using conditional expectations. After imputing the incomplete test data, we can apply estimated $\beta$ directly. To be specific, when observations of features $j = j_1, \ldots, j_k$ for $i$th data point in test are missing, we used

$$\left( \hat{X}_{ij_1}^{test}, \ldots, \hat{X}_{ij_k}^{test} \right) = E \left[ (X_{ij_1}, \ldots, X_{ij_k}) \mid \{X_{ij} \mid j \neq j_1, \ldots, j_k\} \right]$$

where $X_i \sim N_p(\mu, \Sigma)$. (9)

We use the training mean for $\mu$ and $C_{zz} + (|\Lambda_{\text{min}}| + \lambda(1 - \alpha)) I_p$ for $\Sigma$ where $\lambda$ and $\alpha$ are regularization parameters in (7). An extra term $\lambda(1 - \alpha) I_p$ is added to $C_{ZZ}$ which is element-wise unbiased estimator of the true $\Sigma$ to avoid singularity, since the conditional expectation of multivariate normal distribution involves an inverse of submatrix of $\Sigma$. For the case when $\alpha = 1$ and the extra term vanishes, a pseudo inverse is used if a submatrix of interest is singular.

### 3.2.4 Comparison of Non-negative Definite Covariance Approach and Mean Imputation

In this section, we discuss the performance of the non-negative definite covariance approach in comparison to mean imputation via simulated data under various settings. In every instance, the data is generated under a linear model:

$$Y = X \beta + \epsilon, \; \epsilon \sim N(0, \sigma^2 I_p)$$

with fixed $N = 50$ and $p = 15$ where $X$ is generated under multivariate normal distribution:

$$X \sim N(\mu, \Sigma).$$

The coefficient $\beta$ is fixed to be $\beta = (0, 2, 2, 2, 0, \ldots, 0)$ and $\sigma$ is set to have signal-to-ratio of 4. The covariates corresponding to non-zero and zero entries in $\beta$ are considered to be true signals and dummies respectively. We investigated 12 scenarios which are combinations of three types of missing pattern and 4 types of $\Sigma$ of a data matrix $X$. 
For the 3 missing patterns, a case when missing observations are concentrated on the signals, a case when missing rate is uniform over all covariates and a case when missing observations are concentrated on dummy variables are investigated:

\[
O_{ij} \sim \begin{cases} 
\text{Bernoulli}(\gamma) & \text{if missing rate is uniform} \\
\text{Bernoulli}(2\gamma^2 - \frac{2p-2i+1}{2p}) & \text{if missing rate is high on signals} \\
\text{Bernoulli}(2\gamma^2 - \frac{2i-1}{2p}) & \text{if missing rate is high on dummy variables}
\end{cases}
\]

Here \(\gamma\) denotes for the average missing rate in each case and we used \(\gamma = 0.25\) for all cases. For \(\Sigma\), we tried the four following cases:

\[
\Sigma_i = \sigma^2 \begin{bmatrix} 1 & \rho_1 & \ldots & \rho_i \\ \rho_1 & 1 & \ldots & \rho_i \\ \vdots & \vdots & \ddots & \vdots \\ \rho_i & \ldots & \rho_i & 1 \end{bmatrix}
\]

with \(\rho_1 = 0, \rho_2 = 0.5, \) and \(\rho_3 = 0.75\) (10)

and \([\Sigma_4]_{ij} = \rho|i-j|\) with \(\rho = 0.5\). (11)

To investigate the efficacy of the methods, the MSE of \(X\hat{\beta}\) was used. The MSE \(E[(X\hat{\beta} - X\beta)^2]\) is estimated over 300 repetitions where the expectation is over an observation \(O\) and noise \(\epsilon\). Figure 1 and table 1 show that NONDC works better than mean imputation method when missing rate is high on signals while mean imputation method surpasses NONDC when missing rate is high on dummy variables. The non-negative definite covariance technique amplifies values in covariance matrix corresponding to high missing rate by scaling these elements by larger values of \(\frac{1}{N_{jk}}\). As a result, when missingness is concentrated on signals, the role of significant covariates is emphasized leading to a good estimation.

### 3.3 A Combined Approach

The simulated examples show that neither the non-negative definite covariance approach nor the mean imputation method dominates. Thus, an approach embracing both methods might be beneficial. Here we combine these two methods by introducing a new parameter \(\eta\) which can be interpreted as a balancing parameter of the two competing methods.

#### 3.3.1 Implementation

The basis of the non-negative definite covariance approach is to replace the covariance matrix \(X'X\) and \(X'Y\) by \(C_{XX}\) and \(C_{XY}\) defined in (5). The combined approach amends (5) so that it can embrace the mean method:

\[
[C^\eta_{ZZ}]_{ij} = \begin{cases} 
\left(\frac{1-\eta}{N} + \frac{\eta}{N}\right) \langle Z^{(i)}, Z^{(j)} \rangle & \text{if } i \neq j \\
\left(\frac{1-\eta}{N} + \frac{\eta}{N}\right) \|Z\|^2 & \text{if } i = j \end{cases}
\]

and \([C^\eta_{YZ}]_{j} = \left(1-\eta \frac{N}{N} + \eta \frac{N}{N}\right) \langle Y, Z^{(j)} \rangle \) for \(\eta \in [0, 1] \).
Figure 1: Plots of estimated MSE of the 12 scenarios over 300 trials. Error bars contain the mean value and ±1 se of the mean. For each plot, α is fixed at the point which bears the global minimum. The cases in which missing rate is high on signals(left column), the cases in which missing rate is uniform for all covariates(middle column) and the cases in which missing rate is high on dummy variables(right column) are plotted in the figure. The data matrix $X$ in the $i$th row is generated under multivariate normal distribution with covariance matrix proportional to $\Sigma_i$ as in (11).
Penalized Regression with Missing Observations

Global Minimum MSE

| Σ in  | Approach | Missing rate  |
|-------|----------|---------------|
|       |          | High on | Uniform | High on |
|       |          | signals |         | dummy  |
|       |          |         |         | variables |
| Σ₁    | NONDC    | 0.53 (0.42) | 0.29 (0.24) | 0.12 (0.12) |
|       | MI       | 0.80 (0.49) | 0.33 (0.27) | 0.08 (0.07) |
| Σ₂    | NONDC    | 0.97 (0.49) | 0.67 (0.43) | 2.22 (0.53) |
|       | MI       | 1.59 (0.33) | 0.87 (0.44) | 1.16 (0.17) |
| Σ₃    | NONDC    | 0.80 (0.32) | 0.79 (0.37) | 1.56 (0.19) |
|       | MI       | 1.12 (0.22) | 0.83 (0.26) | 0.19 (0.16) |
| Σ₄    | NONDC    | 0.51 (0.40) | 0.27 (0.22) | 0.09 (0.08) |
|       | MI       | 0.70 (0.52) | 0.28 (0.24) | 0.08 (0.06) |

Table 1: Global minimum MSE over regularization parameters α and λ of 12 different scenarios. Each cell represents one scenario with two different methods (the non-negative definite covariance and the mean imputation). Non-negative definite covariance approach and mean imputation method are referred to as NONDC and MI respectively. Global minimum MSE for each case is estimated over 300 trials. The values in parenthesis are corresponding 1 se.

This is identical to the non-negative definite covariance approach when η = 0 while it is equivalent to mean imputation for η = 1. For η between 0 and 1, this approach inherits advantages of both methods. As the only changes in the combined method from the non-negative definite covariance method are $C_{ZZ}$ and $C_{ZY}$, we can estimate $\hat{\beta}$ in the same manner as in the non-negative definite covariance approach just by plugging $C_{ZZ}^\eta$ and $C_{ZY}^\eta$ into the corresponding places in (4). Thus the objective function in this combined approach is

$$\frac{1}{2} (\beta^T C_{ZZ}^\eta \beta - 2C_{YZ}^\eta \beta + ||Y||_2^2) + \lambda \left( \alpha ||\beta||_1 + \frac{1}{2} (1 - \alpha) ||\beta||_2^2 \right).$$

Again $\hat{\beta}$ can be estimated by cyclic coordinate descent as follows:

$$\hat{\beta}_j \leftarrow \frac{S([C_{ZY}^\eta]_j - \sum_{k:\hat{\beta}_k > 0} \hat{\beta}_k [C_{ZZ}^\eta]_{jk}, \lambda \alpha)}{[C_{ZZ}^\eta]_{jj} + \lambda (1 - \alpha)}.$$  

with the range of $\alpha$ and $\lambda$ being

$$\lambda \alpha \in \left[0, \frac{\max_j |C_{YZ}^\eta|}{\Lambda_{\text{min}} I_{\Lambda_{\text{min}} < 0}} \right]$$  

and

$$\alpha \in \left[0, \frac{\max_j |C_{YZ}^\eta|}{\Lambda_{\text{min}} I_{\Lambda_{\text{min}} < 0}} + \max_j |C_{YZ}^\eta| \right]$$

where $\Lambda_{\text{min}}$ is the smallest eigen value of $C_{ZZ}^\eta$. 
Global Minimum MSE

| Σ in X ~ N(µ, σ²Σ) | Approach | Missing rate |
|---------------------|----------|--------------|
|                     |          | High on signals | Uniform | High on dummy variables |
| Σ₁                  | Comb     | 0.53 (0.42)     | 0.29 (0.25)   | 0.08 (0.07)   |
|                     | NONDC    | **0.53 (0.42)** | 0.29 (0.24)   | 0.12 (0.12)   |
|                     | MI       | 0.80 (0.49)     | 0.33 (0.27)   | **0.08 (0.07)** |
| Σ₂                  | Comb     | 0.97 (0.49)     | **0.65 (0.40)** | 0.16 (0.17)   |
|                     | NONDC    | **0.97 (0.49)** | 0.67 (0.43)   | 2.22 (0.53)   |
|                     | MI       | 1.59 (0.33)     | 0.87 (0.44)   | **0.16 (0.17)** |
| Σ₃                  | Comb     | 0.80 (0.32)     | **0.71 (0.33)** | 0.18 (0.15)   |
|                     | NONDC    | **0.80 (0.32)** | 0.79 (0.37)   | 1.56 (0.19)   |
|                     | MI       | 1.12 (0.22)     | 0.83 (0.26)   | 0.19 (0.16)   |
| Σ₄                  | Comb     | 0.51 (0.40)     | **0.26 (0.23)** | 0.07 (0.06)   |
|                     | NONDC    | **0.51 (0.40)** | 0.27 (0.22)   | 0.09 (0.08)   |
|                     | MI       | 0.70 (0.52)     | 0.28 (0.24)   | 0.08 (0.06)   |

Table 2: Global minimum MSEs over regularization parameters α and λ of 12 different scenarios. Each cell represents one scenario with 3 different methods (the combined approach, the non-negative definite covariance approach and the mean imputation). The combined method, the non-negative definite covariance approach and the mean imputation method are referred to as Comb, NONDC and MI respectively. The Global minimum MSE for each case is estimated over 300 trials. The values in parentheses are corresponding 1 se. The smallest value among three different approaches in a cell is represented in bold letter.

In the combined method, predicting the values in an incomplete test set can be conducted in the same manner as in the non-negative definite covariance approach. Like the non-negative definite covariance approach, we use conditional expectation on assuming multivariate normal distribution on a feature space. In the combined method, we estimate Σ by $C_{ZZ}^\alpha + (|\Lambda_{min}| + \lambda(1-\alpha)) I_p$ in which $C_{ZZ}$ in [9] is replaced by $C_{ZZ}^\alpha$. Again, when $\alpha = 1$ and Σ becomes singular, pseudo inverse is used for conditional expectation.

3.3.2 Simulation Results

In this section, we will first compare the performance of the mean imputation method, the non-negative definite covariance approach and the combined method. Second, we will discuss the ability of the combined method in choosing proper regularization parameters using cross validation. Finally, we will evaluate test error values of the combined method. The simulation settings in this section are the same as in section 3.2.4. For an incomplete test set imputation for evaluating both cross validation and test error, we used 3 different types of Σ in [11]: $\Sigma = C_{ZZ} + (|\Lambda_{min}| + \lambda(1-\alpha)) I$, $\Sigma = I$ and $\Sigma = \Sigma_{true}$, the true covariance of a given design matrix $X$. $\Sigma = C_{ZZ} + (|\Lambda_{min}| + \lambda(1-\alpha)) I$ is the
Penalized Regression with Missing Observations

Figure 2: Plots of estimated minimum MSEs over 300 trials of combination of 4 different data structure and 3 different missing patterns. Each line represents the minimum MSEs of one scenario. The minimum MSE at given $\eta$ is achieved over $\alpha$ and $\lambda$. Each plot represents one of the data structures noted in (11). Cases when the covariance matrix of the matrix $X$ is $\Sigma_1$ (top left), $\Sigma_2$ (top right), $\Sigma_3$ (bottom left) or $\Sigma_4$ (bottom right) are shown. Lines in each plot represent 3 different missing patterns. The case in which missing rate is high on signals (red line), the case in which missing rate is uniform over features (green line) and the case in which missing rate is high on dummy variables (blue line) are plotted. A solid dot in each line represents the global minimum of the corresponding case.
Table 3: Test errors evaluated at optimal \((\alpha, \lambda, \eta)\) of 9 different scenarios. Each cell represents one scenario with 3 different \(\Sigma\) used for an incomplete test set imputation. \(\Sigma_{\text{est}}\) represents \(C_{ZZ} + (|\Lambda_{\text{min}}| + \lambda(1 - \alpha))I\) which is the suggested method in this paper while \(\Sigma_{\text{true}}\) denotes the true covariance matrix of the data matrix \(X\). \(\Sigma_{\text{true}}\) and \(I\) are presented for reference. The optimal \((\alpha, \lambda, \eta)\) in each setting is estimated to be the point which yields the global minimum MSE which is estimated over 300 repetitions. Test error values are estimated over 50 trials. The values in parenthesis are corresponding 1 se. The smaller value between \(\Sigma_{\text{est}}\) and \(I\) is represented in bold letter.
Penalized Regression with Missing Observations

Ratio of Global Minimum MSE and MSE at \((\hat{\alpha}, \hat{\lambda}, \hat{\eta})\) Chosen by Cross Validation

| Covariance of X | Σ used for test set imputation | Missing rate | | | |
|----------------|--------------------------------|--------------|---|---|
|                |                                | High on signals | Uniform | High on dummy variables |
| Σ₁              | Σ_{est}                        | 1.55 (0.32)   | 1.62 (0.55) | 2.20 (1.37) |
|                 | I                              | 1.60 (0.29)   | 1.49 (0.61) | 1.92 (0.98) |
|                 | Σ_{true}(= Σ₁)                 | 1.60 (0.29)   | 1.49 (0.61) | 1.92 (0.98) |
| Σ₂              | Σ_{est}                        | 1.50 (0.35)   | 1.64 (0.47) | 1.49 (0.33) |
|                 | I                              | 2.09 (0.32)   | 1.91 (0.68) | 2.01 (0.82) |
|                 | Σ_{true}(= Σ₂)                 | 1.43 (0.27)   | 1.21 (0.23) | 1.49 (0.42) |
| Σ₃              | Σ_{est}                        | 1.34 (0.24)   | 1.44 (0.24) | 1.18 (0.14) |
|                 | I                              | 1.69 (0.15)   | 1.59 (0.29) | 1.73 (0.60) |
|                 | Σ_{true}(= Σ₃)                 | 1.33 (0.25)   | 1.19 (0.30) | 1.20 (0.17) |

Table 4: Ratio of global minimum MSE and MSE at \((\hat{\alpha}, \hat{\lambda}, \hat{\eta})\) chosen by cross validation of 9 different scenarios. Each cell represents one scenario with 3 different Σ used for an incomplete test set imputation. Σ_{est} represents \(CZZ + (|\Lambda_{\min}| + \hat{\lambda}(1 - \hat{\alpha}))I\) which is the suggested method in this paper while Σ_{true} denotes the true covariance matrix of the data matrix X. Σ_{true} and I are presented for reference. The ratio values are estimated over 50 trials. The values in parenthesis are corresponding 1 se. The smaller value between Σ_{est} and I is represented in bold letter.

4 Conclusion

This paper discusses the problem of applying penalized regression when observations are absent. We first proposed the non-negative definite covariance approach, which forms an unbiased estimator of the objective function and then modifies it to ensure convexity. We extended this approach by combining with the mean imputation method. We also discussed practical issues such as choosing the optimization parameters and predicting \(\hat{y}\) in case test observations are incomplete.

Further investigation of these estimators and their properties would be valuable, especially in big data settings.
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