Conditional Uncorrelation and Efficient Non-approximate Subset Selection in Sparse Regression

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Abstract

Given $m$ $d$-dimensional responsors and $n$ $d$-dimensional predictors, sparse regression finds at most $k$ predictors for each respensor for linearly approximation, $1 \leq k \leq d - 1$. The key problem in sparse regression is subset selection, which usually suffers from the high computational cost. Here we consider sparse regression from the view of correlation, and propose the formula of conditional uncorrelation. Then an efficient non-approximate method of subset selection is proposed in which we do not need to calculate any linear coefficients for the candidate predictors. By the proposed method, the computational complexity is reduced from $O(\frac{1}{2}k^3 + kd)$ to $O(\frac{1}{3}k^3)$ for each candidate subset in sparse regression. Because the dimension $d$ is generally the number of observations or experiments and large enough, the proposed method can significantly improve the efficiency of sparse regression.

Key words: conditional uncorrelation, non-approximate method, sparse regression, subset selection, multivariate correlation.

1. INTRODUCTION

The concept of regression, along with the concept of correlation, was firstly discussed by Galton in 1885 [4]. Ten years later, the inner-product correlation coefficient was developed by Pearson. Then the simple regression question can be well solved with the help of Pearson’s correlation coefficient [5]. However, because there was no compact formulation to define the correlation among multiple variables for a long time, people had to analyze the multivariate regression question by the hat-matrix method.

Consider the sparse regression problem with $m$ $d$-dimensional responsors $y_1, y_2, \ldots, y_m$ and $n$ $d$-dimensional predictors $x_1, x_2, \ldots, x_n$. For each respensor $y \in \{y_1, y_2, \ldots, y_m\}$, at most $k$ predictors are selected to linearly predict $y$, $1 \leq k \leq d - 1$. The target of sparse regression is to minimize the $l_2$ distance between $y$ and the optimum linear combination of the selected predictors. At present, the applications of sparse regression
can be classified into two categories. In the problems belonged to the first category, such as approximate sparse representation, the approximate methods of sparse regression play important roles. For the problems in the second category, like association detection in data, the non-approximate sparse regression is widely used. In recent years, many works have been conducted to improve the efficiency of approximate sparse regression. However, the non-approximate method receives little attention.

The sparse regression problem mentioned above is usually discussed with a fixed sparsity parameter $k$. Without loss of generality, suppose that $x_1, x_2, \ldots, x_k$ are the predictors we are considering for the responder $y$, then

$$y = \beta_0 \mathbf{1} + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + e,$$  \hspace{1cm} (1)

where $\mathbf{1}$ is the vector with all ones, $e$ is the residual, and $\beta_i$ is the scalar coefficients of $x_i$, $i = 1, 2, \ldots, k$.

In the traditional multivariate regression, we let $X = [\mathbf{1}, x_1, x_2, \cdots, x_k]$ and $\beta = [\beta_0, \beta_1, \beta_2, \cdots, \beta_k]^T$, then $y = X \beta + e$. Finally, we have

$$\hat{\beta} = (X^T X)^{-1} X^T y$$
$$\hat{y} = X (X^T X)^{-1} X^T y$$
$$e = y - X ((X^T X)^{-1} (X^T y))$$  \hspace{1cm} (2)

where $\hat{\beta}$ and $\hat{y}$ are the estimated vectors of $\beta$ and $y$, respectively, and $X (X^T X)^{-1} X^T$ is the hat matrix. The hat-matrix method appeared no later than the 1960s, and has always been an important tool in various fields.

To select $k$ predictors from the predictor set for a responder $y$, we need to consider all the possible subsets with $k$ predictors ($k$-subset), which is called subset selection. According to Eq. 2 before calculating $e$ and the $l$-2 norm of $e$ for subset selection, we have to compute the linear coefficients for each $k$-subset. Moreover, the dimension $d$ of the responders and predictors is generally the number of observations or experiments in statistics and experimental analysis, which is usually large enough. As the size of hat matrix is $d \times d$, the hat-matrix method has a high computational cost.

In the era of big data, we urgently need an efficient non-approximate sparse regression method to detect associations among data in large data sets. However, hat-matrix method, which has been used over fifty years, does not meet the needs.
According to Equation 1, sparse regression problem is essentially a correlation problem among the predictors $x_1, x_2, \cdots, x_k$ and the responser $y$. Here we discuss it from the view of correlation. We have proposed a pair of measures for multivariate correlation, namely, the unsigned correlation coefficient (UCC) $r$ and the unsigned uncorrelation coefficient (UUC) $\omega$ [7,8]. If $R$ is the correlation matrix of the variables $x_1, x_2, \cdots, x_k$, then $r$ and $\omega$ are defined, respectively, as following:

$$
\begin{align*}
r^2 &= 1 - \det(R) \\
\omega^2 &= \det(R).
\end{align*}
$$

Many important properties and visual figures show that UCC and UUC are general measures for multivariate correlation [8].

In this paper, the formula of conditional uncorrelation are derived based on multivariate correlation firstly, based on which an efficient non-approximate subset selection method is proposed. Compared with the hat-matrix method, the correlation-based method does not need to compute for linear coefficients in subset selection, thereby considerably improving the efficiency of sparse regression.

2. CONDITIONAL UNCORRELATION

In sparse regression, it is the target to minimize the mean square error (MSE) between the target vector $y$ and its estimated vector $\hat{y}$:

$$
\text{MSE}(y, \hat{y}) = \frac{1}{d} \| y - (\beta_0 1 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k) \|_2^2.
$$

where $d$ is the dimension of the involved vectors.

Let the standard deviations of the elements in $y$ and $\hat{y}$ are $\sigma_y$ and $\sigma_{\hat{y}}$, respectively, the means of the elements in $x_i$, $y$, and $\hat{y}$ are $\mu_i$, $\mu_y$, and $\mu_{\hat{y}}$, respectively, and the covariances between $x_i$ and $y$, between $x_i$ and $x_j$, and between $y$ and $\hat{y}$ are $\sigma_{iy}$, $\sigma_{ij}$, and $\sigma_{y\hat{y}}$, respectively, $i, j = 1, 2, \cdots, k$. If $x = (x_1, x_2, \cdots, x_d)^T$ and $y = (y_1, y_2, \cdots, y_d)^T$, here the variance of the elements in $x$ is defined as $\sigma_x^2 = \frac{1}{d} \sum_{i=1}^{n} (x_i - \mu_x)^2$, and the covariance between $x$ and $y$ is defined as $\sigma_{xy} = \frac{1}{d} \sum_{i=1}^{n} (x_i - \mu_x)(y_i - \mu_y)$. Then

$$
\begin{align*}
\sigma_{\hat{y}}^2 &= \sum_i \beta_i^2 \sum_j \beta_j \sigma_{ij} \\
\sigma_{y\hat{y}} &= \sum_i \beta_i \sigma_{iy}.
\end{align*}
$$

3
To minimize the value of MSE between $y$ and $\hat{y}$ by the least square method, we have

$$\mu_y = \mu_{\hat{y}} = \hat{\beta}_0 + \hat{\beta}_1 \mu_1 + \hat{\beta}_2 \mu_2 + \cdots + \hat{\beta}_k \mu_k$$

$$\sum_j \hat{\beta}_j \sigma_{ij} = \sigma_{iy}$$

$$\text{MSE}(y, \hat{y}) = \sigma_y^2 - 2\sigma_y \hat{\sigma} + \hat{\sigma}^2$$

$i = 1, 2, \cdots, k$. Then

$$\sigma_y^2 = \sum_i \hat{\beta}_i \sum_j \hat{\beta}_j \sigma_{ij} = \sum_i \hat{\beta}_i \sigma_{iy} = \sigma_{y\hat{y}}.$$  \hfill (7)

Let $\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1k} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{k1} & \sigma_{k2} & \cdots & \sigma_{kk} \end{bmatrix}$, $\hat{\beta} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix}$, $\sigma_y = \begin{bmatrix} \sigma_{1y} \\ \sigma_{2y} \\ \vdots \\ \sigma_{ky} \end{bmatrix}$. According to the second equation in Eq. (6), we have

$$\hat{\beta} = \sigma^{-1} \sigma_y.$$  \hfill (8)

Combining Eqs. (7) and (8) we can obtain

$$\sigma_{y\hat{y}} = \sigma_{y\hat{y}} \sigma^{-1} \sigma_y.$$  \hfill (9)

Moreover,

$$\det \begin{bmatrix} \sigma & \sigma_y \\ \sigma^T_y & \sigma_y^2 \end{bmatrix} = \det(\sigma)(\sigma_y^2 - \sigma_{y\hat{y}} \sigma^{-1} \sigma_y).$$  \hfill (10)

Hence,

$$\text{MSE}(y, \hat{y}) = \sigma_y^2 - \sigma_{y\hat{y}} = \frac{\det \begin{bmatrix} \sigma & \sigma_y \\ \sigma^T_y & \sigma_y^2 \end{bmatrix}}{\det(\sigma)}$$

$$= \sigma_y^2 \cdot \frac{\omega^2(x_1, x_2, \cdots, x_k, y)}{\omega^2(x_1, x_2, \cdots, x_k)}.$$  \hfill (11)

For a responsor $y$, $\sigma_y^2$ is kept invariant. Then it comes to an interesting conclusion:

$$\min \text{MSE}(y, \hat{y}) \Leftrightarrow \min \frac{\omega^2(x_1, x_2, \cdots, x_k, y)}{\omega^2(x_1, x_2, \cdots, x_k)}.$$  \hfill (12)

The above conclusion in Eq. (12) provides the target function to choose predictors for a responsor $y$ in the correlation-based sparse regression.
Let \( r(y, \hat{y}) \) and \( \omega(y, \hat{y}) \) are the unsigned bivariate correlation coefficient (absolute value of Pearson’s correlation coefficient) and the unsigned bivariate uncorrelation coefficient between \( y \) and its estimated vector \( \hat{y} \), respectively, then

\[
r^2(y, \hat{y}) = \left( \frac{\sigma_{y\hat{y}}}{\sigma_y \sigma_{\hat{y}}} \right)^2 = \frac{\sigma_{y\hat{y}}^2}{\sigma_y^2} = 1 - \frac{\omega^2(x_1, x_2, \ldots, x_k, y)}{\omega^2(x_1, x_2, \ldots, x_k)}.
\]

Therefore,

\[
\omega(y, \hat{y}) = \frac{\omega(x_1, x_2, \ldots, x_k, y)}{\omega(x_1, x_2, \ldots, x_k)}.
\]

(13)

It shows from Eqs. (12 and 13) that the minimization of MSE\((y, \hat{y})\) is equivalent to minimizing the value of UUC between \( y \) and \( \hat{y} \), which is kept the same with the univariate case [6].

Here \( \omega(y, \hat{y}) \) is the uncorrelation between \( y \) and the optimum linear approximation constructed by \( x_1, x_2, \ldots, \) and \( x_k \) for \( y \). We can thus use \( \omega(y|x_1, x_2, \ldots, x_k) \) to denote \( \omega(y, \hat{y}) \). Then

\[
\omega(y|x_1, x_2, \ldots, x_k) = \frac{\omega(x_1, x_2, \ldots, x_k, y)}{\omega(x_1, x_2, \ldots, x_k)}.
\]

(14)

We call Eq. 13 and Eq. 14 as the formula of conditional uncorrelation, which offers the relation among the UUC between the target vector \( y \) and its estimated vector \( \hat{y} \), the UUC among these vector \( x_1, x_2, \ldots, x_m, y \), and the UUC among these predictor vectors \( x_1, x_2, \ldots, x_m \).

Additionally, the coefficient of multiple determination \( R^2 \) [3] can also be simplified as

\[
R^2 = \frac{SSR}{SSTO} = \frac{\sigma_{\hat{y}}^2}{\sigma_y^2} = \frac{\sigma_{y\hat{y}}^2}{\sigma_y^2} = r^2(y, \hat{y}).
\]

(15)

According to Eqs. (12–15), we have

\[
\min \text{MSE}(y, \hat{y}) \Leftrightarrow \max R^2 \Leftrightarrow \min \omega^2(y, \hat{y}).
\]

(16)

Therefore, in sparse regression, it is consistent for a responser \( y \) to select its predictors whether the target is to minimize MSE between \( y \) and \( \hat{y} \) or to maximize the coefficient of multiple determination.

Lastly, by minimizing the conditional uncorrelation of \( y \) we can select the best predictors for \( y \) according to Eq. (12). The linear coefficients of the selected predictors can be
computed by the following equation, which can be easily derived from Eq. (8):

\[
\begin{bmatrix}
\sigma_1 \hat{\beta}_1 \\
\sigma_2 \hat{\beta}_2 \\
\vdots \\
\sigma_k \hat{\beta}_k
\end{bmatrix} = \sigma_y R_{x}^{-1} \begin{bmatrix}
\rho_{1y} \\
\rho_{2y} \\
\vdots \\
\rho_{ky}
\end{bmatrix}
\]

(17)

where \( R_x \) is the correlation matrix of \( x_1, x_2, \ldots, x_k \), and \( \sigma_i \) is the standard deviation of the elements in \( x_i \), \( i = 1, 2, \ldots, k \). Then the formula system of the correlation-based multivariate regression is composed by Eqs. (11), (12), and (17).

3. EFFICIENT SUBSET SELECTION IN SPARSE REGRESSION

In sparse regression, we need to minimize \( l^{-2} \)-norm of the residual vector \( e \). For each subset, the time complexity \( T \) to compute \( l^{-2} \)-norm of \( e \) in the hat-matrix method is related to both \( d \) and \( k \) so that \( T = T(d, k) \) according to Eq. [2]. In the correlation-based sparse regression, we need to compute the ratio of two squared UUCs for each subset according to Eq. (12) so that \( T = T(k) \). As we use \( k \) predictors and the vector 1 to linearly approximate each \( d \)-dimensional response in sparse regression, when \( k = d - 1 \) the responses can be losslessly represented if these predictors are linearly independent. Generally, we have \( k \ll d - 1 \). Hence, the correlation-based sparse regression may be more efficient than the traditional regression method.

According to Eq. (12), we need to compute the ratio between the determinants of two correlation matrices. Here we optimize the computation by the method of matrix diagonalization. After diagonalization of a matrix, the determinant of the matrix is the product of all the diagonal elements. Suppose \( R_{xy} \) is the correlation matrix among \( x_1, x_2, \ldots, x_k, y \), and let the correlation coefficients related to \( y \) lie in the last row and last column of \( R_{xy} \). Because the product of the diagonal elements of \( R_x \) is kept the same with the product of the first \( k \) diagonal elements of \( R_{xy} \), the last diagonal elements of \( R_{xy} \) is just \( \omega^2(y, \hat{y}) \). Hence, we can compute the value of \( \omega^2(y, \hat{y}) \) according to Algorithm[1]. Because the first element is 1 in correlation matrix, we can further optimize the calculation of \( \omega^2(y, \hat{y}) \) according to Algorithm[2].

4. TIME COMPLEXITY ANALYSIS
Algorithm 1: Calculation of $\omega^2(y, \hat{y})$

**Input:** Correlation matrix $R_{xy}$ of $x_1, x_2, \cdots, x_k, y$

**Output:** $\omega^2(y, \hat{y})$

1. for $i \leftarrow 1$ to $k$
2.   recipdiag = $1 / R_{xy}[i][i]$
3.   for $j \leftarrow i + 1$ to $k + 1$
4.     temp = $R_{xy}[j][i] \times \text{recipdiag}$;
5.     for $p \leftarrow i + 1$ to $k + 1$
6.         $R_{xy}[j][p] = R_{xy}[j][p] - R_{xy}[i][p] \times \text{temp}$;
7.   end
8. end
9. return $R_{xy}[k + 1][k + 1]$

In sparse regression, the main time complexity comes from subset selection. Compared with subset selection, the computational complexity of other parts, such as calculation of inner products or correlation coefficients, is negligible. In the proposed method, we firstly obtain all the correlation coefficients between two predictors and all the correlation coefficients between the responsor and each predictor. Then in the process of subset selection, these correlation coefficients can be directly used to construct the correlation matrix $R_{xy}$. In the hat-matrix method, we also firstly compute all the inner products between two predictors and all the inner products between the responsor and each predictor. In the process of subset selection, the inner products can be directly used to construct $X^TX$ and $X^Ty$. Subsequently, we compute $\hat{\beta} = (X^TX)^{-1}X^Ty$ by the method of elementary row operations. Lastly, $e = y - X\hat{\beta}$ and the $l$-2 norm of $e$ are calculated for selecting the best subset.

The numbers of different operations in the proposed method and the hat-matrix method are provided in Table I from which we can see that the time complexity of the proposed method is $O(\frac{1}{3}k^3)$, and the time complexity of hat-matrix method is $O(\frac{1}{2}k^3 + kd)$. Because the dimension $d$ of the variables in regression is generally the number of observations or experiments, which is large enough, the proposed method can significantly improve the efficiency of sparse regression.
Algorithm 2: Calculation of $\omega^2(y, \hat{y})$

**Input:** Correlation matrix $R_{xy}$ of $x_1, x_2, \cdots, x_k, y$

**Output:** $\omega^2(y, \hat{y})$

1. for $i \leftarrow 1$ to $k$ do
   2. if $i \neq 1$ then
      3. recipdiag = $1 / R_{xy}[i][i]$;
      4. for $p \leftarrow i + 1$ to $k + 1$ do
         5. $R_{xy}[i][p] = R_{xy}[i][p] \times$ recipdiag;
      end
   end
   7. end
   8. for $j \leftarrow i + 1$ to $k + 1$ do
      9. temp = $R_{xy}[j][i]$;
      10. for $p \leftarrow i + 1$ to $k + 1$ do
          11. $R_{xy}[j][p] = R_{xy}[j][p] - R_{xy}[i][p] \times$ temp;
      end
   end
13. end
15. return $R_{xy}[k + 1][k + 1]$

| Operation | Ours | Hat-matrix |
|-----------|------|------------|
| $+$       | $k(k^2 + 3k - 1)$ | $(k + 1)d + \frac{3}{2}(k + 2)^2$ |
| $\times$  | $k(k + 1)(2k + 1)$ | $(k + 1)d + \frac{6}{2}k(k + 1)(k + 2)$ |
| $\div$    | $k - 1$ | $k + 1$ |

Table 1: Numbers of different operations in the proposed method and the hat-matrix method. The dimension of the vectors is $d$, and the sparsity parameter is $k$.

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