Computation & optimization for Lasso - part 2

Luyang Han & Janosch Ott

ETH Zürich

22 October 2018

2018-10-14

Computation & optimization

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Overview

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

Digression: Duality in optimization

In various section, I came across terms like "dual" and "dual problem"

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	$\lambda \geq 0$
Optimize	$\max q(\lambda, \mu)$

Why though? - **Dual problem is always convex!**

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Why though? - **Dual problem is always convex!**

$x \in X$ for e.g. solutions in a cone or integer solutions
Terms: Primal problem, Lagrange function with dual variables/Lagrange-multipliers, dual function, dual problem
Dual problem is always convex! - I don't know much about optimization yet, but they really like convexity.
"(Convexity confers two advantages. The first is that, in a constrained problem, a convex feasible region makes it easier to ensure that you do not generate infeasible solutions while searching for an optimum.)
The second advantage is that all local optima are global optima. That allows local search algorithms to guarantee optimal solutions. And local search is often faster." [Rubin, 2016])

Alternating Direction Method of Multipliers (ADMM)

Problem

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

Lagrangian

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

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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decomposable problem and constraints!

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

Lagrangian problem can still be decomposed into β and μ terms
this has nice algorithm where we can execute some stuff in parallel, because we can decompose the Lagrangian

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Augmented: scalar product with ρ gets added,
Method of Multipliers: is a way to make the algorithm more robust
advantage: better convergence
disadvantage: no longer parallel execution of subtasks due to l2-term, no longer decomposable in beta and theta terms, as l2 norm dquares every entry of the vector
alternating direction: semi-decomposable, i.e. keeping one variable fixed while updating the other
ρ is step length of iterative algorithm
All notes on this slide: see the slides by [Boyd]

Dual Variable Update

Alternating Direction Method of Multipliers

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

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

$$\mu^{t+1} = \mu^t + \rho(\mathbf{A}\beta^{t+1} + \mathbf{B}\theta^{t+1} - c)$$

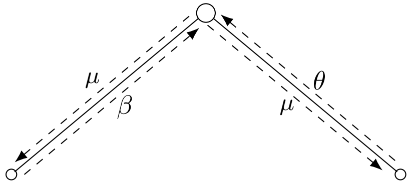
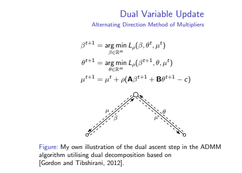


Figure: My own illustration of the dual ascent step in the ADMM algorithm utilising dual decomposition based on [Gordon and Tibshirani, 2012].



Method of Multipliers: is a way to make the algorithm more robust, (if in second line β^t statt β^{t+1})
alternating direction: semi-decomposable, i.e. keeping one variable fixed while updating the other
last step is called a dual variable update, this dual has nothing to do with two, but is connected to what is called a dual problem
dual variable update, we are working in the dual problem as "min L", thus convex problem, thus "dual decomposition" into subproblems which is possible by [Gordon and Tibshirani, 2012]
think of it as only the last line, sending μ to the updaters for β and θ
ρ in last line can be thought of as "step length"

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ADMM - Why?

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

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- blockwise computation
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Details for blockwise computation in Exercise 5.12.

ADMM for the Lasso

Problem

Problem in Lagrangian form

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

Augmented Lagrangian

$$L_\rho(\beta,\theta,\mu) := \left\{ \frac{1}{2}\|\mathbf{y}-\mathbf{X}\beta\|_2^2 + \lambda\|\theta\|_1 \right\} + \langle\mu,\beta-\theta\rangle + \frac{\rho}{2}||\beta-\theta||_2^2$$

ADMM for the Lasso
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In the problem, I can decompose into beta and theta terms, i.e.show $f(\beta)$ and $g(\theta)$
the problem itself and the constraints,
A and B are unit matrices here
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

ADMM for the Lasso

Update

Update

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

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

ADMM for the Lasso
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$\mathcal{S}$ is a soft-thresholding parameter
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

Screening Rules

- 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)

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- 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)

Imagine a big data set, a very big data set, with such a huge design matrix, that you cannot load it into memory (RAM). Wh

What is a good predictor?

includegraphics
correlation is covariance with some factors
covariance is an inner product on a vector space
high absolute correlation (=large absolute inner product) =¿
high predictive power (see plots) =¿ xj with largest inner
product has predictive power, thus for that j we are most
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SAFE 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 $\lambda < \lambda_{\text{max}}$. The global strong rule discards the j^{th} variable if

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

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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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Majorization-Minimization Algorithms work analoguosly.

MMA visually

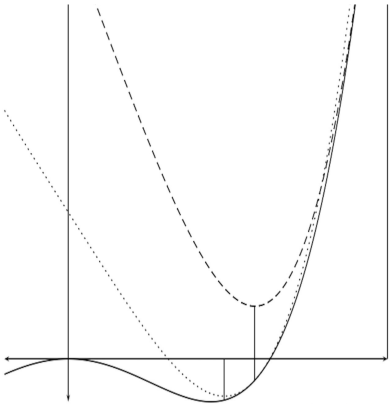
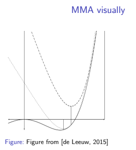


Figure: Figure from [de Leeuw, 2015]



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 $\beta^{t+1} = \arg\min_{\beta \in \mathbb{R}^p} \Psi(\beta, \beta^t)$

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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

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

where

(i) & (iii) Definiton of majorize

(ii) β^{t+1} is a minimizer of $\beta \mapsto \Psi(\beta, \beta^t)$

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for inequalities: show previous slide

Biconvexity

Let's consider an example ...

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

Biconvexity

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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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Comments . . .

Questions . . .

Suggestions . . .

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Thanks for listening.

Fill out your feedback sheets!

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