Coordinate Descent

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Convex Optimization 10-725/36-725

Last time: conditional gradient method

For the problem

$$\min_x \; f(x) \;\; \text{subject to} \;\; x \in C$$

where f is convex, smooth and C is a convex set, the conditional gradient (Frank-Wolfe) method chooses an initial $x^{(0)}$ and repeats for $k = 1, 2, 3, \ldots$

$$\begin{aligned} s^{(k-1)} &\in \operatorname*{argmin}_{s \in C} \; \nabla f(x^{(k-1)})^T s \\ x^{(k)} &= (1-\gamma_k) x^{(k-1)} + \gamma_k s^{(k-1)} \end{aligned}$$

Here γ_k is a step size, either prespecified (as in $\gamma_k = 2/(k+1)$) or chosen by line search

For many problems, linear minimization over C is simpler or more efficient than projection onto C, hence the appeal of Frank-Wolfe

Outline

Today:

- Coordinate descent
- Examples
- Implementation tricks
- Coordinate descent—literally
- Screening rules

Coordinate descent

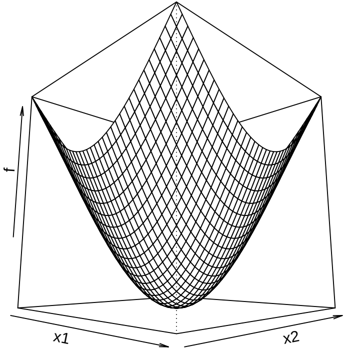
We've seen some pretty sophisticated methods thus far

We now focus on a very simple technique that can be surprisingly efficient, scalable: coordinate descent, or more appropriately called coordinatewise minimization

Q: Given convex, differentiable $f : \mathbb{R}^n \to \mathbb{R}$, if we are at a point x such that $f(x)$ is minimized along each coordinate axis, then *have we found a global minimizer?*

I.e., does $f(x + \delta e_i) \geq f(x)$ for all $\delta, i \quad \Rightarrow \quad f(x) = \min_z \; f(z)$?

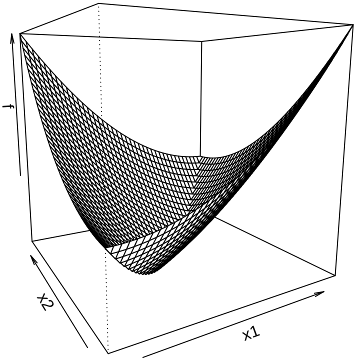
(Here $e_i = (0, \ldots, 1, \ldots 0) \in \mathbb{R}^n$, the ith standard basis vector)

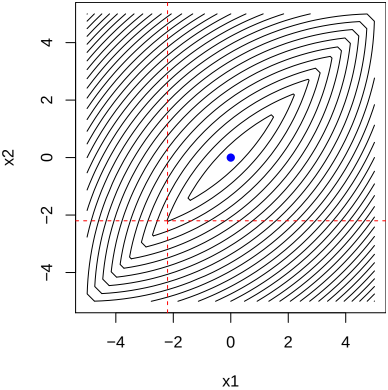


A: Yes! Proof:

$$\nabla f(x) = \left(\frac{\partial f}{\partial x_1}(x), \ldots \frac{\partial f}{\partial x_n}(x) \right) = 0$$

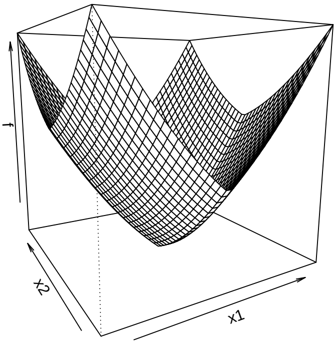
Q: Same question, but now for f convex, and not differentiable?

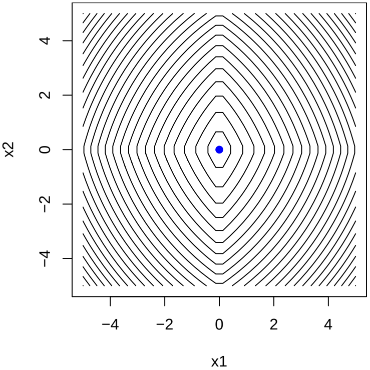




A: No! Look at the above counterexample

Q: Same question again, but now $f(x) = g(x) + \sum_{i=1}^{n} h_i(x_i)$, with g convex, differentiable and each h_i convex? (Here the nonsmooth part is called separable)





A: Yes! Proof: for any y,

$$f(y) - f(x) \geq \nabla g(x)^T (y - x) + \sum_{i=1}^{n} [h_i(y_i) - h_i(x_i)]$$

$$= \sum_{i=1}^{n} \underbrace{[\nabla_i g(x)(y_i - x_i) + h_i(y_i) - h_i(x_i)]}_{\geq 0} \geq 0$$

Coordinate descent

This suggests that for $f(x) = g(x) + \sum_{i=1}^n h_i(x_i)$, with g convex, differentiable and each h_i convex, we can use coordinate descent to find a minimizer: start with some initial guess $x^{(0)}$, and repeat

$$
\begin{aligned}
x_1^{(k)} &\in \underset{x_1}{\operatorname{argmin}} \; f\big(x_1, x_2^{(k-1)}, x_3^{(k-1)}, \ldots x_n^{(k-1)}\big) \\
x_2^{(k)} &\in \underset{x_2}{\operatorname{argmin}} \; f\big(x_1^{(k)}, x_2, x_3^{(k-1)}, \ldots x_n^{(k-1)}\big) \\
x_3^{(k)} &\in \underset{x_2}{\operatorname{argmin}} \; f\big(x_1^{(k)}, x_2^{(k)}, x_3, \ldots x_n^{(k-1)}\big) \\
&\ldots \\
x_n^{(k)} &\in \underset{x_2}{\operatorname{argmin}} \; f\big(x_1^{(k)}, x_2^{(k)}, x_3^{(k)}, \ldots x_n\big)
\end{aligned}
$$

for $k = 1, 2, 3, \ldots$. Important: after solving for $x_i^{(k)}$, we use its new value from then on!

Tseng (2001) proves that for such f (provided f is continuous on compact set $\{x : f(x) \leq f(x^{(0)})\}$ and f attains its minimum), any limit point of $x^{(k)}$, $k = 1, 2, 3, \ldots$ is a minimizer of f[1]

Notes:

- Order of cycle through coordinates is arbitrary, can use any permutation of $\{1, 2, \ldots n\}$
- Can everywhere replace individual coordinates with blocks of coordinates
- "One-at-a-time" update scheme is critical, and "all-at-once" scheme does not necessarily converge
- The analogy for solving linear systems: Gauss-Seidel versus Jacobi method

[1] Using real analysis, we know that $x^{(k)}$ has subsequence converging to $x^\star$ (Bolzano-Weierstrass), and $f(x^{(k)})$ converges to $f^\star$ (monotone convergence)

Example: linear regression

Given $y \in \mathbb{R}^n$, and $X \in \mathbb{R}^{n \times p}$ with columns $X_1, \ldots X_p$, consider linear regression:

$$\min_{\beta} \ \frac{1}{2}\|y - X\beta\|_2^2$$

Minimizing over β_i, with all β_j, $j \neq i$ fixed:

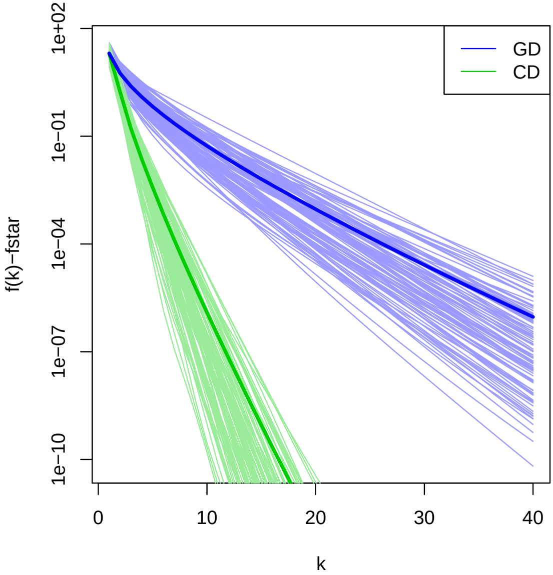
$$0 = \nabla_i f(\beta) = X_i^T(X\beta - y) = X_i^T(X_i\beta_i + X_{-i}\beta_{-i} - y)$$

i.e., we take

$$\beta_i = \frac{X_i^T(y - X_{-i}\beta_{-i})}{X_i^T X_i}$$

Coordinate descent repeats this update for $i = 1, 2, \ldots, p, 1, 2, \ldots$

Coordinate descent vs gradient descent for linear regression: 100 instances with $n = 100$, $p = 20$



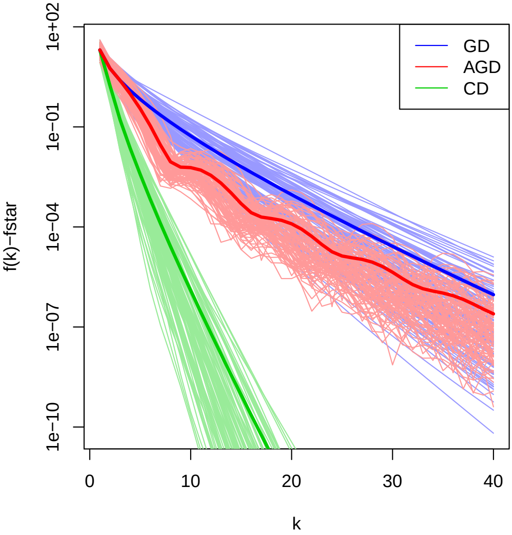
Is it fair to compare 1 cycle of coordinate descent to 1 iteration of gradient descent? Yes, if we're clever

- Gradient descent: $\beta \leftarrow \beta + tX^T(y - X\beta)$, costs $O(np)$ flops
- Coordinate descent, one coordinate update:

$$\beta_i \leftarrow \frac{X_i^T(y - X_{-i}\beta_{-i})}{X_i^T X_i} = \frac{X_i^T r}{\|X_i\|_2^2} + \beta_i$$

  where $r = y - X\beta$

- Each coordinate costs $O(n)$ flops: $O(n)$ to update r, $O(n)$ to compute $X_i^T r$
- One cycle of coordinate descent costs $O(np)$ operations, same as gradient descent



Same example, but now with accelerated gradient descent for comparison

Is this contradicting the optimality of accelerated gradient descent? No! Coordinate descent uses more than first-order information

Example: lasso regression

Consider the lasso problem:

$$\min_{\beta} \ \frac{1}{2}\|y - X\beta\|_2^2 + \lambda\|\beta\|_1$$

Note that the nonsmooth part is separable: $\|\beta\|_1 = \sum_{i=1}^{p} |\beta_i|$

Minimizing over β_i, with β_j, $j \neq i$ fixed:

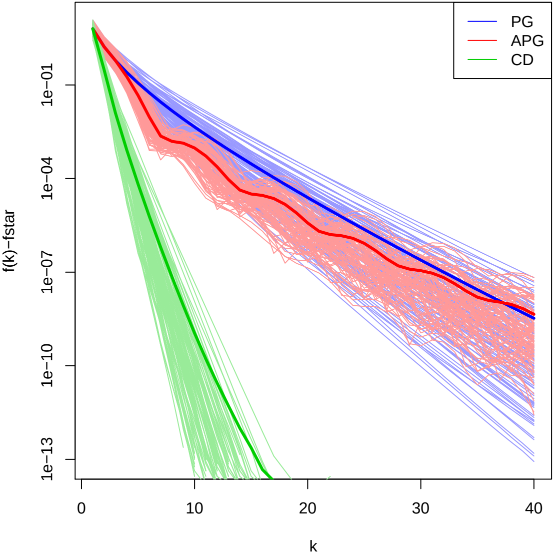
$$0 = X_i^T X_i \beta_i + X_i^T (X_{-i}\beta_{-i} - y) + \lambda s_i$$

where $s_i \in \partial|\beta_i|$. Solution is simply given by soft-thresholding

$$\beta_i = S_{\lambda/\|X_i\|_2^2}\left(\frac{X_i^T(y - X_{-i}\beta_{-i})}{X_i^T X_i}\right)$$

Repeat this for $i = 1, 2, \ldots p, 1, 2, \ldots$

Proximal gradient vs coordinate descent for lasso regression: 100 instances with $n = 100$, $p = 20$



For same reasons as before:

- All methods use $O(np)$ flops per iteration
- Coordinate descent uses much more information

Example: box-constrained QP

Given $b \in \mathbb{R}^n$, $Q \in \mathbb{S}^n_+$, consider box-constrained quadratic program

$$\min_x \ \frac{1}{2} x^T Q x + b^T x \ \ \text{subject to} \ \ l \le x \le u$$

Fits into our framework, as $I\{l \le x \le u\} = \sum_{i=1}^n I\{l_i \le x_i \le u_i\}$

Minimizing over x_i with all x_j, $j \neq i$ fixed: same basic steps give

$$x_i = T_{[l_i, u_i]} \left(\frac{b_i - \sum_{j \neq i} Q_{ij} x_j}{Q_{ii}} \right)$$

where $T_{[l_i,u_i]}$ is the truncation (projection) operator onto $[l_i, u_i]$:

$$T_{[l_i,u_i]}(z) = \begin{cases} u_i & \text{if } z > u_i \\ z & \text{if } l_i \le z \le u_i \\ l_i & \text{if } z < l_i \end{cases}$$

Example: support vector machines

A coordinate descent strategy can be applied to the SVM dual:

$$\min_{\alpha} \ \frac{1}{2}\alpha^T \tilde{X}\tilde{X}^T\alpha - 1^T\alpha \ \text{ subject to } \ 0 \le \alpha \le C1, \ \alpha^T y = 0$$

Sequential minimal optimization or SMO (Platt 1998) is basically blockwise coordinate descent in blocks of 2. Instead of cycling, it chooses the next block greedily

Recall the complementary slackness conditions

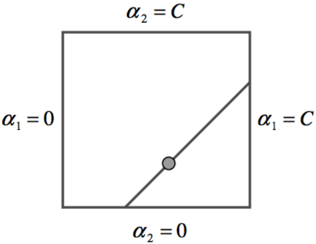
$$\alpha_i\big(1 - \xi_i - (\tilde{X}\beta)_i - y_i\beta_0\big) = 0, \quad i = 1, \ldots n \tag{1}$$

$$(C - \alpha_i)\xi_i = 0, \quad i = 1, \ldots n \tag{2}$$

where β, β_0, ξ are the primal coefficients, intercept, and slacks. Recall that $\beta = \tilde{X}^T\alpha$, β_0 is computed from (1) using any i such that $0 < \alpha_i < C$, and ξ is computed from (1), (2) SMO repeats the following two steps:

- Choose α_i, α_j that do not satisfy complementary slackness, greedily (using heuristics)
- Minimize over α_i, α_j exactly, keeping all other variables fixed

Using equality constraint, reduces to minimizing univariate quadratic over an interval (From Platt 1998)



Note this does not meet separability assumptions for convergence from Tseng (2001), and a different treatment is required

Many further developments on coordinate descent for SVMs have been made; e.g., a recent one is Hsiesh et al. (2008)

Coordinate descent in statistics and ML

History in statistics:

- Idea appeared in Fu (1998), and again in Daubechies et al. (2004), but was inexplicably ignored
- Three papers around 2007, especially Friedman et al. (2007), really sparked interest in statistics and ML communities

Why is it used?

- Very simple and easy to implement
- Careful implementations can be near state-of-the-art
- Scalable, e.g., don't need to keep full data in memory

Examples: lasso regression, lasso GLMs (under proximal Newton), SVMs, group lasso, graphical lasso (applied to the dual), additive modeling, matrix completion, regression with nonconvex penalties

Pathwise coordinate descent for lasso

Here is the basic outline for pathwise coordinate descent for lasso, from Friedman et al. (2007), Friedman et al. (2009)

Outer loop (pathwise strategy):

- Compute the solution over a sequence $\lambda_1 > \lambda_2 > \ldots > \lambda_r$ of tuning parameter values
- For tuning parameter value λ_k, initialize coordinate descent algorithm at the computed solution for λ_{k+1} (warm start)

Inner loop (active set strategy):

- Perform one coordinate cycle (or small number of cycles), and record active set A of coefficients that are nonzero
- Cycle over coefficients in A until convergence
- Check KKT conditions over all coefficients; if not all satisfied, add offending coefficients to A, go back one step

Notes:

- Even when the solution is desired at only one λ, the pathwise strategy (solving over $\lambda_1 > \ldots > \lambda_r = \lambda$) is typically much more efficient than directly performing coordinate descent at λ
- Active set strategy takes advantage of sparsity; e.g., for very large problems, coordinate descent for lasso is much faster than it is for ridge regression
- With these strategies in place (and a few more clever tricks), coordinate descent can be competitve with fastest algorithms for ℓ_1 penalized minimization problems
- Fast Fortran implement glmnet, easily linked to R or MATLAB

What's in a name?

The name coordinate descent is confusing. For a smooth function f, the method that repeats

$$\begin{aligned}
x_1^{(k)} &= x_1^{(k-1)} - t_{k,1} \cdot \nabla_1 f\big(x_1^{(k-1)}, x_2^{(k-1)}, x_3^{(k-1)}, \ldots x_n^{(k-1)}\big) \\
x_2^{(k)} &= x_2^{(k-1)} - t_{k,2} \cdot \nabla_2 f\big(x_1^{(k)}, x_2^{(k-1)}, x_3^{(k-1)}, \ldots x_n^{(k-1)}\big) \\
x_3^{(k)} &= x_3^{(k-1)} - t_{k,3} \cdot \nabla_3 f\big(x_1^{(k)}, x_2^{(k)}, x_3^{(k-1)}, \ldots x_n^{(k-1)}\big) \\
&\ldots \\
x_n^{(k)} &= x_n^{(k-1)} - t_{k,n} \cdot \nabla_n f\big(x_1^{(k)}, x_2^{(k)}, x_3^{(k)}, \ldots x_n^{(k-1)}\big)
\end{aligned}$$

for $k = 1, 2, 3, \ldots$ is also (rightfully) called coordinate descent. If $f = g + h$, where g is smooth and h is separable, then the proximal version of the above is also called coordinate descent

These versions are often easier to apply that exact coordinatewise minimization, but the latter makes more progress per step

Convergence analyses

Theory for coordinate descent moves quickly. The list given below is incomplete (may not be the latest and greatest). Warning: some references below treat coordinatewise minimization, some do not

- Convergence of coordinatewise minimization for solving linear systems, the Gauss-Seidel method, is a classic topic. E.g., see Golub and van Loan (1996), or Ramdas (2014) for a modern twist that looks at randomized coordinate descent
- Nesterov (2010) considers randomized coordinate descent for smooth functions and shows that it achieves a rate $O(1/\epsilon)$ under a Lipschitz gradient condition, and a rate $O(\log(1/\epsilon))$ under strong convexity
- Richtarik and Takac (2011) extend and simplify these results, considering smooth plus separable functions, where now each coordinate descent update applies a prox operation

- Saha and Tewari (2013) consider minimizing ℓ_1 regularized functions of the form $g(\beta) + \lambda\|\beta\|_1$, for smooth g, and study both cyclic coordinate descent and cyclic coordinatewise min. Under (very strange) conditions on g, they show both methods dominate proximal gradient descent in iteration progress
- Beck and Tetruashvili (2013) study cyclic coordinate descent for smooth functions in general. They show that it achieves a rate $O(1/\epsilon)$ under a Lipschitz gradient condition, and a rate $O(\log(1/\epsilon))$ under strong convexity. They also extend these results to a constrained setting with projections
- Nutini et al. (2015) analyze greedy coordinate descent (called Gauss-Southwell rule), and show it achieves a faster rate than randomized coordinate descent for certain problems
- Wright (2015) provides some unification and a great summary. Also covers parallel versions (even asynchronous ones)
- General theory is still not complete; still unanswered questions (e.g., are descent and minimization strategies the same?)

Graphical lasso

Consider a data matrix $X \in \mathbb{R}^{n \times p}$, whose rows $x_1, \ldots x_n \in \mathbb{R}^p$ are independent observations from $N(0, \Sigma)$, with unknown covariance matrix Σ. Want to estimate Σ. For $Z \sim N(0, \Sigma)$, normality theory tells us

$$\Sigma^{-1}_{ij} = 0 \iff Z_i, Z_j \text{ conditionally independent given } Z_\ell,\, \ell \neq i, j$$

If we believe that many components are conditionally independent given others (often reasonable for large p) then we want a sparse estimate of Σ^{-1}. Solve graphical lasso problem (Banerjee et al. 2007, Friedman et al. 2007):

$$\min_{\Theta \in \mathbb{S}^p_+} \; -\log\det\Theta + \mathrm{tr}(S\Theta) + \lambda\|\Theta\|_1$$

Minimizer $\hat{\Theta}$ is an estimate for Σ^{-1}. (Note here $S = X^T X/n$ is the empirical covariance matrix, and $\|\Theta\|_1 = \sum_{i,j=1}^p |\Theta_{ij}|$)

Graphical lasso KKT conditions (stationarity):

$$-\Theta^{-1} + S + \lambda\Gamma = 0$$

where $\Gamma_{ij} \in \partial|\Theta_{ij}|$. Let $W = \Theta^{-1}$; we will solve in terms of W. Note $W_{ii} = S_{ii} + \lambda$, because $\Theta_{ii} > 0$ at solution. Now partition:

$$W = \begin{bmatrix} W_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \quad \Theta = \begin{bmatrix} \Theta_{11} & \theta_{12} \\ \theta_{21} & \theta_{22} \end{bmatrix} \quad S = \begin{bmatrix} S_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \quad \Gamma = \begin{bmatrix} \Gamma_{11} & \gamma_{12} \\ \gamma_{21} & \gamma_{22} \end{bmatrix}$$

where $W_{11} \in \mathbb{R}^{(p-1)\times(p-1)}$, $w_{12} \in \mathbb{R}^{(p-1)\times 1}$, and $w_{21} \in \mathbb{R}^{1\times(p-1)}$, $w_{22} \in \mathbb{R}$; same with others

Coordinate descent strategy: solve for w_{12}, the last column of W (note w_{22} is known), with all other columns fixed; then solve for second-to-last column, etc., and cycle around until convergence. (Solve for Θ along the way, so we don't have to invert W to get Θ)

Now consider $(1,2)$-block of KKT conditions:

$$-w_{12} + s_{12} + \lambda\gamma_{12} = 0$$

Because $\begin{bmatrix} W_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \begin{bmatrix} \Theta_{11} & \theta_{12} \\ \theta_{21} & \theta_{22} \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & 1 \end{bmatrix}$, we know that $w_{12} = -W_{11}\theta_{12}/\theta_{22}$. Substituting this into the above,

$$W_{11}\frac{\theta_{12}}{\theta_{22}} + s_{12} + \lambda\gamma_{12} = 0$$

Letting $\beta = \theta_{12}/\theta_{22}$ and noting that $\theta_{22} > 0$ at solution, this is

$$W_{11}\beta + s_{12} + \lambda\rho = 0$$

where $\rho \in \partial\|\beta\|_1$. What does this condition look like?

These are exactly the KKT conditions for

$$\min_{\beta} \ \beta^T W_{11} \beta + s_{12}^T \beta + \lambda \|\beta\|_1$$

which is (basically) a lasso problem and can be itself solved quickly via coordinate descent

From β we get $w_{12} = -W_{11}\beta$, and set $w_{21} = w_{12}^T$. Then θ_{12}, θ_{22} are obtained from $\left[\begin{array}{cc} W_{11} & w_{12} \\ w_{21} & w_{22} \end{array}\right] \left[\begin{array}{cc} \Theta_{11} & \theta_{12} \\ \theta_{21} & \theta_{22} \end{array}\right] = \left[\begin{array}{cc} I & 0 \\ 0 & 1 \end{array}\right]$, and we set $\theta_{21} = \theta_{12}^T$

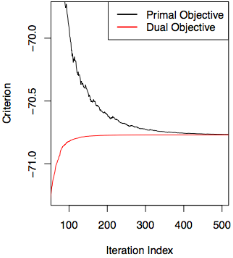
The next step moves on to a different column of W, and so on; hence we have reduced the graphical lasso problem to a repeated sequence of lasso problems

This coordinate descent approach for the graphical lasso, usually called glasso algorithm (Friedman et al. 2007) is very efficient and scales well

Meanwhile, people have noticed that using glasso algorithm, it can happen that the objective function doesn't decrease monotonically across iterations — is this a bug?

No! The glasso algorithm makes a variable transformation and solves in terms of coordinate blocks of W; note that these are not coordinate blocks of original variable Θ, so strictly speaking it is not a coordinate descent algorithm

However, it can be shown that glasso is doing coordinate ascent on the dual problem (Mazumder et al. 2011)



Screening rules

In some problems, screening rules can be used in combination with coordinate descent to further wittle down the active set. Screening rules themselves have amassed a sizeable literature recently. Here is an example, the SAFE rule for the lasso[2]:

$$|X_i^T y| < \lambda - \|X_i\|_2 \|y\|_2 \frac{\lambda_{\text{max}} - \lambda}{\lambda_{\text{max}}} \;\Rightarrow\; \hat{\beta}_i = 0, \quad \text{all } i = 1, \ldots p$$

where $\lambda_{\text{max}} = \|X^T y\|_\infty$ (the smallest value of λ such that $\hat{\beta} = 0$)

Note: this is not an if and only if statement! But it does give us a way of eliminating features apriori, without solving the lasso

(There have been many advances in screening rules for the lasso, but SAFE is the simplest, and was the first)

[2] El Ghaoui et al. (2010), "Safe feature elimination in sparse learning"

Why is the SAFE rule true? Construction comes from lasso dual:

$$\max_u \; g(u) \;\; \text{subject to} \;\; \|X^T u\|_\infty \le \lambda$$

where $g(u) = \frac{1}{2}\|y\|_2^2 - \frac{1}{2}\|y-u\|_2^2$. Suppose that u_0 is dual feasible (e.g., take $u_0 = y \cdot \lambda/\lambda_{\mathsf{max}}$). Then $\gamma = g(u_0)$ is a lower bound on the dual optimal value, so dual problem is equivalent to

$$\max_u \; g(u) \;\; \text{subject to} \;\; \|X^T u\|_\infty \le \lambda, \; g(u) \ge \gamma$$

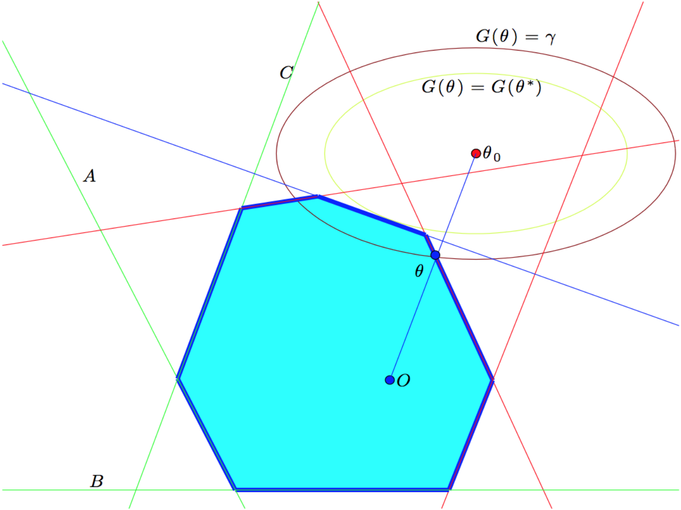
Now consider computing

$$m_i = \max_u \; |X_i^T u| \;\; \text{subject to} \;\; g(u) \ge \gamma, \quad \text{for } i = 1, \ldots p$$

Then we would have

$$m_i < \lambda \;\; \Rightarrow \;\; |X_i^T \hat{u}| < \lambda \;\; \Rightarrow \;\; \hat{\beta}_i = 0, \quad i = 1, \ldots p$$

The last implication comes from the KKT conditions



(From El Ghaoui et al. 2010)

Another dual argument shows that

$$\begin{aligned} &\max_u \; X_i^T u \;\; \text{subject to} \;\; g(u) \geq \gamma \\ =&\min_{\mu > 0} \; -\gamma\mu + \frac{1}{\mu}\|\mu y - X_i\|_2^2 \\ =&\|X_i\|_2 \sqrt{\|y\|_2^2 - 2\gamma} - X_i^T y \end{aligned}$$

where the last equality comes from direct calculation

Thus m_i is given the maximum of the above quantity over $\pm X_i$,

$$m_i = \|X_i\|_2 \sqrt{\|y\|_2^2 - 2\gamma} + |X_i^T y|, \quad i = 1, \ldots p$$

Lastly, subtitute $\gamma = g(y \cdot \lambda / \lambda_{\mathsf{max}})$. Then $m_i < \lambda$ is precisely the safe rule given on previous slide

Screening rules for graphical lasso

Graphical lasso computations can be significantly accelerated by using a clever screening rule (this is analogous to the SAFE rules for the lasso)

Mazumder et al. (2011), Witten et al. (2011) examine the KKT conditions:

$$-\Theta^{-1} + S + \lambda\Gamma = 0$$

and conclude that Θ is block diagonal over variables C_1, C_2 if and only if $|S_{ij}| \leq \lambda$ for all $i \in C_1$, $j \in C_2$. Why?

- If Θ is block diagonal, then so is Θ^{-1}, and thus $|S_{ij}| \leq \lambda$ for $i \in C_1$, $j \in C_2$
- If $|S_{ij}| \leq \lambda$ for $i \in C_1$, $j \in C_2$, then the KKT conditions are satisfied with Θ^{-1} block diagonal, so Θ is block diagonal

Exact same idea extends to multiple blocks. Hence group structure in graphical lasso solution is just given by covariance thresholding

References

Early coordinate descent references in optimization:

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- Z. Luo and P. Tseng (1992), "On the convergence of the coordinate descent method for convex differentiable minimization"
- J. Ortega and W. Rheinboldt (1970), "Iterative solution of nonlinear equations in several variables"
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Early coordinate descent references in statistics and ML:

- I. Daubechies and M. Defrise and C. De Mol (2004), "An iterative thresholding algorithm for linear inverse problems with a sparsity constraint"
- J. Friedman and T. Hastie and H. Hoefling and R. Tibshirani (2007), "Pathwise coordinate optimization"
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- T. Wu and K. Lange (2008), "Coordinate descent algorithms for lasso penalized regression"
- A. van der Kooij (2007), "Prediction accuracy and stability of regresssion with optimal scaling transformations"

Applications of coordinate descent:

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- J. Friedman and T. Hastie and R. Tibshirani (2007), "Sparse inverse covariance estimation with the graphical lasso"
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