Luyang Han & Janosch Ott

Coordinat Descent

Least Angle Regression

Optimization

Recall: Duality

ADMM

Rules

Minor-Max Algorithms

Alternating Minimizations

Computation & optimization for Lasso - part 2

Luyang Han & Janosch Ott

ETH Zürich

22 October 2018

Luyang Han & Janosch Ott

- 1. Coordinate Descent
- 2. Least Angle Regression
- 3. Comparison of Optimization Methods
- 4. Recall: Duality
- 5. ADMM
- 6. Screening Rules

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization
Methods

Recall: Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Coordinate Descent Algorithm

What is the Coordinate Descent (CD) Algorithm?

$$\beta_k^{t+1} = \underset{\beta_k}{\operatorname{argmin}} \ f(\beta_1^t , \beta_2^t , ... \beta_k , \beta_{k+1}^t , ... \beta_p^t)$$
 (1)

and
$$\beta_j^{t+1} = \beta_j^t$$
 for $j \neq k$

• An iterative algorithm that updates from β^t to β^{t+1} by choosing a single coordinate, and minimizing over this coordinate.

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization Methods

Recall:

ADMN

Screenin

Minor-Max Algorithms

Alternating

Separability Condition

Motivation

Does CD procedure converge to the global minimum of a convex function?

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization Methods

Recall: Duality

ADMN

Screenii Rules

Minor-Max Algorithms

Alternating Minimizations

Separability Condition

Motivation

Does CD procedure converge to the global minimum of a convex function?

- **Sufficient Condition:** the function is continuously differentiable and strictly convex in each coordinate.
- ⇒ restrictive

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMM

Screenin Rules

Minor-Max Algorithms

Alternating Minimizations

Separability Condition

Suppose the cost function f has the additive decomposition:

$$f(\beta_1, ..., \beta_p) = g(\beta_1, ..., \beta_p) + \sum_{j=1}^p h_j(\beta_j)$$
 (2)

where $g: \mathbb{R}^p \to \mathbb{R}$ is differentiable and convex, and the univariate functions $h_j: \mathbb{R} \to \mathbb{R}$ is convex.

• <u>Lasso</u>: $g(\beta) = \frac{1}{2N} ||\mathbf{y} - \mathbf{X}\beta||_2^2$ and $h_j(\beta_j) = \lambda |\beta_j|$ satisfies the condition

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

A D I A I

Screeni

Minor-Ma:

Alternating Minimizations

Separability Condition: Example

An Example of failure of Coordinate Descent

$$\underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \ \frac{1}{2N} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \ \lambda_1 \sum_{j=1}^p |\beta_j| + \ \lambda_2 \sum_{j=2}^p |\beta_j - \beta_{j-1}|$$

- $h(\beta)$ is not separable
- Fused Lasso: coordinate descent procedure is not guaranteed to find the global minimum

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization
Methods

Recall:

ΔΡΜΜ

Screenin

Minor-Max Algorithms

Alternating

Separability Condition: Example

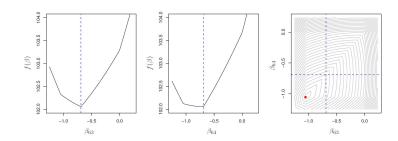


Figure: Fused Lasso: CD fail to reach the global minimum

1

¹Picture taken from Statistical Learning with Sparsity page 111

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization Methods

Recall:

ADMN

Rules

Minor-Max Algorithms

Alternating Minimizations

Lasso & Coordinate Descent

Optimality Condition:

$$-\frac{1}{2N}\sum_{i=1}^{N}(y_i - \beta_0 - \sum_{k=1}^{p}x_{ik}\beta_k)x_{ij} + \lambda s_j = 0$$

where $s_j \in sign(\beta_j)$ for j = 1, 2, ...p

- Define the **partial residual**: $r_i^{(j)} = y_i \sum_{k \neq j} x_{ik} \hat{\beta}_k$
- Then the solution for $\hat{\beta}_j$ satisfies:

$$\hat{\beta}_{j} = \frac{S_{\lambda}(\frac{1}{N}\sum_{i=1}^{N}r_{i}^{(j)}x_{ij})}{\frac{1}{N}\sum_{i=1}^{N}x_{ij}^{2}}$$

where
$$S_{\lambda}(\theta) = sign(\theta)(|\theta| - \lambda)_{+}$$

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMN

Rules
Minor-Ma

Algorithm

Alternating Minimizations

Lasso & Coordinate Descent

Illustration of Coordinate Descent in R

Strategies to make the operation efficient:

Naive Updating

$$r_{i}^{(j)} = y_{i} - \sum_{k \neq j} x_{ik} \hat{\beta}_{k} = r_{i} + x_{ij} \hat{\beta}_{j}$$

$$\frac{1}{N} \sum_{i=1}^{N} x_{ii} r_{i}^{(j)} = \frac{1}{N} \sum_{i=1}^{N} x_{ji} r_{i} + \hat{\beta}_{i}$$

Covariance Updating

$$\sum_{i=1}^{N} x_{ij} r_i = \langle x_j, y \rangle - \sum_{k \mid |\beta_{\hat{k}}| > 0} \langle x_j, x_k \rangle \beta_{\hat{k}}$$

Warm Starts: For a decreasing sequence of values $\{\lambda_0^L\}$, $\hat{\beta}(\lambda_l)$ is typically a very good warm start for the solution $\hat{\beta}(\lambda_{l+1})$. We set $\lambda_0 = \frac{1}{N} \max |\langle x_i, y \rangle|$ and $\lambda_L \approx 0$

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison o Optimization Methods

Recall: Duality

ADMM

Screenin Rules

Minor-Max Algorithms

Alternating Minimizations

Lasso & Coordinate Descent

Active-set Convergence: Define the active set A and iterate the algorithm using only variables in A.

Strong-set Convergence: Define the strong set S and iterate the algorithm using only variables in S.

Sparsity: Sparsity of the design matrix X makes the operation of inner product efficient.

Details in page 113 and page 114.

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison o Optimization Methods

Recall:

Duality

ADMN

Screenin

Minor-Max Algorithms

Alternating Minimizations

Elastic Net & Coordinate Descent

$$minimize_{\beta_0,\beta_p} \frac{1}{2} \sum_{i=1}^{N} (y_i - \beta_0 - x_i^T \beta)^2 + \lambda \left[\frac{1}{2} (1 - \alpha) ||\beta||_2^2 + \alpha ||\beta|| \right]_1$$

- Combination of L1 and L2 penaLty
- Satisfy the separability condition
- The solution satisfies:

$$\hat{\beta}_{j} = \frac{S_{\alpha\lambda}(\frac{1}{N}\sum_{i=1}^{N}r_{i}^{(j)}x_{ij})}{\frac{1}{N}\sum_{i=1}^{N}x_{ij}^{2} + (1-\alpha)\lambda}$$

Luyang Han & Janosch Ott

Coordinate Descent

Regression

Optimization
Methods

Recall:

ADMN

Screeni Rules

Minor-Max Algorithms

Alternating Minimizations

Logistic Regression & Coordinate Descent

Background

• Class Label G: Take values 1 and -1

Denote
$$p(x_i; \beta_0, \beta) = Pr(G = 1|x_i)$$

Define log odds:
$$log \frac{Pr(G=-1|x)}{Pr(G=1|x)} = \beta_0 + x^T \beta$$

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization Methods

Recall:

ADMN

Screeni Rules

Minor-Ma Algorithm

Alternating Minimizations

Logistic Regression & Coordinate Descent

Background

• Class Label G: Take values 1 and -1

Denote
$$p(x_i; \beta_0, \beta) = Pr(G = 1|x_i)$$

Define log odds:
$$log \frac{Pr(G=-1|x)}{Pr(G=1|x)} = \beta_0 + x^T \beta$$

Maximize penalized log-likelihood:

$$\frac{1}{N} \sum_{i=1}^{N} \{ I(g_i = 1) \cdot logp(x_i; \beta_0, \beta) + I(g_i = -1) \cdot log(1 - p(x_i; \beta_0, \beta)) \} - \lambda ||\beta||_1$$
Denote $y_i = I(g_i = -1)$

Explicit form of log likelihood (without penalty):

$$I(\beta_0, \beta) = \frac{1}{N} \sum_{i=1}^{N} \left[y_i \cdot (\beta_0 + x_i^T \beta) - log(1 + e^{\beta_0 + x_i^T \beta}) \right]$$

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMN

Screenin Rules

Minor-Max Algorithms

Alternating Minimizations

Logistic Regression & Coordinate Descent

Background

• Form a quadratic objective function using Taylor expansion about current estimates $(\tilde{\beta}_0, \tilde{\beta})$: Idea of Newton method, Iterated Weighted Least Square problem

$$I_Q(\beta_0, \beta) = -\frac{1}{2N} \sum_{i=1}^{N} (w_i (z_i - \beta_0 - x_i^T \beta)^2 + C(\tilde{\beta_0}, \tilde{\beta})$$

• Use Coordinate Descent to solve the problem $minimize_{(\beta_0,\beta)}\{I_Q\{\beta_0,\beta\}+\lambda||\beta||_1\}$

Luyang Han & Janosch Ott

Coordinate Descent

Regression

Optimization
Methods

Recall: Duality

ADMN

Rules
Minor Ma

Algorithms

Alternating Minimizations

Logistic Regression & Coordinate Descent

Algorithm

OUTER LOOP: Decrement λ

MIDDLE LOOP: Update the quadratic approximation I_Q

using the current parameters (β_0, β)

INNER LOOP: Run the coordinate descent algorithm on the

penalized weighted least squares problem

Luyang Han & Janosch Ott

Least Angle Regression

Comparison of Optimization

Recall:

A D I A I

Screenin

Minor-Max Algorithms

Alternating Minimizations

Least Angle Regression

Introduction

- Relates to Forward Selection method
- Relates to Lasso method
- Able to deliver the entire solution path of the lasso problem with squared-error loss as a function of the regularization parameter λ

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison o Optimization Methods

Recall: Duality

ADMM

Rules

Minor-Max Algorithms

Alternating Minimizations

Least Angle Regression: Algorithm

- Start with all coefficients β_j equal to zero
- Find the predictor X_j most correlated with y
- Increase the coefficient β_j in the direction of the sign of its correlation with y
- Take **residuals** $r = y \hat{y}$ along the way; Stop when some other predictor X_k has **as much correlation** with r as X_j has
- Increase β_j, β_k in their joint least squares direction, until some other predictor has as much correlation with the residual r

Continue until: all predictors are in the model

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ΔΡΜΙΛ

Screenin Rules

Minor-Max Algorithms

Alternating Minimizations

Least Angle Regression: Algorithm

Algorithm 5.1 Least Angle Regression.

- 1. Standardize the predictors to have mean zero and unit ℓ_2 norm. Start with the residual $\mathbf{r}_0 = \mathbf{y} \bar{\mathbf{y}}, \, \beta^0 = (\beta_1, \beta_2, \dots, \beta_p) = \mathbf{0}$.
- 2. Find the predictor \mathbf{x}_j most correlated with r_0 ; i.e., with largest value for $|\langle \mathbf{x}_j, r_0 \rangle|$. Call this value λ_0 , define the active set $\mathcal{A} = \{j\}$, and $\mathbf{X}_{\mathcal{A}}$, the matrix consisting of this single variable.
- 3. For $k = 1, 2, ..., K = \min(N 1, p)$ do:
 - (a) Define the least-squares direction $\delta = \frac{1}{\lambda_{k-1}} (\mathbf{X}_{\mathcal{A}}^T \mathbf{X}_{\mathcal{A}})^{-1} \mathbf{X}_{\mathcal{A}}^T r_{k-1}$, and define the *p*-vector Δ such that $\Delta_{\mathcal{A}} = \delta$, and the remaining elements are zero.
 - (b) Move the coefficients β from β^{k-1} in the direction Δ toward their least-squares solution on $\mathbf{X}_{\mathcal{A}}$: $\beta(\lambda) = \beta^{k-1} + (\lambda_{k-1} \lambda)\Delta$ for $0 < \lambda \leq \lambda_{k-1}$, keeping track of the evolving residuals $\mathbf{r}(\lambda) = \mathbf{y} \mathbf{X}\beta(\lambda) = \mathbf{r}_{k-1} (\lambda_{k-1} \lambda)\mathbf{X}\Delta$.
 - (c) Keeping track of $|\langle \mathbf{x}_{\ell}, \mathbf{r}(\lambda) \rangle|$ for $\ell \notin \mathcal{A}$, identify the largest value of λ at which a variable "catches up" with the active set; if the variable has index j, that means $|\langle \mathbf{x}_{j}, \mathbf{r}(\lambda) \rangle| = \lambda$. This defines the next "knot" λ_{k} .
 - (d) Set $\mathcal{A} = \mathcal{A} \cup \{j\}$, $\beta^k = \beta(\lambda_k) = \beta^{k-1} + (\lambda_{k-1} \lambda_k)\Delta$, and $\mathbf{r}_k = \mathbf{y} \mathbf{X}\beta^k$.
- 4. Return the sequence $\{\lambda_k, \beta^k\}_0^K$.

Luyang Han & Janosch Ott

Coordinat

Least Angle Regression

Comparison of Optimization

Recall:

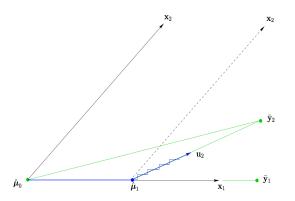
A DIAM

Screening Rules

Minor-Max

Alternating

Least Angle Regression: Geometric Representation



³

³Figure taken from Efron, Hastie, Johnstore and Tibschirani (2004)

Computatio	n
&	
optimization	1
Luyang Han	&

Janosch Ott

Comparison of Optimization Methods

Luyang Han & Janosch Ott

Coordinat

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

A D. 44

_

Rules Minor May

Algorithms

Alternating Minimizations

Connection between LAR and Lasso

LAR

$$\mathbf{x}_{j}^{T}(\mathbf{y} - \mathbf{X}\beta(\lambda)) = \lambda \cdot \mathbf{s}_{j}, \ \forall j \in \mathbb{A}$$
 where \mathbf{s}_{j} is the sign of inner product λ . [3(c)]

Luyang Han & Janosch Ott

Coordinate

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMN

Rules

Minor-Max Algorithms

Alternating Minimizations

Connection between LAR and Lasso

LAR

 $\mathbf{x}_{j}^{T}(\mathbf{y} - \mathbf{X}\beta(\lambda)) = \lambda \cdot s_{j}, \ \forall j \in \mathbb{A} \ \text{ where } s_{j} \text{ is the sign of inner product } \lambda. \ [3(c)]$

LASSO

Let \mathbb{B} be the active set of variables in the solution for a given value of λ .

$$R(\beta) = \frac{1}{2}||\mathbf{y} - \mathbf{X}\beta||_2^2 + \lambda||\beta||_1$$

For differentiable $R(\beta)$, the stationary conditions give:

$$\mathbf{x}_i^T(\mathbf{y} - \mathbf{X}eta) = \lambda \cdot sign(eta_j), orall j \in \mathbb{B}$$

If sign (β_j) matches s_j , the coefficient would be identical.

Luyang Han & Janosch Ott

Coordinat Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMN

NA:

Minor-Max Algorithms

Alternating Minimization

Connection between LAR and Lasso

- R Example
- LAR algorithm explains that the coefficient paths for the lasso are piecewise linear
- Coefficient paths differ if $sign(\beta_j)$ is different from s_j
- Modification of LAR for computing Lasso solution [3(c)+]:

If a **nonzero** coefficient **crosses zero** before the next variable enters, **drop** it from \mathbb{A} and recompute the current joint least squares direction.

Luyang Han & Janosch Ott

Coordinate

Least Angle Regression

Comparison of Optimization Methods

Recall:

ΔΡΜΝ

Screening Rules

Minor-Max Algorithms

Alternating

Connection between LAR and Lasso

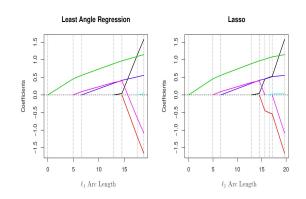


Figure: Cases where signs of λ and β disagree

4

⁴Picture taken from Statistical Learning with Sparsity page 120

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMN

Screenin Rules

Minor-Max Algorithms

Alternating Minimization

Algorithm Performance

Simulation: Comparison of computation efficiency between CD and LAR

Set Up: 5

- Generate Gaussian data with N observations and p predictors, with each pair of predictors X_j , X_k having the same population correlation ρ .
- Try different combination of N and p; Range ρ from 0 to 0.95.

$$Y = \sum_{j=1}^{p} X_j \beta_j + kZ$$
 where $\beta_j = (-1)^j exp(\frac{-2(j-1)}{20}), Z \sim N(0,1)$ and k is a constant.

⁵Friedman, Hastie, Tibshirani (2010)

Luyang Han & Janosch Ott

Coordinat Descent

Regression

Comparison of Optimization Methods

Recall: Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating

Algorithm Performance

	L	inear Re	gression	— Dens	e Featur	es
			Corre	lation		
	0	0.1	0.2	0.5	0.9	0.95
			N = 1000	p = 100)	
glmnet-naive	0.05	0.06	0.06	0.09	0.08	0.07
glmnet-cov	0.02	0.02	0.02	0.02	0.02	0.02
lars	0.11	0.11	0.11	0.11	0.11	0.11
			N = 5000	p = 100)	
glmnet-naive	0.24	0.25	0.26	0.34	0.32	0.31
glmnet-cov	0.05	0.05	0.05	0.05	0.05	0.05
lars	0.29	0.29	0.29	0.30	0.29	0.29
			N = 100,	p = 1000)	
glmnet-naive	0.04	0.05	0.04	0.05	0.04	0.03
glmnet-cov	0.07	0.08	0.07	0.08	0.04	0.03
lars	0.73	0.72	0.68	0.71	0.71	0.67
			N = 100,	p = 5000)	
glmnet-naive	0.20	0.18	0.21	0.23	0.21	0.14
glmnet-cov	0.46	0.42	0.51	0.48	0.25	0.10
lars	3.73	3.53	3.59	3.47	3.90	3.52
		i i	V = 100,	p = 2000	0	
glmnet-naive	1.00	0.99	1.06	1.29	1.17	0.97
glmnet-cov	1.86	2.26	2.34	2.59	1.24	0.79
lars	18.30	17.90	16.90	18.03	17.91	16.39
			V = 100.	p = 5000	0	

Figure: Comparison of computing time

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMN

Screenin Rules

Minor-Max Algorithms

Alternating Minimizations

Algorithm Performance

Simulation: Comparison of computation efficiency between Coordinate Descent, Proximal Gradient Descent and Nestrov Method

Set Up: ⁷

- Generated an N × p predictor matrix X with standard Gaussian entries and pairwise correlation 0 or 0.5 between the features.
- $|\beta_j| = \exp\left[-0.5(u(j-1))^2\right]$ and $u = \sqrt{\frac{\pi}{20}}$ and alternating signs -1,+1,-1...

⁷Statistical Learning with Sparsity Page 117

Luyang Han &

Coordinate

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMIN

Rules

Algorithms

Alternating Minimizations

Algorithm Performance

Table 5.1 Lasso for linear regression: Average (standard error) of CPU times over ten realizations, for coordinate descent, generalized gradient, and Nesterov's momentum methods. In each case, time shown is the total time over a path of 20λ values.

	N = 10000, p = 100		N = 200, p = 10000		
Correlation	0	0.5	0	0.5	
Coordinate descent	0.110 (0.001)	0.127 (0.002)	0.298 (0.003)	0.513 (0.014)	
Proximal gradient	0.218 (0.008)	0.671 (0.007)	1.207 (0.026)	2.912(0.167)	
Nesterov	0.251 (0.007)	0.604 (0.011)	1.555 (0.049)	$2.914\ (0.119)$	

 $0 \quad 1 \quad i1 \quad \cdot \quad 1 \quad \cdot \quad i \quad \cdots \quad i \quad 1$

Figure: Comparison of computing efficiency between 3 methods

8

⁸Statistical Learning with Sparsity Page 117

Luyang Han & Janosch Ott

Coordinat

Least Angle Regression

Optimization
Methods

Recall: Duality

ADMN

Screenin Rules

Minor-Max Algorithms

Alternating Minimizations

Recall: Duality in optimization

Luyang Han & Janosch Ott

Coordinate Descent

Regression

Optimization Methods

Recall: Duality

ADMIN

Rules

Algorithms

Alternating Minimizations

	Primal	
Optimize	$\min f(x)$	
Constraints	$g_i(x) \leq 0, h_j(x) = 0, x \in X$	
Function	$L(x, \lambda, \mu) := f(x) + \sum_{i} \lambda_{i} g_{i}(x) + \sum_{j} \mu_{j} h_{j}(x)$	
Dual		
Function	$q(\lambda,\mu) = \inf_{x \in X} L(x,\lambda,\mu)$	
Constraints	$\lambda \ge 0$	
Optimize	$\max_{\lambda \geq 0, \mu} q(\lambda, \mu)$	
	_	

Why though? - Dual problem is always convex!

Luyang Han & Janosch Ott

Coordinate

Least Angle Regression

Comparison o Optimization Methods

Recall: Duality

ADMM

Rules

Minor-Max Algorithms

Alternating Minimizations

Alternating Direction Method of Multipliers (ADMM)

Problem

$$\min_{\beta \in \mathbb{R}^m, \theta \in \mathbb{R}^n} f(\beta) + g(\theta) \quad \text{subject to } \mathbf{A}\beta + \mathbf{B}\theta - c = 0$$

Lagrangian

$$f(\beta) + g(\theta) + \langle \mu, \mathbf{A}\beta + \mathbf{B}\theta - c \rangle$$

Augmented Lagrangian

$$L_
ho(eta, heta,\mu):=f(eta)+g(heta)+\langle\mu,\mathbf{A}eta+\mathbf{B} heta-c
angle+rac{
ho}{2}||\mathbf{A}eta+\mathbf{B} heta-c||_2^2$$

Luyang Han & Janosch Ott

Coordinate Descent

Comparison of Optimization

Methods Recall:

Duality

ADMM

Minau Ma

Minor-Max Algorithms

Alternating Minimizations

Alternating Direction Method of Multipliers (ADMM)

Problem - decomposable!

$$\min_{\beta \in \mathbb{R}^m, \theta \in \mathbb{R}^n} f(\beta) + g(\theta) \quad \text{subject to } \mathbf{A}\beta + \mathbf{B}\theta - c = 0$$

Lagrangian

$$f(\beta) + g(\theta) + \langle \mu, \mathbf{A}\beta + \mathbf{B}\theta - c \rangle$$

Augmented Lagrangian

$$L_{
ho}(eta, heta,\mu):=f(eta)+g(heta)+\langle\mu,\mathbf{A}eta+\mathbf{B} heta-c
angle+rac{
ho}{2}||\mathbf{A}eta+\mathbf{B} heta-c||_2^2$$

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMM

ADIVIIV

Minor-Ma

Algorithms

Alternating Minimizations

Alternating Direction Method of Multipliers (ADMM)

Problem - decomposable !

Lagrangian - decomposable!

$$f(\beta) + g(\theta) + \langle \mu, \mathbf{A}\beta + \mathbf{B}\theta - c \rangle$$

Augmented Lagrangian

$$L_{
ho}(eta, heta,\mu):=f(eta)+g(heta)+\langle\mu,\mathbf{A}eta+\mathbf{B} heta-c
angle+rac{
ho}{2}||\mathbf{A}eta+\mathbf{B} heta-c||_2^2$$

Luyang Han & Janosch Ott

Coordinate Descent

Comparison of

Optimization Methods

Recall: Duality

ADMM

, ,,,,,,,,,

Minor M

Algorithms

Alternating Minimizations

Alternating Direction Method of Multipliers (ADMM)

Problem - decomposable!

$$\min_{\beta \in \mathbb{R}^m, \theta \in \mathbb{R}^n} f(\beta) + g(\theta) \quad \text{subject to } \mathbf{A}\beta + \mathbf{B}\theta - c = 0$$

Lagrangian - decomposable !

$$f(\beta) + g(\theta) + \langle \mu, \mathbf{A}\beta + \mathbf{B}\theta - c \rangle$$

Augmented Lagrangian - NOT decomposable !

$$L_
ho(eta, heta,\mu):=f(eta)+g(heta)+\langle\mu,\mathbf{A}eta+\mathbf{B} heta-c
angle+rac{
ho}{2}||\mathbf{A}eta+\mathbf{B} heta-c||_2^2$$

Luyang Han & Janosch Ott

Coordinat Descent

Least Angle Regression

Optimization Methods

Recall: Duality

ADMM

Screenir Rules

Minor-Max Algorithms

Alternating Minimization

Dual Variable Update

Alternating Direction Method of Multipliers

$$\begin{split} \beta^{t+1} &= \operatorname*{arg\;min}_{\beta \in \mathbb{R}^m} L_{\rho}(\beta, \theta^t, \mu^t) \\ \theta^{t+1} &= \operatorname*{arg\;min}_{\theta \in \mathbb{R}^m} L_{\rho}(\beta^{t+1}, \theta, \mu^t) \\ \mu^{t+1} &= \mu^t + \rho(\mathbf{A}\beta^{t+1} + \mathbf{B}\theta^{t+1} - c) \end{split}$$

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization Methods

Recall: Duality

ADMM

Rules

Minor-Max Algorithms

Alternating Minimizations

Dual Variable Update

Alternating Direction Method of Multipliers

$$\begin{split} \beta^{t+1} &= \operatorname*{arg\,min}_{\beta \in \mathbb{R}^m} L_{\rho}(\beta, \theta^t, \mu^t) \\ \theta^{t+1} &= \operatorname*{arg\,min}_{\theta \in \mathbb{R}^m} L_{\rho}(\beta^{t+1}, \theta, \mu^t) \\ \mu^{t+1} &= \mu^t + \rho(\mathbf{A}\beta^{t+1} + \mathbf{B}\theta^{t+1} - c) \end{split}$$

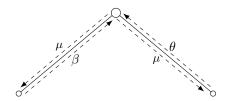


Figure: My own illustration of the dual ascent step in the ADMM algorithm utilising dual decomposition based on [Gordon and Tibshirani, 2012].

Luyang Han & Janosch Ott

Coordinat

Least Angle Regression

Optimization
Methods

Recall: Duality

ADMM

Kules

Minor-Max Algorithms

Alternating Minimizations

ADMM - Why?

- convex problems with nondifferentiable constraints
- blockwise computation
 - sample blocks
 - feature blocks

Luyang Han & Janosch Ott

Coordinate

Least Angle Regression

Comparison o Optimization Methods

Recall: Duality

ADMM

Kules

Minor-Max Algorithms

Alternating Minimizations

ADMM for the Lasso

Problem in Lagrangian form

$$\underset{\beta \in \mathbb{R}^{p}, \theta \in \mathbb{R}^{p}}{\operatorname{minimize}} \left\{ \frac{1}{2} \left\| \mathbf{y} - \mathbf{X} \beta \right\|_{2}^{2} + \lambda \left\| \theta \right\|_{1} \right\} \quad \text{such that } \beta - \theta = 0$$

Augmented Lagrangian

$$\mathcal{L}_{
ho}(eta, heta,\mu) := \left\{rac{1}{2}\left\|\mathbf{y}-\mathbf{X}eta
ight\|_{2}^{2} + \lambda\left\| heta
ight\|_{1}
ight\} + \langle\mu,eta- heta
angle + rac{
ho}{2}||eta- heta||_{2}^{2}$$

Luyang Han & Janosch Ott

ADMM for the Lasso Update

Least Angle

Comparison of Optimization

Recall: Duality

ADMM

Rules

Minor-Max Algorithms

Alternating Minimizations

Update

$$\begin{split} \boldsymbol{\beta}^{t+1} &= (\mathbf{X}^T \mathbf{X} + \rho \mathbf{I})^{-1} (\mathbf{X}^T \mathbf{y} + \rho \boldsymbol{\theta}^t - \boldsymbol{\mu}^t) \\ \boldsymbol{\theta}^{t+1} &= \mathcal{S}_{\lambda/\rho} (\boldsymbol{\beta}^{t+1} + \boldsymbol{\mu}^t/\rho) \\ \boldsymbol{\mu}^{t+1} &= \boldsymbol{\mu}^t + \rho (\boldsymbol{\beta}^{t+1} - \boldsymbol{\theta}^{t+1}) \end{split}$$

where
$$S_{\lambda/\rho}(z) = \operatorname{sign}(z)(|z| - \frac{\lambda}{\rho})_+$$
.

Luyang Han & Janosch Ott

Coordinat Descent

Comparison o

Optimization Methods

Recall: Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Screening Rules

- Pre-processing to eliminate features
- very big data set, esp. huge number of predictors
- maybe too big to load into memory
- Screening rules eliminate predictors with minor calculation
- and very high / safe certainty (i.e. eliminated predictors would not show up in lasso model based on full data)

They achieve a reduction in the number of variables, typically by an order of magnitude

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization
Methods

Recall: Duality

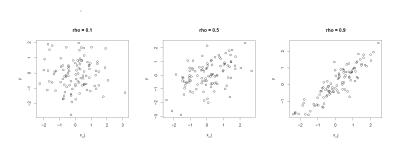
ADMN

Screening Rules

Minor-Ma Algorithm

Alternating

What is a good predictor?



correlation is an inner product
high absolute correlation (=large absolute inner product)

- > high predictive power (compare plots)
- $->x_j$ with largest inner product has highest predictive power, thus for that j we are most willing to accept some penalty from λ

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison o Optimization Methods

Recall: Duality

ADMN

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Lasso - an iterative algorithm

Let $\mathcal A$ be the active set of predictors. Let λ take values on a decreasing sequence.

iterate

- 1. order predictors x_j not in \mathcal{A} by their "effectiveness" using $\left|x_j^T y\right|$ or better $\left|x_j^T (y \hat{y}_{\lambda})\right|$, call the best predictor $x_{j_{\text{max}}}$
- 2. move λ such that the positive effect from the best predictor $x_{i_{\max}}$ compensates the penalty by λ
- 3. calculate solution for chosen λ

Luyang Han & Janosch Ott

Coordinate

Least Angle Regression

Optimization
Methods

Recall:

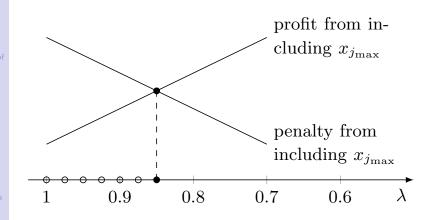
V D M M

Screening Rules

Minor-Max

Algorithms

Lasso - a visual intepretation



Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Back to screening rules

Let λ take values on a decreasing sequence. Let λ_{\max} be the λ where the first predictor has a non-zero coefficient.

$$\lambda_{\max} = \max_{j} \left| x_{j}^{T} y \right|$$

Let A be the active set of predictors.

$$\forall j \in \mathcal{A} \ \lambda = \left| x_j^T (y - \hat{y}) \right|$$

$$\forall j \notin \mathcal{A} \ \lambda \geq \left| x_j^T (y - \hat{y}) \right|$$

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization Methods

Recall: Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Back to screening rules

Let λ take values on a decreasing sequence. Let λ_{\max} be the λ where the first predictor has a non-zero coefficient.

$$\lambda_{\max} = \max_{j} \left| x_{j}^{T} y \right|$$

Let A be the active set of predictors.

$$\forall j \in \mathcal{A} \ \lambda = \left| x_j^T (y - \hat{y}) \right|$$

$$\forall j \notin \mathcal{A} \ \lambda \geq \left| x_j^T (y - \hat{y}) \right|$$

R example

Luyang Han & Janosch Ott

Coordinat Descent

Regression

Optimization Methods

Recall: Duality

ΔDMN

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Global vs. Sequential

Global (one-time screening):

Suppose we want to calculate a lasso solution at $\lambda < \lambda_{\max}$.

Sequential (iterative screening):

Suppose we have the lasso solution $\hat{\beta}(\lambda')$ at λ' and want to screen variables for solutions at $\lambda < \lambda'$.

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMN

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Dual Polytope Projection (DPP)

Suppose we want to calculate a lasso solution at $\lambda < \lambda_{\max}$. The DPP rule discards the j^{th} variable if

$$\left|\mathbf{x}_{j}^{T}\mathbf{y}\right|<\lambda_{\mathsf{max}}-\left\|\mathbf{x}_{j}\right\|_{2}\left\|\mathbf{y}\right\|_{2}\frac{\lambda_{\mathsf{max}}-\lambda}{\lambda}$$

Sequential DPP rule

Suppose we have the lasso solution $\hat{\beta}(\lambda')$ at λ' and want to screen variables for solutions at $\lambda < \lambda'$. We discard the j^{th} variable if

$$\left|\mathbf{x}_{j}^{T}(\mathbf{y} - \mathbf{X}\hat{eta}(\lambda'))\right| < \lambda' - \left\|\mathbf{x}_{j}\right\|_{2} \left\|\mathbf{y}\right\|_{2} \frac{\lambda_{\mathsf{max}} - \lambda}{\lambda}$$

Luyang Han & Janosch Ott

Coordinate Descent

Regression

Optimization Methods

Recall: Duality

ADMN

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Global Strong Rule

Suppose we want to calculate a lasso solution at $\lambda < \lambda_{\max}$. The global strong rule discards the j^{th} variable if

$$\left|\mathbf{x}_{j}^{\mathsf{T}}\mathbf{y}\right|<\lambda-\left(\lambda_{\mathsf{max}}-\lambda
ight)=2\lambda-\lambda_{\mathsf{max}}$$

Sequential Strong Rule

Suppose we have the lasso solution $\hat{\beta}(\lambda')$ at λ' and want to screen variables for solutions at $\lambda < \lambda'$. We discard the j^{th} variable if

$$\left|\mathbf{x}_{j}^{T}(\mathbf{y}-\mathbf{X}\hat{eta}(\lambda'))\right|<2\lambda-\lambda'$$

Luyang Han & Janosch Ott

Coordinat Descent

Comparison of Optimization

Methods

Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Screening Rules - Example Setup

- simulated dataset
- N = 200, p = 5000 uncorrelated Gaussian predictors,
- 1/4 true non-zero coefficients
- 100 decreassing lambda values equally spaced on the log-scale
- Compare Global DPP, Global Strong, Sequential DDP, Sequential Strong
- no violations for either of the strong rules

Luyang Han & Janosch Ott

Coordinate

Least Angle Regression

Optimization
Methods

Recall:

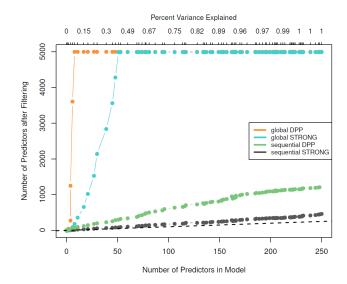
ADMN

Screening Rules

Minor-Max Algorithms

Alternating

Figure: From [Hastie et al., 2015]



Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison o Optimization Methods

Recall: Duality

ADMN

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Summary I

Coordinate Descent

- An efficient algorithm implemented in glmnet but requires separability condition
- Application: Ridge, Lasso, Elastic Net, Logistic Regression, etc.

Least Angle Regression

- Similar to the idea of Forward Selection
- Computationally efficient but does not scale well to large problems

Connection between LASSO and LAR

- LAR could be modified to obtain Lasso solution
- Explains the fact that Lasso coefficient solution path is piece-wise linear

Luyang Han & Janosch Ott

Coordinate Descent

Comparison

Optimization Methods

Recall: Duality

ADMN

Screening Rules

Minor-Ma:

Alternating Minimizations

Summary II

ADMM

- Use duality to your advantage
- Limitations in speed for Lasso, but useful in more complex settings

Screening Rules

- Promising for very large p's
- Difficult to find best rule, field in development

Luyang Han & Janosch Ott

Coordinat Descent

Comparison

Optimization Methods

Recall: Duality

ADMN

Rules

Minor-Max Algorithms

Alternating

Minorization-Maximization Algorithms (MMA)

- Problem: minimize $f(\beta)$ over $\beta \in \mathbb{R}^p$ for f possibly non-convex
- Introduce additional variable θ
- Use θ to majorize (bound from above) the objective function to be minimized

Majorization-Minimization Algorithms work analoguosly.

Luyang Han & Janosch Ott

Coordinat

Least Angl Regression

Optimization
Methods

Recall: Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating

MMA visually

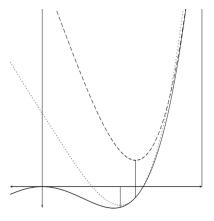


Figure: Figure from [de Leeuw, 2015]

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Comparison of Optimization Methods

Recall: Duality

ADMM

Screenin

Minor-Max Algorithms

Alternating Minimizations

MMA analytically I

Def. $\Psi : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ majorizes f at $\beta \in \mathbb{R}^p$ if

$$\forall \theta \in \mathbb{R}^p \quad \Psi(\beta, \theta) \geq f(\beta)$$

with equality for $\theta = \beta$.

Minor-Maxxalgorithm

- initialize β^0
- update with $eta^{t+1} = rg\min_{eta \in \mathbb{R}^p} \Psi(eta, eta^t)$

Luyang Han & Janosch Ott

Coordinate Descent

Regression

Comparison of Optimization Methods

Recall: Duality

ADMM

Screeni

Minor-Max Algorithms

Alternating Minimizations

MMA analytically II

This scheme generates a sequence of β 's for which the cost $f(\beta^t)$ is nonincreasing, because

$$f(\beta^t) \stackrel{(i)}{=} \Psi(\beta^t, \beta^t) \stackrel{(ii)}{\geq} \Psi(\beta^{t+1}, \beta^t) \stackrel{(iii)}{\geq} f(\beta^{t+1})$$

where

- (i) & (iii) Definiton of majorize
 - (ii) β^{t+1} is a minimizer of $\beta \mapsto \Psi(\beta, \beta^t)$

Luyang Han & Janosch Ott

Coordinat Descent

Comparison of

Optimization Methods

Recall: Duality

ADMN

Screeni

Minor-Max Algorithms

Alternating Minimizations Let's consider an example . . .

$$f(\alpha,\beta) = (1 - \alpha\beta)^2$$

Least Angle Regression

Comparison o Optimization Methods

Recall: Duality

ADMM

Rules

Minor-Max Algorithms

Alternating Minimizations Let's consider an example . . .

$$f(\alpha,\beta) = (1 - \alpha\beta)^2$$

Def. A function $f(\alpha, \beta): \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}$ is biconvex, if for each $\alpha \in \mathbb{R}^m$ the function $\alpha \mapsto f(\alpha, \beta)$ is convex and for each $\beta \in \mathbb{R}^n$ the function $\beta \mapsto f(\alpha, \beta)$ is convex. Analoguosly, a set $\mathcal{C} \subseteq \mathcal{A} \times \mathcal{B}$, for \mathcal{A}, \mathcal{B} convex sets, is called <u>biconvex</u>, if it is convex

Luyang Han & Janosch Ott

Coordinate

Least Angle Regression

Comparison o Optimization Methods

Recall: Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

Alternate Convex Search

Block coordinate descent applied to α and β blocks

- 1. Initialize (α^0, β^0) at some point in the biconvex set to minimize over
- 2. For t = 0, 1, 2, ...
 - (i) Fix $\beta = \beta^t$ and update $\alpha^{t+1} \in \arg\min_{\alpha \in \mathcal{C}_{\beta^t}} f(\alpha, \beta^t)$
 - (ii) Fix $\alpha = \alpha^{t+1}$ and update $\beta^{t+1} \in \operatorname*{arg\,min}_{\alpha \in \mathcal{C}_{\alpha^{t+1}}} f(\alpha^{t+1}, \beta)$

For a function bounded from below, the algorithm converges to a partial optimum (i.e. as biconvexity, only optimal in one coordinate if the other coordinate is fixed).

Luyang Han & Janosch Ott

Coordinate Descent

Least Angle Regression

Optimization
Methods

Recall: Duality

ADMN

Screenin

Minor-Ma:

Alternating Minimizations

References I



Trevor Hastie, Robert Tibshirani, and Martin Wainwright (2015) Statistical learning with sparsity: the Lasso and generalizations *CRC Press:* Boca Raton. FL



Jan De Leeuw (2015)

Block Relaxation Methods in Statistics

doi.org/10.13140/RG.2.1.3101.9607 (last accessed: 02.10.18)



S. Boyd

Alternating Direction Method of Multipliers

https://web.stanford.edu/~boyd/papers/pdf/admm_slides.pdf (last accessed: 14.10.18)



Geoff Gordon and Ryan Tibshirani (2012)

Uses of Duality

https://www.cs.cmu.edu/~ggordon/10725-F12/slides/ 18-dual-uses.pdf (last accessed: 14.10.18)

Luyang Han & Janosch Ott

Coordinat Descent

Least Angle Regression

Optimization

Recall:

A DIMIN

Screenin

Minor-Max

Alternating Minimizations

References II



Paul Rubin (2016)

What are the advantages of convex optimization compared to more general optimization problems?

https://www.quora.com/

What-are-the-advantages-of-convex-optimization-compared-to-

(last accessed: 14.10.18)

Luyang Han & Janosch Ott

Coordinat Descent

Least Angle Regression

Comparison o Optimization Methods

Recall: Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating Minimizations Comments . . . Questions . . . Suggestions . . .

Luyang Han & Janosch Ott

Coordinat Descent

Least Angle Regression

Optimization Methods

Recall: Duality

ADMM

Screening Rules

Minor-Max Algorithms

Alternating Minimizations

That's it. Thanks for listening.

Fill out your feedback sheets!