Computation & optimization

Luyang Han & Janosch Ott

Computation & optimization for Lasso - part 2

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ETH Zürich

22 October 2018

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Overview

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└Overview

Overview

1. Coordinate Descent
2. A Simulation Study
3. Least Angle Regression
4. ADMM
5. Minor-Max Algorithms
6. Alternating Minimizations
7. Screening Rules

Alternating Direction Method of Multipliers (ADMM)

Problem

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

Lagrangian

$$f(\beta)+g(\theta)+\rho||\mathbf{A}\beta+\mathbf{B}\theta-c||_2^2$$

Augmented Lagrangian

$$L_\rho(\beta,\theta,\mu):=f(\beta)+g(\theta)+\langle\mu,\mathbf{A}\beta+\mathbf{B}\theta-c\rangle+\frac{\rho}{2}||\mathbf{A}\beta+\mathbf{B}\theta-c||_2^2$$

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Augmented: scalar product with μ gets added

Dual variable update

$$\beta^{t+1} = \arg\min_{\beta \in \mathbb{R}^m} L_\rho(\beta, \theta^t, \mu^t)$$
$$\theta^{t+1} = \arg\min_{\theta \in \mathbb{R}^m} L_\rho(\beta^{t+1}, \theta, \mu^t)$$
$$\mu^{t+1} = \mu^t + \rho(\mathbf{A}\beta^{t+1} + \mathbf{B}\theta^{t+1} - c)$$

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ADMM - Why?

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

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Detailsfor blockwise computation in Exercise 5.12.

ADMM for the Lasso

Problem in Lagrangian form

$$\underset{\beta \in \mathbb{R}^p, \theta \in \mathbb{R}^p}{\text{minimize}} \left\{ \frac{1}{2} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \|\theta\|_1 \right\} \quad \text{such that } \beta - \theta = 0$$

Update

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

where $\mathcal{S}_{\lambda/\rho}(z) = \text{sign}(z)(|z| - \frac{\lambda}{\rho})_+$.

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where $\mathcal{S}_{\lambda/\rho}(z) = \text{sign}(z)(|z| - \frac{\lambda}{\rho})_+$.

Computational cost: Initially $\mathcal{O}(p^3)$, which is a lot, for the SVD(singular value decomposition of $\mathbf{X}$), after that comparable to coordinate descent or composite gradient from earlier

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.

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MMA visually

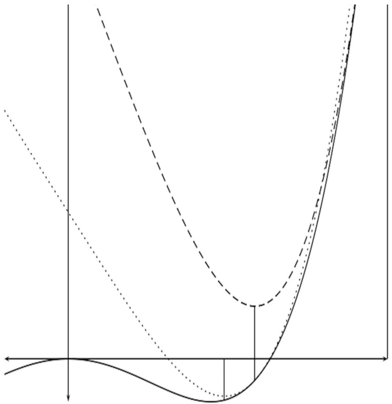

Figure: Figure from [de Leeuw, 2015]

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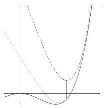

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MMA analytically I

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-Max algorithm

- initialize β^0
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MMA analytically II

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

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

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for inequalities: show previous slide

Biconvexity

Let's consider an example . . .

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

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Mathematica: `3D plot (1-xy)^2, x in [-2,2], y in [-2,2]`

The formula is a link.

Biconvexity

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 biconvex, if it is convex

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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 $t = 0, 1, 2, \dots$
   - (i) Fix $\beta = \beta^t$ and update $\alpha^{t+1} \in \underset{\alpha \in \mathcal{C}_{\beta^t}}{\arg\min} f(\alpha, \beta^t)$
   - (ii) Fix $\alpha = \alpha^{t+1}$ and update $\beta^{t+1} \in \underset{\alpha \in \mathcal{C}_{\alpha^{t+1}}}{\arg\min} f(\alpha^{t+1}, \beta)$

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).

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Screening Rules

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

$$\left|\mathbf{x}_j^T \mathbf{y}\right| < \lambda_{\max} - \|\mathbf{x}_j\|_2 \, \|\mathbf{y}\|_2 \, \frac{\lambda_{\max} - \lambda}{\lambda}$$

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

$$\left|\mathbf{x}_j^T (\mathbf{y} - \mathbf{X}\hat{\beta}(\lambda'))\right| < \lambda' - \|\mathbf{x}_j\|_2 \, \|\mathbf{y}\|_2 \, \frac{\lambda_{\max} - \lambda}{\lambda}$$

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Global Strong Rule

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

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

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References

Trevor Hastie, Robert Tibshirani, and Martin Wainwright (2015)
Statistical learning with sparsity: the Lasso and generalizations
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