A Homotopic Method to Solve the Lasso Problems — an Improved Upper Bound of Convergence Rate

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Homotopic Lasso Solver

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Lasso (Tibshirani, 1996)



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$$y = X\beta^* + w.$$



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$$y = X\beta^* + w.$$

The Lasso estimator $\widehat{\beta}$ is

$$\widehat{\beta} = \arg\min_{\beta} \left\{ \frac{1}{2n} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1 \right\},\tag{1}$$

where parameter λ controls the trade-off between the sparsity and model's goodness of fit.



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Essentially, an optimization problem, aiming to minimize the objective function

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 (2)

with respect to β .



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Introduction

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- No close form for $\widehat{\beta}$.
- Most Lasso-algorithms are recursive with an iteration index k. That is, $\beta^{(k)}$ is the kth estimate in an iteration of a Lasso-algorithm.
- In this talk, we focus on ϵ -precision.

$$F(\beta^{(k)}) - F(\widehat{\beta}) \le \epsilon \tag{3}$$

and evaluate how many numerical operations are needed to achieve the above. (Note, we are not using k as the ultimate measurement of performance.)



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- Don't use the total number of iterations, as it may depend on what to compute within the iterations.
- Don't use the running time, as it depends on the implementation and platform.



Theoretical Results

Main Result/Our Contribution

The state-of-the-art Lasso-algorithms we compare include

- the Iterative Shrinkage-Thresholding Algorithm (ISTA)
- the Fast Iterative Shrinkage-Thresholding Algorithm (FISTA)
- a Coordinate Descent (CD) algorithm, and
- the Smooth Lasso (SL)

These algorithms are representative in the literature.

Table: The available orders of complexity of four existing Lasso-algorithms and ours (in the last column) for achieving the ϵ -precision. The common factor that involves n (the sample size) and p (the dimensionality of the parameter) is omitted for simplicity.

| Method | ISTA | FISTA | CD | SL | Ours |
|---------------------|-----------------|------------------------|-----------------|-----------------|--------------------------------------|
| Order of complexity | $O(1/\epsilon)$ | $O(1/\sqrt{\epsilon})$ | $O(1/\epsilon)$ | $O(1/\epsilon)$ | $O\left([\log(1/\epsilon)]^2\right)$ |



State-of-the-Art Lasso Algorithms



What can ISTA solve?

ISTA aims at the minimization of a summation of two functions, g + f, where the first function $g: \mathbb{R}^p \to \mathbb{R}$ is continuous convex and the other function $f: \mathbb{R}^p \to \mathbb{R}$ is smooth convex with Lipschitz continuous gradient.



Introduction

- What can ISTA solve? ISTA aims at the minimization of a summation of two functions, g + f, where the first function $g: \mathbb{R}^p \to \mathbb{R}$ is continuous convex and the other function $f: \mathbb{R}^p \to \mathbb{R}$ is smooth convex with Lipschitz continuous gradient.
- Lasso is a specially case of ISTA. If we let $g(\beta) = \lambda \|\beta\|_1$ and $f(\beta) = \frac{1}{2n} \|Y - X\beta\|_2^2$ with Lipschitz continuous gradient L taking the largest eigenvalue of matrix X'X/n.



Introduction

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- Lasso is a specially case of ISTA. If we let $g(\beta) = \lambda \|\beta\|_1$ and $f(\beta) = \frac{1}{2n} \|Y - X\beta\|_2^2$ with Lipschitz continuous gradient L taking the largest eigenvalue of matrix X'X/n.
- What is the updating rule from $\beta^{(k)}$ to $\beta^{(k+1)}$, i.e., $\beta^{(k)} \to \beta^{(k+1)}$? It is realized by updating $\beta^{(k+1)}$ through the quadratic approximation function of $f(\beta)$ at value $\beta^{(k)}$:

$$\beta^{(k+1)} = \arg\min_{\beta} f(\beta^{(k)}) + \langle (\beta - \beta^{(k)}), \nabla f(\beta^{(k)}) \rangle + \frac{\sigma_{\max}(X'X/n)}{2} \|\beta - \beta^{(k)}\|_2^2 + \lambda \|\beta\|_1.$$

Simple algebra shows that (ignoring constant terms in β), minimization of equation above is equal to the minimization of the following equation:

$$\beta^{(k+1)} = \arg\min_{\beta} \frac{\sigma_{\max}(X'X/n)}{2} \left\|\beta - \left(\beta^{(k)} - \frac{\frac{1}{n}(X'X\beta^{(k)} - X'y)}{\sigma_{\max}(X'X/n)}\right)\right\|_2^2 + \lambda \|\beta\|_1,$$

where soft-thresholding function can be used.

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Iterative Shrinkage-Thresholding Algorithms (ISTA)

Algorithm 1: Iterative Shrinkage-Thresholding Algorithms (ISTA)

Input: $y_{n\times 1}, X_{n\times p}, L = \sigma_{\max}(X'X/n)$

```
Output: an estimator of \beta satisfies the \epsilon-precision, noted as \beta^{(k)}

1 initialization;

2 \beta^{(0)}, k=0

3 while F(\beta^{(k)}) - F(\widehat{\beta}) > \epsilon do

4 \beta^{(k+1)} = S(\beta^{(k)} - \frac{1}{n'}(X'X\beta^{(k)} - X'y), \lambda/L)
```

Number of operations in each iteration: $O(p^2)$



k = k + 1

6 end

2: Algorithm Iterative Shrinkage-Thresholding Algorithms (ISTA)

Input: $y_{n\times 1}, X_{n\times p}, L = \sigma_{\max}(X'X/n)$ **Output:** an estimator of β satisfies the ϵ -precision,

- noted as $\beta^{(k)}$ initialization:
- $\beta^{(0)}, k=0$

Introduction

- 3 while $F(\beta^{(k)}) F(\widehat{\beta}) > \epsilon$ do
- $\beta^{(k+1)} = S(\beta^{(k)} \frac{1}{n!}(X'X\beta^{(k)} X'y), \lambda/L)$
- k = k + 1
- 6 end

- Number of operations in each iteration: $O(p^2)$
- Number of iterations needed to achieve the ϵ -precision:

$$\sigma_{\max}(X'X/n)\|\beta^{(0)}-\widehat{\beta}\|_2^2$$

(Beck and Teboulle, 2009, Theorem 3.1)



Algorithm 3: Iterative Shrinkage-Thresholding Algorithms (ISTA)

Input: $y_{n\times 1}, X_{n\times p}, L = \sigma_{\max}(X'X/n)$ **Output:** an estimator of β satisfies the ϵ -precision, noted as $\beta^{(k)}$

- initialization:
- $\beta^{(0)}, k=0$

6 end

Introduction

- 3 while $F(\beta^{(k)}) F(\widehat{\beta}) > \epsilon$ do
- $\beta^{(k+1)} = S(\beta^{(k)} \frac{1}{n!}(X'X\beta^{(k)} X'y), \lambda/L)$
- k = k + 1

- Number of operations in each iteration: $O(p^2)$
- Number of iterations needed to achieve the ϵ -precision:

$$\sigma_{\max}(X'X/n)\|\beta^{(0)}-\widehat{\beta}\|_2^2$$

(Beck and Teboulle, 2009, Theorem 3.1)

Order of complexity: $O(p^2/\epsilon)$



Fast Iterative Shrinkage-Thresholding Algorithms (FISTA)

Motivation: Based on ISTA and Accelerated Gradient Descent.



Motivation:

Introduction

Based on ISTA and Accelerated Gradient Descent.

Difference of ISTA and FISTA:

FISTA employs the second-order Taylor expansion in equation (9) at the an auxiliary variable $\alpha^{(k)}$ to update from $\beta^{(k)}$ to $\beta^{(k+1)}$, i.e.,

$$\beta^{(k+1)} = \arg\min_{\alpha} f(\alpha^{(k)}) + \langle (\alpha - \alpha^{(k)}), \nabla f(\alpha^{(k)}) \rangle + \frac{\sigma_{\max}(X'X/n)}{2} \|\alpha - \alpha^{(k)}\|_2^2 + \lambda \|\alpha\|_1,$$

where $\alpha^{(k)}$ is a specific linear combination of the previous two estimator $\beta^{(k-1)}, \beta^{(k-2)}$, i.e., we have $\alpha^{(k)} = \beta^{(k-1)} + \frac{t_{k-1}-1}{t_k} (\beta^{(k-1)} - \beta^{(k-2)})$.



Fast Iterative Shrinkage-Thresholding Algorithms (FISTA)

- Motivation: Based on ISTA and Accelerated Gradient Descent.
- Difference of ISTA and FISTA: FISTA employs the second-order Taylor expansion in equation (9) at the an auxiliary variable $\alpha^{(k)}$ to update from $\beta^{(k)}$ to $\beta^{(k+1)}$. i.e.,

$$\beta^{(k+1)} = \arg\min_{\alpha} f(\alpha^{(k)}) + \langle (\alpha - \alpha^{(k)}), \nabla f(\alpha^{(k)}) \rangle + \frac{\sigma_{\max}(X'X/n)}{2} \|\alpha - \alpha^{(k)}\|_2^2 + \lambda \|\alpha\|_1,$$

where $\alpha^{(k)}$ is a specific linear combination of the previous two estimator $\beta^{(k-1)}, \beta^{(k-2)}, \text{ i.e., we have } \alpha^{(k)} = \beta^{(k-1)} + \frac{t_{k-1}-1}{t} (\beta^{(k-1)} - \beta^{(k-2)}).$

FISTA falls in the framework of Accelerate Gradient Descent(AGD), because it takes additional past information to take an extra gradient step via the auxiliary sequence $\alpha^{(k)}$, which is constructed by adding a "momentum" term $\beta^{(k-1)} - \beta^{(k-2)}$ that incorporates the effect of second-order changes.



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Homotopic Lasso Solver

Algorithm 4: Fast Iterative Shrinkage-Thresholding Algorithms (FISTA)

Input:
$$y_{n \times 1}, X_{n \times p}, L = \sigma_{\max}(X'X/n)$$

Output: an estimator of β , noted as $\beta^{(k)}$, which satisfies the ϵ -precision.

1 initialization:

Introduction

$$2 \beta^{(0)}, t_1 = 1, k = 0$$

$$3 \text{ while } F(\beta^{(k)}) - F(\hat{\beta}) > \epsilon \text{ do}$$

$$4 \beta^{(k)} = S(\alpha^{(k)} - \frac{1}{nL}(X'X\alpha^{(k)} - X'y), \lambda/L)$$

$$5 t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2}$$

$$6 \alpha^{(k+1)} = \beta^{(k)} + \frac{t_{k-1}}{t_{k+1}} (\beta^{(k)} - \beta^{(k-1)})$$

$$7 k = k + 1$$

Number of operations in each iteration: $O(p^2)$



8 end

Algorithm 5: Fast Iterative Shrinkage-Thresholding Algorithms (FISTA)

Input:
$$y_{n \times 1}, X_{n \times p}, L = \sigma_{\max}(X'X/n)$$

Output: an estimator of β , noted as $\beta^{(k)}$, which satisfies the ϵ -precision.

1 initialization:

Introduction

2
$$\beta^{(0)}$$
, $t_1 = 1, k = 0$
3 while $F(\beta^{(k)}) - F(\hat{\beta}) > \epsilon$ do
4 $\beta^{(k)} = S(\alpha^{(k)} - \frac{1}{nL}(X'X\alpha^{(k)} - X'y), \lambda/L)$
5 $t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2}$
6 $\alpha^{(k+1)} = \beta^{(k)} + \frac{t_{k-1}}{t_{k+1}}(\beta^{(k)} - \beta^{(k-1)})$
7 $k = k + 1$

 $\frac{2\sigma_{\max}(X'X/n)\|\beta^{(0)}-\widehat{\beta}\|_2^2}{\sqrt{\epsilon}}$

 ϵ -precision:

(Beck and Teboulle, 2009, Theorem 4.4)

Number of operations in each iteration:
$$O(p^2)$$

Number of iterations needed to achieve the

8 end

Algorithm 6: Fast Iterative Shrinkage-Thresholding Algorithms (FISTA)

Input:
$$y_{n\times 1}, X_{n\times p}, L = \sigma_{\max}(X'X/n)$$

Output: an estimator of β , noted as $\beta^{(k)}$, which satisfies the ϵ -precision.

1 initialization:

Introduction

$$\begin{array}{ll} \mathbf{2} & \beta^{(0)}, \ t_1 = 1, k = 0 \\ \mathbf{3} & \text{while } \frac{F(\beta^{(k)}) - F(\widehat{\beta}) > \epsilon \ do}{4} \\ \mathbf{4} & \beta^{(k)} = S(\alpha^{(k)} - \frac{1}{nL}(X'X\alpha^{(k)} - X'y), \lambda/L) \\ \mathbf{5} & t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2} \\ \mathbf{6} & \alpha^{(k+1)} = \beta^{(k)} + \frac{t_{k-1}}{t_{k+1}} (\beta^{(k)} - \beta^{(k-1)}) \\ \mathbf{7} & k = k+1 \end{array}$$

8 end

- Number of operations in each iteration: $O(p^2)$
- Number of iterations needed to achieve the ϵ -precision:

$$\frac{2\sigma_{\max}(X'X/n)\|\beta^{(0)}-\widehat{\beta}\|_2^2}{2}$$

(Beck and Teboulle, 2009, Theorem 4.4)

Order of complexity:

$$O(p^2/\sqrt{\epsilon})$$



Coordinate Descent (CD)

Difference between CD and the two previous algorithms: The updating rule in both ISTA and FISTA is global. In contrast, Friedman et al. (2010) proposed a Lasso-algorithm which cyclically chooses one entry at a time and performs a simple analytical update through coordinate gradient descent.



Coordinate Descent (CD)

- Difference between CD and the two previous algorithms: The updating rule in both ISTA and FISTA is global. In contrast, Friedman et al. (2010) proposed a Lasso-algorithm which cyclically chooses one entry at a time and performs a simple analytical update through coordinate gradient descent.
- What is the updating rule from $\beta^{(k)}$ to $\beta^{(k+1)}$, i.e., $\beta^{(k)} \to \beta^{(k+1)}$? The updating rule from $\beta^{(k)}$ to $\beta^{(k+1)}$ in CD is that, it partially optimizes with respect to only j-th entry of $\beta^{(k+1)}$, $(j=1\cdots p)$, where the gradient at $\beta^{(k)}_j$ in the following equation is used for the updating process.

$$\frac{\partial}{\partial \beta_i} F(\beta^{(k)}) = \frac{1}{n} \left(e_j' X' X \beta^{(k)} - y' X e_j \right) + \lambda \operatorname{sign}(\beta_j)$$



Coordinate Descent (CD)

Algorithm 7: Coordinate Descent(CD)

```
Input: y_{n\times 1}, X_{n\times D}, \lambda
```

Output: an estimator of β , noted as $\beta^{(k)}$, which

```
satisfies the \epsilon-precision.
  initialization:
\beta^{(0)}, k=0
3 while F(\beta^{(k)}) - F(\widehat{\beta}) > \epsilon do
           for i = 1 \cdot \cdot \cdot p do
                  \beta_i^{(k+1)} =
                     S\left(y'Xe_{j}-\sum_{l
eq j}\left(X'X
ight)_{il}eta_{k}^{(k)},n\lambda
ight)/\left(X'X
ight)_{ij}
7 end
```

Number of operations in each iteration: $O(p^2)$



Coordinate Descent (CD)

Algorithm 8: Coordinate Descent(CD)

```
Input: y_{n\times 1}, X_{n\times n}, \lambda
```

Output: an estimator of β , noted as $\beta^{(k)}$, which satisfies the ϵ -precision.

initialization:

7 end

$$\begin{array}{ll} 2 & \beta^{(0)}, k = 0 \\ 3 & \text{while } F(\beta^{(k)}) - F(\widehat{\beta}) > \epsilon \text{ do} \\ 4 & \text{ for } j = 1 \cdots p \text{ do} \\ 5 & \beta_j^{(K+1)} = \\ & S\left(y'Xe_j - \sum_{l \neq j} (X'X)_{jl} \, \beta_k^{(K)}, n\lambda\right) / \left(X'X\right)_{jj} \end{array}$$

Number of operations in each iteration: $O(p^2)$

Theoretical Results

achieve the ϵ -precision: $\frac{4\sigma_{\max}(X'X/n)(1+p)\|\beta^{(0)}-\widehat{\beta}\|_{2}^{2}}{\epsilon} - \frac{8}{n}$ ((Beck and Tetruashvili, 2013, Corollary 3.8)

Number of iterations needed to



Coordinate Descent (CD)

Algorithm 9: Coordinate Descent(CD)

```
Input: y_{n\times 1}, X_{n\times n}, \lambda
```

Output: an estimator of β , noted as $\beta^{(k)}$, which satisfies the ϵ -precision.

1 initialization:

$$\beta^{(0)}$$
, $k = 0$

3 while
$$F(\beta^{(k)}) - F(\widehat{\beta}) > \epsilon$$
 do
4 | for $j = 1 \cdots p$ do
5 | $\beta_i^{(k+1)} =$

$$S\left(y'Xe_{j}-\sum_{l\neq j}\left(X'X\right)_{jl}\beta_{k}^{(k)},n\lambda\right)/\left(X'X\right)_{jj}$$

7 end

- Number of operations in each iteration:
 O(p²)
- Number of iterations needed to achieve the ϵ -precision:

$$\frac{4\sigma_{\max}(X'X/n)(1+p)\|\beta^{(0)}-\widehat{\beta}\|_2^2}{((\text{Beck and Tetruashvili, 2013, } \text{Corollary 3.8})} - \frac{8}{p}$$

Order of complexity: $O(p^2/\epsilon)$



Smooth Lasso (SL)

Main idea:

It use a smooth function— $\phi_{\alpha}(u)=\frac{2}{u}\log(1+e^{\alpha u})-u$ — to approximate ℓ_1 penalty, and Accelerated Gradient Descent (AGD) algorithm is applied after the replacement.



Smooth Lasso (SL)

Algorithm 10: Smooth Lasso (SL)

Input:
$$y_{n \times 1}, X_{n \times p},$$

$$\mu = \left[\sigma_{\max}^2(X/\sqrt{n}) + \lambda \alpha/2 \right]^{-1}$$

Output: an estimator of β , noted as $\beta^{(k)}$, which satisfies the ϵ -precision.

1 initialization:

7 end

2
$$\beta^{(0)}$$
, $k = 0$
3 while $F(\beta^{(k)}) - F(\hat{\beta}) > \epsilon$ do
4 $w^{(k+1)} = \beta^{(k)} + \frac{k-2}{k+1} (\beta^{(k)} - \beta^{(k-1)})$
5 $\beta^{(k+1)} = w^{(k+1)} - \mu \nabla F_{\alpha}(w^{(k)})$
6 $k = k + 1$

 $O(p^2)$

Number of operations in each iteration:



Smooth Lasso (SL)

Algorithm 11: Smooth Lasso (SL)

Input:
$$y_{n \times 1}, X_{n \times p},$$

$$\mu = \left[\sigma_{\max}^2 (X/\sqrt{n}) + \lambda \alpha/2 \right]^{-1}$$

Output: an estimator of β , noted as $\beta^{(k)}$, which satisfies the ϵ -precision.

1 initialization:

$$\begin{array}{ll} \mathbf{2} & \beta^{(0)} \text{ , } k = 0 \\ \mathbf{3} & \text{ while } \frac{F(\beta^{(k)}) - F(\widehat{\beta}) > \epsilon}{k + 1} \text{ do} \\ \mathbf{4} & | w^{(k+1)} = \beta^{(k)} + \frac{k-2}{k+1} (\beta^{(k)} - \beta^{(k-1)}) \\ \mathbf{5} & | \beta^{(k+1)} = w^{(k+1)} - \mu \nabla F_{\alpha}(w^{(k)}) \\ \mathbf{6} & | k = k+1 \end{array}$$

7 end

- Number of operations in each iteration: $O(p^2)$
- Number of iterations needed to achieve the ε-precision:

 $O(1/\epsilon)$ (Mukherjee and Seelamantula (2016))



Smooth Lasso (SL)

Algorithm 12: Smooth Lasso (SL)

Input:
$$y_{n \times 1}, X_{n \times p},$$

$$\mu = \left[\sigma_{\max}^2 (X/\sqrt{n}) + \lambda \alpha/2 \right]^{-1}$$

Output: an estimator of β , noted as $\beta^{(k)}$, which satisfies the ϵ -precision.

1 initialization:

$$\beta^{(0)}, k=0$$

3 while
$$F(\beta^{(k)}) - F(\widehat{\beta}) > \epsilon$$
 do

4 |
$$w^{(k+1)} = \beta^{(k)} + \frac{k-2}{k+1} (\beta^{(k)} - \beta^{(k-1)})$$

5 | $\beta^{(k+1)} = w^{(k+1)} - \mu \nabla F_{\alpha}(w^{(k)})$
6 | $k = k+1$

7 end

Number of operations in each iteration: $O(p^2)$

Number of iterations needed to achieve the ε-precision:

 $O(1/\epsilon)$ (Mukherjee and Seelamantula (2016))

Order of complexity:

$$O(p^2/\epsilon)$$



Comparison between the state-of-the-art algorithms with ours

Recall the following table that has been shown earlier.

Table: The available orders of complexity of four existing Lasso-algorithms and ours (in the last column) for achieving the ϵ -precision. The common factor that involves n (the sample size) and p (the dimensionality of the parameter) is omitted for simplicity.

| Method | ISTA | FISTA | CD | SL | Ours |
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Our proposed Algorithm



Introduction

Motivation

We know: if the objective function is strongly convex and well conditioned, then a gradient descent method (or an accelerated gradient descent method) can achieve very fast convergence rate.



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- Function of the ℓ_1 norm (i.e., $\|\beta\|_1$) does not have derivative at the origin. (Subgradient has to be used here.)



Introduction

Motivation

- We know: if the objective function is strongly convex and well conditioned, then a gradient descent method (or an accelerated gradient descent method) can achieve very fast convergence rate.
- Function of the ℓ_1 norm (i.e., $\|\beta\|_1$) does not have derivative at the origin. (Subgradient has to be used here.)
- We consider surrogate function approach:

$$F_t(\beta) = \frac{1}{2n} \|y - X\beta\|_2^2 + \lambda f_t(\beta)$$



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Let $f_t(\beta) \to \|\beta\|_1$ as $t \to 0$.



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- Function of the ℓ_1 norm (i.e., $\|\beta\|_1$) does not have derivative at the origin. (Subgradient has to be used here.)
- We consider surrogate function approach:

$$F_t(\beta) = \frac{1}{2n} \|y - X\beta\|_2^2 + \lambda f_t(\beta)$$

- Let $f_t(\beta) \to ||\beta||_1$ as $t \to 0$.
- **Each** $f_t(\beta)$ is strongly convex and well conditioned.



Homotopic Method

Introduction

Motivation

Recall that when $t \to 0$, we have $f_t(\beta) \to \|\beta\|_1$.



Homotopic Method

- Recall that when $t \to 0$, we have $f_t(\beta) \to \|\beta\|_1$.
- Design $t_0 > t_1 > t_2 > \cdots > t_k > \cdots$ for $j = 1, 2, 3, \ldots$, (outer loop)



Homotopic Method

- Recall that when $t \to 0$, we have $f_t(\beta) \to \|\beta\|_1$.
- Design $t_0 > t_1 > t_2 > \cdots > t_k > \cdots$ for $j = 1, 2, 3, \ldots$, (outer loop)
 - Minimize the following

$$\frac{1}{2n}\|y-X\beta\|_2^2+\lambda f_{t_j}(\beta)$$

via a few Accelerated Gradient Descent steps (inner loop)



Motivation

- Recall that when $t \to 0$, we have $f_t(\beta) \to ||\beta||_1$.
- 2 Design $t_0 > t_1 > t_2 > \cdots > t_k > \cdots$ for $j = 1, 2, 3, \dots$, (outer loop)
 - Minimize the following

$$\frac{1}{2n}\|y-X\beta\|_2^2+\lambda f_{t_j}(\beta)$$

via a few Accelerated Gradient Descent steps (inner loop)

 The stopping point of the previous subproblem is the initial point of the current subproblem



Algorithm Overview

Our algorithm has two layers.

Algorithm 13: Pseudo code of the proposed Homotopy-Shrinkage algorithm

Input: A response vector y, a model matrix X, a parameter λ that relates to the Lasso

Output: an estimator of β , which satisfies the ϵ -precision

- 1 Hypter-parameter initialization initialize t
- 2 ► Outer-Iteration: \triangleleft while the precision ϵ is not achieved do
- 3 shrink t;
- 4 ► Inner-Iteration:
 - use Accelerated Gradient Descent steps to minimize $F_t(\beta)$ until the precision of the inner-iteration is achieved
- 6 end

5



Condition for the surrogate function

To narrow down the difference between the surrogate $(F_t(\beta))$ and the origins $(F(\beta))$, $f_t(\beta)$ is designed to get more and more close to the ℓ_1 penalty when t approaches 0, i.e., $t \to 0$. The condition below lists all the requirement of $f_t(x)$.

Condition

Assume function $f_t(x)$ satisfies the following conditions.

- When $t \to 0$, we have $f_0(x) = |x|$, where |x| is the absolute value function.
- For fixed t > 0, function $x \mapsto f_t(x)$ is quadratic on [-t, t], here \mapsto indicates that the left hand side (i.e., x) is the variable in the function in the right hand side (i.e., $f_t(x)$). We following this convention in the rest of this paper.
- Functions $x \mapsto f_t(x)$ and $t \mapsto f_t(x)$ are C^1 , i.e., continuously differentiable functions.



The Designed surrogate function

Following the requirements in condition we mentioned, we design $f_t(x)$ in the following equation, where the input variable x is a scalar.

$$f_t(x) = \begin{cases} \frac{1}{3t^3} [\log(1+t)]^2 x^2, & \text{if } |x| \le t, \\ \left\lceil \frac{\log(1+t)}{t} \right\rceil^2 |x| + \frac{1}{3|x|} [\log(1+t)]^2 - \frac{1}{t} [\log(1+t)]^2, & \text{otherwise.} \end{cases}$$
(4)



The Designed surrogate function

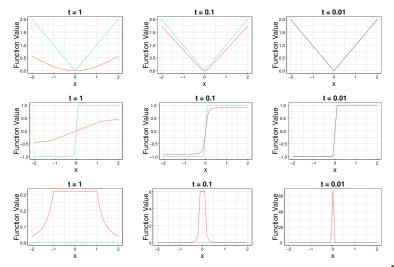
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 (4)

After the replacement of the surrogate function, we have $F_t(\beta) = \frac{1}{2n} \|y - X\beta\|_2^2 + \lambda f_t(\beta)$



The Designed surrogate function



Our proposed Algorithm 0000000000

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Figure: Comparison between $f_t(x)$ and |x| when t changes (the first row), the comparison between their first derivative (the second row) and the comparison between their second derivative (the third row),

Detailed Algorithm

The following is the detailed algorithm.

```
Algorithm 2: A detailed version of our proposed algorithm
```

Input: $y_{n\times 1}, X_{n\times p}, \lambda, t_0, h, \epsilon, B$ Output: an estimator of β , noted as $\beta^{(k)}$, which achieves the ϵ -precision.

1 initialization
$$t_0$$
, h , $k = 1$, $\beta^{(0)} = \left[X'X + \frac{2n\lambda[\log(1+t_0)]^2}{3t_0^2} I \right]^{-1} X'y$

2 \blacktriangleright Outer-Iteration: \blacktriangleleft while $F(\beta^{(k-1)}) - F_{\min} > \epsilon$ do

3 $s = 1$

4 $\beta^{(k)}[0] = \beta^{(k-1)}$

5 $\bar{\beta}^{(k)}[0] = \beta^{(k-1)}$

6 $\tilde{\epsilon}_k = \frac{\lambda p}{3B} [\log(1+t_k)]^2$

7 \blacktriangleright Inner-Iteration: \blacktriangleleft while $F_{t_k}(\bar{\beta}^{(k)}[s-1]) - F_{\min,k} > \tilde{\epsilon}_k$ do

8 $\underline{\beta}^{(k)}[s] = (1-q_s)\bar{\beta}^{(k)}[s-1] + q_s\beta^{(k)}[s-1]$

9 $\beta^{(k)}[s] = \arg\min_{\beta} \left\{ \gamma_s \left[\beta' \nabla F_{t_k}(\underline{\beta}^{(k)}[s]) + \mu_k V(\underline{\beta}^{(k)}[s], \beta) \right] + V(\beta^{(k)}[s-1], \beta) \right\}$

10 $\bar{\beta}^{(k)}[s] = (1-\alpha_s)\bar{\beta}^{(k)}[s-1] + \alpha_s\beta^{(k)}[s]$

11 $s = s+1$

12 $\beta^{(k)}[s] = \bar{\beta}^{(k)}[s]$

13 $t_k = t_{k-1}(1-h)$

14 $t_k = k+1$



Detailed Algorithm

Some details supporting the previous figure.

In line 2, $F_{\min} = \min_{\beta} F(\beta)$.

In line 4 and the rest of this paper, we use parenthesis (k) to denote the kth outer-iteration, and we use bracket [s] to denote the sth inner-iteration.

In line 7, $F_{\min,k} = \min_{\beta} F_{t_k}(\beta)$.

In line 8, in this paper, we choose q_s as $q_s = q = \frac{\alpha_k - \mu_k/L_k}{1 - \mu_k/L_k}$ for $s = 1, 2, \ldots$

where $\alpha_k = \sqrt{\frac{\mu_k}{L_k}}$. And L_k, μ_k is defined as $\|\nabla F_{t_k}(x) - \nabla F_{t_k}(y)\|_2^2 \le \|L_k\|x - y\|_2$,

 $F_{t_k}(y) \ge F_{t_k}(x) + \nabla F_{t_k}(x)(y-x) + \frac{\mu_k}{2} \|y-x\|_2^2$

In line 9, we choose γ_s as $\gamma_s = \gamma = \frac{\alpha}{\mu_k(1-\alpha_k)}$ for $s = 1, 2, \ldots$ Here V(x,z) is defined as

$$V(x,z) = v(z) - [v(x) + \nabla v(x)'(z-x)], \text{ with } v(x) = ||x||_2^2/2.$$



Initial Point

Lemma

Suppose in a Lasso problem, we have the response vector $y \in \mathbb{R}^n$ and a model matrix $X \in \mathbb{R}^{n \times p}$. For our proposed algorithm, there exist a value t_0 that satisfies the following:

$$t_0 \in \left\{ t : \left| \sum_{j=1}^{\rho} M(t)_{ij} (X'y/n)_j \right| \le t \right\}, \quad \forall i = 1, \dots, \rho,$$
 (5)

where $M(t) = \left(\frac{X'X}{n} + \frac{\lambda}{3t^3} [\log(1+t)]^2 I\right)^{-1}$. Here X' represents the transpose of matrix X, and we use this notation in the remaining of the paper. When one chooses the aforementioned t_0 as the initial point in the proposed algorithm, we have $\left|\beta_i^{(0)}\right| \leq t_0$ for any $1 \leq i \leq p$, where $\beta_i^{(0)}$ denotes the ith entry in the vector $\beta_i^{(0)} = M(t_0)X'y/n$.



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update of the hyper-parameter

Shrink the
$$t_k$$
 to $t_{k+1} = t_k(1-h)$



update of the hyper-parameter

- Shrink the t_k to $t_{k+1} = t_k(1-h)$
- Early Stopping in the Inner-Loop: in the kth outer-iteration, the inner-iteration is stopped when

$$F_{t_k}(\beta^{(k)[s]}) - F_{\min,k} < \widetilde{\epsilon}_k,$$

where $\beta^{(k)[s]}$ denotes the iterative estimator in the *s*th inner-iteration of the *k*th outer iteration, and we have

$$F_{\min,k}=\min_{\beta}F_{t_k}(\beta).$$

Here, we set $\tilde{\epsilon}_k = \frac{\lambda p}{3B} [\log(1 + t_k)]^2$, where *B* is the upper bound of $\left| \beta_i^{(k)} \right|$ for all $i = 1, 2, \ldots, p$ and $k = 1, 2, \ldots$



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Theoretical Results



Theorems

Introduction

Theorem (Inner-Loop)

Recall that a Lasso problem has a response vector $y \in \mathbb{R}^n$ and a model matrix $X \in \mathbb{R}^{n \times p}$. To minimize the Lasso objective function $F(\beta) = \frac{1}{2n} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1$, we design a homotopic approach, i.e., in the kth outer-iteration of our proposed algorithm, we use AGD algorithm to minimize a surrogate function $F_{t_k}(\beta) = \frac{1}{2n} \|y - X\beta\|_2^2 + \lambda f_{t_k}(\beta)$. Instead of converging to the minimizer of $F_{t_k}(\beta)$, we do an early stopping to control the total number of numerical operations. And we denote the early stopping estimation as $\beta^{(k)[s]}$, where s is the number of AGD-iterations (inner-iterations). We assume that for any $k = 1, 2, \ldots, s = 1, 2, \ldots$, we have $\left|\beta_i^{(k)[s]}\right| \leq B$, where $\beta_i^{(k)[s]}$ is the ith entry of vector $\beta^{(k)[s]}$ ($i = 1, 2, \ldots, p$), and B is a constant. And we further assume that our proposed algorithm stops when $t_k < \tau$. Under the above assumption, we know that in the kth outer-iteration, the condition $\frac{3B^3 \lambda_{min}(\frac{X'X}{2})}{2B^3 \lambda_{min}(\frac{X'X}{2})}$

number of function $F_{t_k}(\cdot)$ can be bounded by $\frac{3B^3\lambda_{\max}\left(\frac{X'X}{n}\right)}{2\lambda[\log(1+\tau)]^2}+\left(\frac{B}{\tau}\right)^3$. Accordingly, after $C_1\log(1/\widetilde{\epsilon}_k)$ inner-iterations, one is guaranteed to achieve the following precision

$$F_{t_k}(\beta^{(k)}) - F_{\min,k} \leq \widetilde{\epsilon}_k,$$

where $F_{\min,k} = \min_{\beta} F_{t_k}(\beta)$, $\widetilde{\epsilon}_k = \frac{\lambda p}{3B} [\log(1+t_k)]^2$ and C_1 is a constant that does not depend on the value of t_k .



Theorems

Theorem (Number of outer-iteration)

With the conditions in Theorem 3 being satisfied, and suppose the following conditions are also satisfied:

- I For k = 1, 2, ..., we have $t_k = t_0(1 h)^k$ where t_0 , h are pre-specified.
- The precision of AGD in minimizing function $F_{l_k}(\beta)$ is set as $\widetilde{\epsilon}_k = \frac{\lambda \rho}{3B}[\log(1+t_k)]^2$, i.e., we run the AGD until the following inequality is achieved: $F_{l_k}(\beta^{(k)[s]}) F_{k,\min} < \widetilde{\epsilon}_k$, where quantity $\beta^{(k)[s]}$ is the iterative estimator in the sth inner-iteration at the kth outer-iteration, and recall that $F_{k,\min} = \min_{\beta} F_{l_k}(\beta)$.

Then when $k \ge \frac{-1}{\log(1-h)} \log \left(\frac{\lambda p t_0(2B+1)}{\epsilon} \right)$, our proposed algorithm finds a point $\beta^{(k)}$ such that

$$F(\beta^{(k)}) - F_{\min} \leq \epsilon$$

where $F_{\min} = \min_{\beta} F(\beta)$ with $F(\beta) = \frac{1}{2n} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1$, which is defined in (2).



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Theorems

Introduction

Theorem (Main Theory)

Under the conditions that are listed in Theorem 3 and Theorem 4, we can find $\beta^{(k)}$ such that

$$F(\beta^{(k)}) - F_{\min} \le \epsilon$$

with the number of numerical operations has the order of complexity

$$\rho^2 O\left(\left[\frac{-1}{\log(1-h)}\log\left(\frac{\lambda \rho t_0(2B+1)}{\epsilon}\right)\right]^2\right).$$



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Remark

For our proposed algorithm, when $t \rightarrow 0$, we have the perdition error

$$\frac{1}{n} \| X \left(\widetilde{\beta} - \widehat{\beta} \right) \|_2^2 \to 0$$
, where $\widetilde{\beta} = \arg \min_{\beta} \frac{1}{2n} \| y - X \beta \|_2^2 + \lambda f_t(\beta)$ for a general t and $f_t(\beta)$ defined in (4). And $\widehat{\beta} = \arg \min_{\beta} \frac{1}{2n} \| y - X \beta \|_2^2 + \lambda \| \beta \|_1$.



Remark

Suppose the model matrix X in the Lasso problem has the following three properties:

- $\left\| \left(X_{\mathcal{S}}' X_{\mathcal{S}} \right)^{-1} X_{\mathcal{S}}' \right\|_{F} \text{ can be bounded by a constant, where } \mathcal{S} = \{i: \widehat{\beta}_{i} \neq 0, \forall i = 1, 2, \ldots, \rho\} \text{ with }$ $\widehat{\beta} = \frac{1}{2n} \| y X \beta \|_{2}^{2} + \lambda \|\beta\|_{1} \text{ . And } \|\cdot\|_{F} \text{ is the Frobenius norm defined as } \left\| A_{m \times n} \right\|_{F} = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^{2}}, \text{ where }$ $a_{ii} \text{ is the } (i, j) \text{th entry in matrix } A.$
- $\|X_{S^C}^{\dagger}\|_F$ can be bounded by a constant, where S^C is the complement set of S. And $X_{S^C}^{\dagger}$ is the pseudo-inverse of matrix X_{S^C} . The mathematical meaning of pseudo-inverse is that, suppose $X_{S^C} = U\Sigma V$, which is the singular value decomposition (SVD) of X_{S^C} . Then $X_{S^C}^{\dagger} = V'\Sigma^{\dagger}U'$. For the rectangular diagonal matrix Σ , we get Σ^{\dagger} by taking the reciprocal of each non-zero elements on the diagonal, leaving the zeros in place, and then transposing the matrix.
- $\begin{array}{ll} \boxed{\mathbf{3}} & \sigma_{\max}\left(\Sigma_{1}\right) < \min\left\{2,2\sigma_{\min}\left(\Sigma_{2}\right)\right\}, \text{ where } \sigma_{\max}\left(\Sigma_{1}\right) \text{ returns the maximal absolute diagonal values of matrix } \Sigma_{1}, \text{ and } \sigma_{\min}\left(\Sigma_{2}\right) \text{ returns the minimal absolute diagonal values of matrix } \Sigma_{2}. \text{ Matrix } \Sigma_{1} \text{ is the diagonal matrix in the SVD of matrix } \left(X_{S}'X_{S}\right)^{-1}X_{S}'X_{SC} + \left(X_{S}^{\dagger}C_{S}X_{S}\right)', \text{ i.e., } \left(X_{S}'X_{S}\right)^{-1}X_{S}'X_{SC} + \left(X_{S}^{\dagger}C_{S}X_{S}\right)' = U_{1}\Sigma_{1}V_{1}. \text{ Matrix } \Sigma_{2} \text{ is the diagonal matrix of the SVD of matrix } \frac{1}{2}X_{S}^{\dagger}C_{S}C_{S} + \frac{1}{2}\left(X_{S}^{\dagger}C_{S}X_{S}\right)', \text{ i.e., } \frac{1}{2}X_{S}^{\dagger}C_{S}C_{S} + \frac{1}{2}\left(X_{S}^{\dagger}C_{S}X_{S}\right)' = U_{2}\Sigma_{2}V_{2}. \end{array}$

Then we have $\left\|\widetilde{\beta}-\widehat{\beta}\right\|_2^2 \to 0$ when $t\to 0$.



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Numerical Example



Introduction

We generated Gaussian data with *n* observations and *p* predictors, with each pair of predictors noted as X_i , and the explanatory matrix is noted as $X = (X_1 \cdots X_i \cdots X_D).$



Introduction

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- Here we assume that X_i having the same population correlation ρ and we tried a number of ρ varying from 0 to 0.9. (We choose $\rho = 0.5$ in this section.)



Introduction

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- Accordingly, the outcome values were generated by

$$y = X\beta + qz$$
.

where the *i*-th (1 < *i* < *p*) entry in vector $\beta = (\beta_1 \cdots \beta_p)^i$ is generated by $\beta_i = (-1)^i \exp(-2(i-1)/20)$, which are constructed to have alternating signs and to be exponentially decreasing.



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Introduction

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Besides, $z = (z_1 \cdots z_p)'$ is the white noise with normal distribution of z_i as N(0,1)and q is chosen so that the signal-to-noise ratio is 3.0.



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Simulation 1

Introduction

Table: Numerical complexity of ISTA, FISTA, HS in the first simulation

| | | | | Pre | cision ϵ | | | | |
|--------|---------|---------|---------|----------|-------------------|----------|----------|----------|---------|
| method | 0.05 | 0.03 | 0.02 | 0.01 | 0.009 | 0.008 | 0.007 | 0.006 | 0.005 |
| | | | | n = 50 | 0, p = 20 | | | | |
| ISTA | 5, 070 | 6, 016 | 7, 005 | 9, 585 | 10, 101 | 10, 703 | 11, 434 | 12, 294 | 13, 369 |
| FISTA | 4, 781 | 5, 117 | 5, 453 | 6, 461 | 6,685 | 6, 797 | 7, 021 | 7, 133 | 7, 357 |
| Ours | 5, 478 | 5, 478 | 5, 479 | 5, 479 | 5,479 | 5, 479 | 5, 479 | 5, 479 | 6,005 |
| | | | | n = 50 | 0, p = 80 | | | | |
| ISTA | 37, 400 | 50, 277 | 65, 273 | 109, 772 | 119, 226 | 130, 799 | 145, 306 | 164, 377 | 190, 13 |
| FISTA | 31, 237 | 34, 533 | 37, 417 | 45, 657 | 47, 305 | 48, 541 | 50, 189 | 52, 249 | 55, 133 |
| Ours | 30, 919 | 30, 919 | 32, 765 | 34, 611 | 34, 611 | 34, 611 | 36, 457 | 36, 457 | 36, 457 |

There is the parameters settings of our HS algorithm: $t_0 = 3, h = 0.1, \lambda = 1e - 3, \beta^{(0)} = \mathbf{1}_{p \times 1}$.



Numerical Example

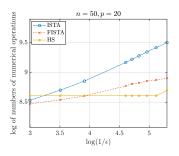
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Homotopic Lasso Solver

Simulation Result



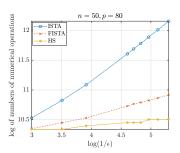


Figure: Number of Operations of ISTA, FISTA, and our algorithm under different ϵ in the first simulation



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Homotopic Lasso Solver

Simulation 2

Introduction

Table: Numerical complexity of ISTA, FISTA, HS in the second simulation

| | | | | Pre | cision ϵ | | | | |
|--------|---------|---------|---------|----------|-------------------|----------|----------|----------|---------|
| method | 0.05 | 0.03 | 0.02 | 0.01 | 0.009 | 0.008 | 0.007 | 0.006 | 0.005 |
| | | | | n = 50 | 0, p = 20 | | | | |
| ISTA | 5, 242 | 6, 274 | 7, 263 | 9, 370 | 9, 757 | 10, 187 | 10, 703 | 11, 305 | 12, 122 |
| FISTA | 4, 781 | 5, 229 | 5, 565 | 6, 125 | 6,349 | 6, 461 | 6, 573 | 6, 797 | 7, 021 |
| Ours | 5, 479 | 5, 479 | 5, 479 | 6,005 | 6,005 | 6,005 | 6,005 | 6,005 | 6,005 |
| | | | | n = 50 | 0, p = 80 | | | | |
| ISTA | 39, 519 | 55, 330 | 72, 119 | 112, 869 | 120, 693 | 130, 473 | 142, 698 | 158, 346 | 179, 37 |
| FISTA | 31,649 | 35, 769 | 39, 065 | 45, 657 | 46, 893 | 48, 129 | 49, 365 | 51,013 | 53, 485 |
| Ours | 30, 918 | 32, 763 | 32, 763 | 32, 763 | 32, 763 | 32, 763 | 32, 763 | 32, 763 | 32, 763 |

The parameters settings of our HS algorithm: $t_0 = 3, h = 0.1, \lambda = 1e - 3, \beta^{(0)} = 0.1_{p \times 1}$



Numerical Example

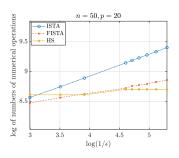
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 State-of-the-Art Lasso Algorithms
 Our proposed Algorithm
 Theoretical Results
 Numerical Example

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Simulation 2



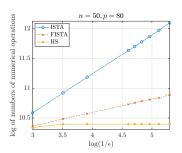


Figure: Number of Operations of ISTA, FISTA, and our algorithm under different ϵ in the second simulation.



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Start at some initial objective problem, which is a Lasso-type objective function:

$$\frac{1}{2n} \|y - X\beta\|_2^2 + \lambda^{(0)} \|\beta\|_1, \tag{6}$$

and then they gradually decrease the large $\lambda^{(0)}$ until the target regularization $\lambda^{(\mathrm{target})}$ is reached.



Other Related Homotopic Ideas

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A close related topic: path-following approach



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- When the path-following approaches work, it is a very nice algorithm; however, contrary to general beliefs, they only work in special cases.



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- Counterexample, where path-following conditions are violated, can be constructed.



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Introduction

 A newly designed homotopic approach that can solve the Lasso-type of problem with better theoretical guarantees (on numerical complexity)



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- Thank You!!!

