Robust, Efficient, and Scalable Subset Selection via Block Grouping Effects

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Abstract

1 Introduction

2 Motivation

Problem 1: The linear model is restrictive on real applications since many problems exhibit nonlinear properties.

Problem 2: The original model need to process all the data samples, which is not scalable to large datasets.

Problem 3: Block grouping effects of the least square regression is able to group

Problem 4:

Problem 5:

3 RES Model

The proposed robust, efficient, and scalable (RES) subset selection model can be formulated as follows:

$$\min_{\mathbf{A}} \|\mathbf{X} - \mathbf{X}\mathbf{A}\|_p^p + \lambda \|\mathbf{A}\|_F^2, \tag{1}$$

where $0 \le p \le 1$. For analysis simplicity, we just set p = 1.

Then the model above can be

$$\min_{\mathbf{A}} \|\mathbf{X} - \mathbf{X}\mathbf{A}\|_p^p + \lambda \|\mathbf{A}\|_F^2. \tag{2}$$

By introducing auxiliary variables into the optimization program, we can set E=X-XA . The program (??) can be transformed into

$$\min_{\boldsymbol{A},\boldsymbol{E}} \|\boldsymbol{E}\|_p^p + \lambda \|\boldsymbol{A}\|_F^2 \text{ s.t. } \boldsymbol{E} = \boldsymbol{X} - \boldsymbol{X}\boldsymbol{A}.$$
 (3)

By introducing a Lagrangian multiplier Δ , the Lagrangian function of the Eq. (??) can be written as

$$\mathcal{L}(\boldsymbol{A}, \boldsymbol{E}, \boldsymbol{\Delta}, \rho) = \|\boldsymbol{E}\|_p^p + \lambda \|\boldsymbol{A}\|_F^2 + \frac{\rho}{2} \|\boldsymbol{E} - \boldsymbol{X} + \boldsymbol{X}\boldsymbol{A} + \rho^{-1}\boldsymbol{\Delta}\|_F^2$$
(4)

Denote by (A_k, E_k) the optimization variables at iteration k, and by Δ the Lagrangian multipliers at iteration k. Taking detivatives of \mathcal{L} with respect to the variables and setting the derivatives to be zeros, we can alternatively update the variables as follows:

(1) Obtain A_{k+1} by minimizing \mathcal{L} with respect to A, while fixing (E_k, Δ_k) . This is equivalent to solve the following problem:

$$A_{k+1} = \arg\min_{A} \frac{\rho_k}{2} ||P_k - XA||_F^2 + \lambda ||A||_F^2$$
 (5)

where $P_k = X - E_k - \rho_k^{-1} \Delta_k$. This is a least squares regression problem which has a closed-form solution as

$$\boldsymbol{A}_{k+1} = (\boldsymbol{X}^{\top} \boldsymbol{X} + 2\lambda \rho_k^{-1} \boldsymbol{I})^{-1} \boldsymbol{X}^{\top} \boldsymbol{P}_k.$$
 (6)

(3) Obtain E_{k+1} by minimizing \mathcal{L} with respect to E, while fixing (A_{k+1}, Δ_k) . This is equivalent to solve the following problem:

$$\min_{E} \frac{\rho_k}{2} \| Q_k - E \|_F^2 + \| E \|_p^p, \tag{7}$$

where $Q_k = X - XA_{k+1} - \rho_k^{-1}\Delta_k$. Since this problem is seperable, it can be decoupled into $m \times n$ scalable subproblems which share the following form:

$$\min_{y} = \frac{1}{2}(c - y)^{2} + \rho_{k}^{-1}|y|^{p}.$$
 (8)

This problem can be solved by the generalized soft-thresholding algorithm [?] as

$$\hat{y} = \text{sign}(c) * \max(|c| - \tau_p(\rho_k^{-1}), 0) * \mathcal{S}_p(|c|; \rho_k^{-1}),$$
 (9)

where

$$\tau_p(\rho_k^{-1}) = \left[2\rho_k^{-1}(1-p)\right]^{\frac{1}{2-p}} + \rho_k^{-1}p\left[2\rho_k^{-1}(1-p)\right]^{\frac{p-1}{2-p}} \tag{10}$$

and $\mathcal{S}_p(|c|;\rho_k^{-1})$ can be obtained by solving the following equation:

$$S_p(|c|; \rho_k^{-1}) - c + \rho_k^{-1} p(S_p(|c|; \rho_k^{-1}))^{p-1} = 0.$$
 (11)

(4) Obtain the Lagrangian multipliers (Δ_{k+1}) while fixing (A_{k+1}, E_{k+1}) :

$$\Delta_{k+1} = \Delta_k + \tau \rho_k (\boldsymbol{E}_{k+1} - \boldsymbol{X} + \boldsymbol{X} \boldsymbol{A}_{k+1}), \quad (12)$$

where $\tau \in (0, \frac{\sqrt{5}+1}{2})$ is the dual step size and is usually set as $\tau = 1$.

(5) Update the penalty parameter ρ as $\rho_{k+1} = \mu \rho_k$, where $\mu > 1$.

4 RES with Diagonal Constraint

We can also restrict that diag(A) = 0 to avoid the samples to be self-represented. However, I want to mention that the proposed model solved by ADMM algorithm with three variables and does not have convergence results.

Then the model above can be

$$\min_{\mathbf{A}} \|\mathbf{X} - \mathbf{X}\mathbf{A}\|_{p}^{p} + \lambda \|\mathbf{A}\|_{F}^{2} \quad \text{s.t.} \quad \text{diag}(\mathbf{A}) = \mathbf{0}. \tag{13}$$

By introducing auxiliary variables into the optimization program, we can set E = X - XA and A = 0. The program (??) can be transformed into

$$\min_{\boldsymbol{A},\boldsymbol{E}} \|\boldsymbol{E}\|_p^p + \lambda \|\boldsymbol{A}\|_F^2$$
 s.t. $\boldsymbol{E} = \boldsymbol{X} - \boldsymbol{X}\boldsymbol{A}$, diag $(\boldsymbol{A}) = \boldsymbol{0}$.

Besides, we can further introduce an auxiliary matrix variable \boldsymbol{C} and consider the following program

$$\min_{\boldsymbol{A},\boldsymbol{C},\boldsymbol{E}} \|\boldsymbol{E}\|_p^p + \lambda \|\boldsymbol{A}\|_F^2$$
s.t. $\boldsymbol{E} = \boldsymbol{X} - \boldsymbol{X}\boldsymbol{C}, \boldsymbol{C} = \boldsymbol{A} - \operatorname{diag}(\boldsymbol{A})$

whose solution for (A, E) coincides with the solution of Eq. $(\ref{eq:condition})$. By introducing two Lagrangian multipliers Δ, δ , the Lagrangian function of the Eq. $(\ref{eq:condition})$ can be written as

$$\mathcal{L}(\boldsymbol{A}, \boldsymbol{C}, \boldsymbol{E}, \boldsymbol{\Delta}, \boldsymbol{\delta}, \rho) = \|\boldsymbol{E}\|_{p}^{p} + \lambda \|\boldsymbol{A}\|_{F}^{2}$$

$$+ \frac{\rho}{2} \|\boldsymbol{E} - \boldsymbol{X} + \boldsymbol{X}\boldsymbol{C} + \rho^{-1}\boldsymbol{\Delta}\|_{F}^{2}$$

$$+ \frac{\rho}{2} \|\boldsymbol{C} - \boldsymbol{A} + \operatorname{diag}(\boldsymbol{A}) + \rho^{-1}\boldsymbol{\delta}\|_{F}^{2}$$
(16)

Denote by (C_k, A_k, E_k) the optimization variables at iteration k, by (Δ_k, δ_k) the Lagrangian multipliers at iteration k, and by ρ_k the penalty parameter at iteration k. Taking detivatives of \mathcal{L} with respect to the variables and setting the derivatives to be zeros, we can alternatively update the variables as follows:

(1) Obtain A_{k+1} by minimizing \mathcal{L} with respect to A, while fixing $(C_k, E_k, \Delta_k, \delta_k)$. This is equivalent to solve the following problem:

$$\mathbf{A}_{k+1} = \mathbf{J} - \operatorname{diag}(\mathbf{J}),$$

$$\mathbf{J} = (\rho_k + 2\lambda)^{-1}(\rho_k \mathbf{C}_k + \boldsymbol{\delta}_k)$$
(17)

(2) Obtain C_{k+1} by minimizing \mathcal{L} with respect to C, while fixing $(A_{k+1}, E_k, \Delta_k, \delta_k)$. This is equivalent to solve the following problem:

$$C_{k+1} = \arg\min_{C} \frac{\rho_{k}}{2} \| E_{k} - X + XC + \rho_{k}^{-1} \Delta_{k} \|_{F}^{2} + \frac{\rho_{k}}{2} \| C - A_{k+1} + \rho_{k}^{-1} \delta_{k} \|_{F}^{2}$$
(18)

This is a least squares regression problem which has a closed-form solution as

$$C_{k+1} = H - \operatorname{diag}(H),$$

 $(X^{\top}X + I)H = X^{\top}P_k + Q_k,$ (19)

where $P_k = X - E_k - \rho_k^{-1} \Delta_k$ and $Q_k = A_{k+1} - \rho_k^{-1} \delta_k$. (3) Obtain E_{k+1} by minimizing \mathcal{L} with respect to E, while fixing $(C_{k+1}, A_{k+1}, \Delta_k, \delta_k)$. This is equivalent to solve the following problem:

(15)
$$\min_{\mathbf{E}} \frac{1}{2} \| (\mathbf{X} - \mathbf{X} \mathbf{C}_{k+1} - \rho_k^{-1} \mathbf{\Delta}_k) - \mathbf{E} \|_F^2 + \rho_k^{-1} \| \mathbf{E} \|_1.$$
(20)

The solution of E can be computed in closed-form as

$$E_{k+1} = S_{\rho_k^{-1}} (X - X C_{k+1} - \rho_k^{-1} \Delta_k), \tag{21}$$

where $S_{\tau}(x) = \text{sign}(x) * \max(|x| - \tau, 0)$ is the softthresholding operator.

(4) Obtain the Lagrangian multipliers $(\Delta_{k+1}, \delta_{k+1})$ while fixing $(C_{k+1}, A_{k+1}, E_{k+1})$:

$$\Delta_{k+1} = \Delta_k + \tau \rho_k (\boldsymbol{E}_{k+1} - \boldsymbol{X} + \boldsymbol{X} \boldsymbol{C}_{k+1}),$$

$$\delta_{k+1} = \delta_k + \tau \rho_k (\boldsymbol{C}_{k+1} - \boldsymbol{A}_{k+1}),$$
 (22)

where $\tau \in (0, \frac{\sqrt{5}+1}{2})$ is the dual step size and is usually

(5) Update the penalty parameter ρ as $\rho_{k+1} = \mu \rho_k$, where $\mu > 1$.

Large Scale Subset Selection Via Woodbury Identity

The Woodbury Identity is

$$(A+UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$
 and transform this problem as

We can also restrict that diag(A) = 0 to avoid the samples to be self-represented. However, I want to mention that the proposed model solved by ADMM algorithm with three variables and does not have convergence results.

Then the model above can be

$$\min_{\mathbf{A}} \|\mathbf{X} - \mathbf{X}\mathbf{A}\|_F^2 + \lambda \|\mathbf{A}\|_{p,1}. \tag{24}$$

By introducing an auxiliary variable C into the optimization program, we can get

$$\min_{\mathbf{A}, \mathbf{C}} \|\mathbf{X} - \mathbf{X}\mathbf{A}\|_F^2 + \lambda \|\mathbf{C}\|_{p, 1} \text{ s.t. } \mathbf{C} = \mathbf{A},$$
 (25)

whose solution for A coincides with the solution of Eq. (??). By introducing two Lagrangian multipliers Δ , the Lagrangian function of the Eq. (??) can be written as

$$\mathcal{L}(\boldsymbol{A}, \boldsymbol{C}, \boldsymbol{\Delta}, \rho) = \|\boldsymbol{X} - \boldsymbol{X}\boldsymbol{A}\|_F^2 + \lambda \|\boldsymbol{C}\|_{p,1} + \langle \boldsymbol{\Delta}, \boldsymbol{C} - \boldsymbol{A} \rangle + \frac{\rho}{2} \|\boldsymbol{C} - \boldsymbol{A}\|_F^2$$
(26)

Denote by (C_k, A_k) the optimization variables at iteration k, by Δ_k the Lagrangian multipliers at iteration k, and by ρ_k the penalty parameter at iteration k. Taking detivatives of \mathcal{L} with respect to the variables and setting the derivatives to be zeros, we can alternatively update the variables as follows:

(1) Obtain A_{k+1} by minimizing \mathcal{L} with respect to A, while fixing (C_k, Δ_k) . This is equivalent to solve the fol-

$$\min_{\mathbf{A}} \|\mathbf{X} - \mathbf{X}\mathbf{A}\|_F^2 + \frac{\rho}{2} \|\mathbf{A} - (\mathbf{C}_k + \rho_k^{-1} \mathbf{\Delta}_k)\|_F^2, (27)$$

which is equalivalently to solve the following problem

$$\boldsymbol{A} = (\boldsymbol{X}^{\top} \boldsymbol{X} + \frac{\rho_k}{2} \boldsymbol{I})^{-1} (\boldsymbol{X}^{\top} \boldsymbol{X} + \frac{\rho_k}{2} \boldsymbol{C}_k + \frac{1}{2} \boldsymbol{\Delta}_k)$$
(28)

Since the matrices $X^{T}X$ is of $N \times N$ dimension. It is computational expensive when N is very large. By employing the Woodburry Identity mentioned above, we can

$$\left(\frac{\rho_k}{2}\mathbf{I} + \mathbf{X}^{\top}\mathbf{X}\right)^{-1} = \frac{2}{\rho_k}\mathbf{I} - \left(\frac{2}{\rho_k}\right)^2 \mathbf{X}^{\top} \left(\mathbf{I} + \frac{2}{\rho_k}\mathbf{X}\mathbf{X}^{\top}\right)^{-1} \mathbf{X}.$$
(29)

$$\mathbf{A} = \left(\frac{2}{\rho_k}\mathbf{I} - \left(\frac{2}{\rho_k}\right)^2 \mathbf{X}^\top \left(\mathbf{I} + \frac{2}{\rho_k} \mathbf{X} \mathbf{X}^\top\right)^{-1} \mathbf{X}\right)$$

$$* \left(\mathbf{X}^\top \mathbf{X} + \frac{\rho_k}{2} \mathbf{C}_k + \frac{1}{2} \mathbf{\Delta}_k\right)$$
(30)

which will save a lot of computational costs.

(2) Obtain C_{k+1} by minimizing \mathcal{L} with respect to C, while fixing (A_{k+1}, Δ_k) . This is equivalent to solve the following problem:

$$\min_{C} \frac{1}{2} \| (\boldsymbol{A}_{k+1} - \rho_k^{-1} \boldsymbol{\Delta} k) - C \|_F^2 + \frac{\lambda}{\rho_k} \| C \|_{p,1}.$$
 (31)

Since the $\ell_{p,1}$ norm is separable with respect to each row, we can write the above problem as

$$\min_{\mathbf{C}} \sum_{i=1}^{M} \frac{1}{2} \| (\mathbf{A}_{k+1})_{i*} - \rho_k^{-1} (\mathbf{\Delta}_k)_{i*} - \mathbf{C}_{i*} \|_2^2 + \frac{\lambda}{\rho_k} \| \mathbf{C}_{i*} \|_p,$$
(32)

where F_{i*} is the *i*th row of the matrix F. Since this step is separable w.r.t. each row, we can employ parallel processing resources and reduce its computational time.

(3) Obtain the Lagrangian multipliers (Δ_{k+1}) while fixing (C_{k+1}, A_{k+1}) :

$$\Delta_{k+1} = \Delta_k + \rho_k (C_{k+1} - A_{k+1}).$$
 (33)

(5) Update the penalty parameter ρ as $\rho_{k+1} = \mu \rho_k$, where $\mu > 1$.

6 Robust Large Scale Subset Selection via Dissimilarity based Outlier Detection

We can also introduce a dissimilarity based matrix D to replace the ℓ_p or $\ell_{2,1}$ norms to ensure robustness. This can also remore the additional term Z on modeling the outliers with the restriction of ℓ_1 norm. The matrix D should better be diagonal matrix. How to design the matrix D is another problem need to be solved.

Then the proposed model can be formulated as

$$\min_{\mathbf{A}} \| (\mathbf{X} - \mathbf{X}\mathbf{A})\mathbf{D} \|_F^2 + \lambda \|\mathbf{A}\|_{p,1}.$$
 (34)

By introducing an auxiliary variable C into the optimization program, we can get

$$\min_{A,C} \|(X - XA)D\|_F^2 + \lambda \|C\|_{p,1} \text{ s.t. } C = A.$$
 (35)

By introducing a Lagrangian multiplier Δ , the Lagrangian function of the Eq. (??) can be written as

$$\mathcal{L}(\boldsymbol{A}, \boldsymbol{C}, \boldsymbol{\Delta}, \rho) = \|(\boldsymbol{X} - \boldsymbol{X}\boldsymbol{A})\boldsymbol{D}\|_F^2 + \lambda \|\boldsymbol{C}\|_{p,1} + \langle \boldsymbol{\Delta}, \boldsymbol{C} - \boldsymbol{A} \rangle + \frac{\rho}{2} \|\boldsymbol{C} - \boldsymbol{A}\|_F^2$$
(36)

Denote by (A_k, C_k) the optimization variables at iteration k, by Δ_k the Lagrangian multiplier at iteration k, and by ρ_k the penalty parameter at iteration k. Taking detivatives of $\mathcal L$ with respect to the variables and setting the derivatives to be zeros, we can alternatively update the variables as follows:

(1) Obtain A_{k+1} by minimizing \mathcal{L} with respect to A, while fixing (C_k, Δ_k) . This is equivalent to solve the following problem:

$$\min_{\mathbf{A}} \| (\mathbf{X} - \mathbf{X}\mathbf{A})\mathbf{D} \|_F^2 + \frac{\rho}{2} \| \mathbf{A} - (\mathbf{C}_k - \rho_k^{-1} \mathbf{\Delta}_k) \|_F^2,$$
(37)

which is equalivalently to solve the following problem

$$\boldsymbol{X}^{\top} \boldsymbol{X} \boldsymbol{A} \boldsymbol{D} \boldsymbol{D}^{\top} + \frac{\rho_k}{2} \boldsymbol{A} = \boldsymbol{X}^{\top} \boldsymbol{X} \boldsymbol{D} \boldsymbol{D}^{\top} + \frac{\rho_k}{2} (\boldsymbol{C}_k - \rho_k^{-1} \boldsymbol{\Delta}_k)$$
(38)

Since the matrices $X^{T}X$ and $D^{T}D$ are positive semidefinite and positive definite, respectively. The above equation is a standard Sylvester equation which has a unique solution.

(2) Obtain C_{k+1} by minimizing \mathcal{L} with respect to C, while fixing (A_{k+1}, Δ_k) . This is equivalent to solve the following problem:

$$\min_{\mathbf{C}} \frac{1}{2} \| (\mathbf{A}_{k+1} + \rho_k^{-1} \mathbf{\Delta} k) - \mathbf{C} \|_F^2 + \frac{\lambda}{\rho_k} \| \mathbf{C} \|_{p,1}.$$
 (39)

Since the $\ell_{p,1}$ norm is separable with respect to each row, we can write the above problem as

$$\min_{C} \sum_{i=1}^{M} \frac{1}{2} \| (\boldsymbol{A}_{k+1})_{i*} + \rho_{k}^{-1} (\boldsymbol{\Delta}_{k})_{i*} - \boldsymbol{C}_{i*} \|_{2}^{2} + \frac{\lambda}{\rho_{k}} \| \boldsymbol{C}_{i*} \|_{p},$$
(40)

where F_{i*} is the *i*th row of the matrix F. Since this step is separable w.r.t. each row, we can employ parallel processing resources and reduce its computational time.

(3) Obtain the Lagrangian multipliers (Δ_{k+1}) while fixing (C_{k+1}, A_{k+1}) :

$$\Delta_{k+1} = \Delta_k + \rho_k (C_{k+1} - A_{k+1}).$$
 (41)

(5) Update the penalty parameter ρ as $\rho_{k+1} = \mu \rho_k$, where $\mu > 1$.

7 Large Scale Subset Selection Via Row-Column Separation

We can also restrict that diag(A) = 0 to avoid the samples to be self-represented. However, I want to mention that the proposed model solved by ADMM algorithm with three variables and does not have convergence results.

Then the model above can be

$$\min_{\mathbf{A}} \|\mathbf{X} - \mathbf{X}\mathbf{A}\|_F^2 + \lambda \|\mathbf{A}\|_{p,1} \quad \text{s.t.} \quad \text{diag}(\mathbf{A}) = \mathbf{0}.$$
(42)

By introducing an auxiliary variable C into the optimization program, we can get

$$\min_{\boldsymbol{A},\boldsymbol{C}} \|\boldsymbol{X} - \boldsymbol{X}\boldsymbol{C}\|_F^2 + \lambda \|\boldsymbol{A}\|_{p,1}$$
s.t. $\boldsymbol{C} = \boldsymbol{A} - \operatorname{diag}(\boldsymbol{A}),$ (43)

whose solution for A coincides with the solution of Eq. $(\ref{eq:condition})$. By introducing two Lagrangian multipliers Δ , the Lagrangian function of the Eq. $(\ref{eq:condition})$ can be written as

$$\mathcal{L}(\boldsymbol{A}, \boldsymbol{C}, \boldsymbol{\Delta}, \rho) = \|\boldsymbol{X} - \boldsymbol{X}\boldsymbol{C}\|_F^2 + \lambda \|\boldsymbol{A}\|_{p,1}$$
$$+ \langle \boldsymbol{\Delta}, \boldsymbol{C} - (\boldsymbol{A} - \operatorname{diag}(\boldsymbol{A})) \rangle + \frac{\rho}{2} \|\boldsymbol{C} - (\boldsymbol{A} - \operatorname{diag}(\boldsymbol{A}))\|_F^2$$
(44)

Denote by (C_k, A_k) the optimization variables at iteration k, by Δ_k the Lagrangian multipliers at iteration k, and by ρ_k the penalty parameter at iteration k. Taking detivatives of $\mathcal L$ with respect to the variables and setting the derivatives to be zeros, we can alternatively update the variables as follows:

(1) Obtain A_{k+1} by minimizing \mathcal{L} with respect to A, while fixing (C_k, Δ_k) . This is equivalent to solve the following problem:

$$\mathbf{A}_{k+1} = \mathbf{J} - \operatorname{diag}(\mathbf{J}),$$

$$\mathbf{J} = \arg\min_{\mathbf{J}} \frac{1}{2} \|\mathbf{C}_k + \rho_k^{-1} \mathbf{\Delta}_k - \mathbf{J}\|_F^2 + \frac{\lambda}{\rho_k} \|\mathbf{J}\|_{p,1}.$$
(45)

(2) Obtain C_{k+1} by minimizing \mathcal{L} with respect to C, while fixing (A_{k+1}, Δ_k) . This is equivalent to solve the following problem:

$$\min_{C} \|X - XC\|_F^2 + \frac{\rho_k}{2} \|C - A_{k+1} + \frac{1}{\rho_k} \Delta_k\|_F^2$$
 (46)

This is a least squares regression problem which has a closed-form solution as

$$C_{k+1} = (X^{\top}X + \frac{\rho_k}{2}I)^{-1}(X^{\top}X + \frac{\rho_k}{2}A_{k+1} - \frac{1}{2}\Delta_k).$$
(47)

(3) Obtain the Lagrangian multipliers (Δ_{k+1}) while fixing (C_{k+1}, A_{k+1}) :

$$\Delta_{k+1} = \Delta_k + \rho_k (C_{k+1} - A_{k+1}).$$
 (48)

(5) Update the penalty parameter ρ as $\rho_{k+1} = \mu \rho_k$, where $\mu > 1$.