CS7301: Advanced Topics in Optimization for Machine Learning

Lecture 5.1: Second Order Methods Cont. and Coordinate Descent

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https://github.com/rishabhk108/AdvancedOptML

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Summary of Algorithms so Far

First Order Methods (Unconstrained)

- Gradient Descent
- Proximal Gradient Descent (if non-smooth function is simple – i.e. proximal operator of that function can be computed efficiently.
- Accelerated Gradient versions in the unconstrained case, projected case and proximal case.

First Order Methods (Constrained)

- Projected Gradient Descent (whenever the Projection step is easy)
- Conditional Gradient Descent

Last Class

Second Order Methods

- Newtons Method
- General Quasi Newton Template
- Symmetric Rank One Update
- BFGS Update
- DFP Update

Outline of Lecture 5.1

- LBFGS (Limited Memory BFGS)
- Conjugate Gradient Descent
- Barzelia Borowein Gradient Descent
- Coordinate Descent Algorithms

Recall: BFGS Update

- BFGS update is a rank two update:

$$B_k = B_{k-1} + auu^T + bvv^T$$

- Recall BFGS update:

$$B_k = B_{k-1} - \frac{B_{k-1}s_{k-1}s_{k-1}^T B_{k-1}}{s_{k-1}^T B_{k-1}s_{k-1}} + \frac{y_{k-1}y_{k-1}^T}{y_{k-1}^T s_{k-1}}$$

- BFGS Inverse Update:

$$B_{k+1}^{-1} = (I - \frac{s_{k-1}y_{k-1}^T}{s_{k-1}^T y_{k-1}})B_k^{-1}(I - \frac{y_{k-1}s_{k-1}^T}{y_{k-1}^T s_{k-1}}) + \frac{s_{k-1}s_{k-1}^T}{y_{k-1}^T s_{k-1}}$$

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- Instead store upto l (e.g. $l = 30$) values of s_k and y_k and compute B_k^{-1} using the recursive BFGS equation and assuming $B_{k-l} = I$:

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- This makes the cost per iteration of $O(dl)$ and storage also as $O(dl)$ instead of $O(d^2)$.

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- Next: Can we achieve Newton like behaviour with Gradient Descent like algorithms?

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Conjugate Gradient Descent for Quadratic Functions

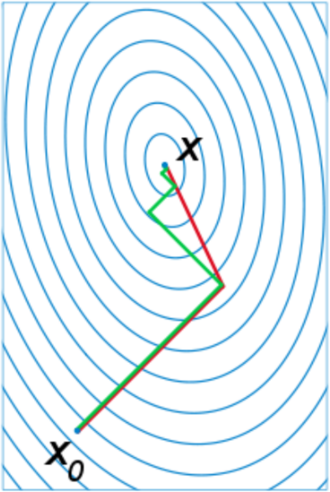
A comparison of

* gradient descent with optimal step size (in green) and

* conjugate vector (in red)

for minimizing a quadratic function.

Conjugate gradient converges in at most n steps (here n=2).



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- Hestenes–Stiefel:

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- Moreover, similar to Newton and BFGS, one can also show superlinear local convergence and global convergence results for CG!
- Advantage of CG is that the complexity is exactly identical to Gradient Descent and yet it has some of the properties of Quasi Newton algorithms!

Hessian Free Optimization (James Martin, ICML 2010)

- Recall the quadratic expansion:

$$f(x) \approx f(x_t) + \nabla f(x_t)^T (x - x_t) + \frac{1}{2}(x - x_t)^T \nabla^2 f(x_t)(x - x_t)$$

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- This is the directional derivative of $\frac{\partial f}{\partial x_i}$ in the direction of v! and can be computed numerically!

Barzelai Borwein (BB) Gradient Descent

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- Typically used with non-monotone line search as convergence safeguard against non-quadratic problems (we won't cover this in class).

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- Solve this using least squares!

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  - Approach 2: Least squares in α directly:

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- However, $f(x_k)$ and $\nabla f(x_k)$ are not monotonic!
- Non Monotonic line search required for convergence analysis.

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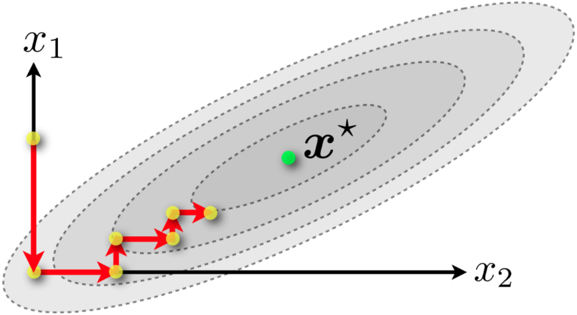
- BFGS improves it to $O(d^2)$ which is further improved to $O(d)$ by LBFGS!
- CG and BB are variants of Gradient Descent but try to mimic Newton's methods and in practice are much faster than simple GD while maintaining the simplicity!

Coordinate Descent

-
- Coordinate Descent: Basic Idea
- Optimality w.r.t co-ordinate descent
- Two variants of Coordinate Descent
- Convergence of coordinate descent algorithms.

Coordinate Descent

Goal: Find $\mathbf{x}^\star \in \mathbb{R}^d$ minimizing $f(\mathbf{x})$.



Idea: Update one coordinate at a time, while keeping others fixed.

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  in closed form.
- Also how do we select the coordinate i_k?
- Two strategies: One is to pick it up randomly (called randomized coordinate descent) and second it to pick it up greedily (greedy coordinate descent).

Randomized Coordinate Descent

select $i_t \in [d]$ uniformly at random
$$\mathbf{x}_{t+1} := \mathbf{x}_t - \frac{1}{L}\nabla_{i_t} f(\mathbf{x}_t)\, \mathbf{e}_{i_t}$$

- Faster convergence than gradient descent
  (if coordinate step is significantly cheaper than full gradient step)

Randomized Coordinate Descent: Convergence Analysis

- Key ingredient: **Coordinate wise Smoothness**:

$$f(x + \gamma e_i) \leq f(x) + \gamma \nabla_i f(x) + \frac{L_i}{2}\gamma^2, \forall x \in \mathbb{R}^d, \forall \gamma \in \mathbb{R}$$

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- Similar to Gradient Descent, this is $O(1/\epsilon)$ convergence!
- However, we just need to update a single dimension at a time, and hence the per iteration cost of CD can be $O(d)$ cheaper compared to GD!

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$$E(f(x_k)) - f_* \leq (1 - \frac{\mu}{dL})^k (f(x_0) - f_*)$$

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- This means that similar to GD, CD improves the objective value at every iteration!

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- Note that $\bar{L} \leq L$ and can in fact be significantly smaller!

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Exact Coordinate Minimization

- So far, we went over coordinate descent in a way akin to gradient descent, i.e. taking a coordinate step in each coordinate.
- Next, consider exact minimization in each coordinate.

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

for $k = 1, 2, 3, \ldots$

Note: after we solve for $x_i^{(k)}$, we use its new value from then on!

DALLAS

Exact Coordinate Minimization: Linear Regression

Consider linear regression

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{2}\|y - X\beta\|_2^2$$

where $y \in \mathbb{R}^n$, and $X \in \mathbb{R}^{n \times p}$ with columns $X_1, \ldots X_p$

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

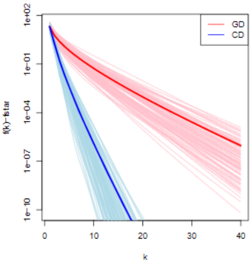
$$\beta_i = \frac{X_i^T(y - X_{-i}\beta_{-i})}{X_i^T X_i}$$

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

LAS

Exact Coordinate Minimization: Linear Regression

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



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

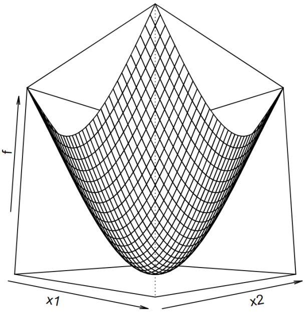
$$\beta_i \leftarrow \frac{X_i^T(y - X_{-i}\beta_{-i})}{X_i^T X_i} = \frac{X_i^T r}{\|X_i\|_2^2} + \beta_i$$

where $r = y - X\beta$. Therefore each coordinate update takes $O(n)$ operations — $O(n)$ to update r, and $O(n)$ to compute $X_i^T r$ — and one cycle requires $O(np)$ operations, just like gradient descent

Optimality Conditions with Coordinate Descent

- Coordinate Descent Family of Algorithms try to make progress every iteration!
- What is the stopping/optimality condition?
- One way to think of this is: If we are a point x such that it is minimum along each coordinate axis! In other words, no coordinate descent algorithm can make progress!
- Does this mean we are at a global minimum?
- Mathematically this means: Does a point x satisfying $f(x + \delta e_i) \geq f(x), \forall \delta, i \Rightarrow f(x) = \min_z f(z)$?

Optimality Conditions: Differentiable Functions

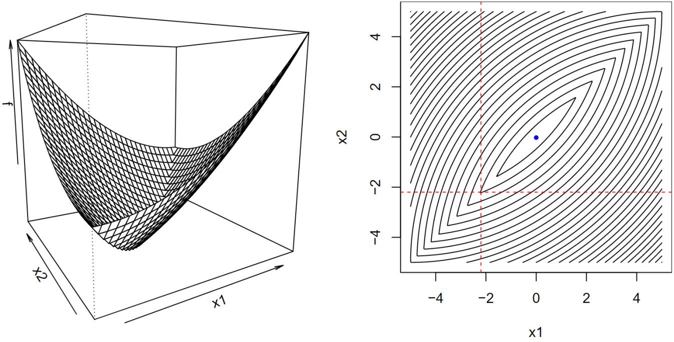


A: Yes! Proof:

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

Q: Same question, but for f convex (not differentiable) ... ?

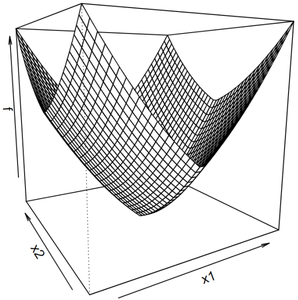
Optimality Conditions: Non Differentiable Functions

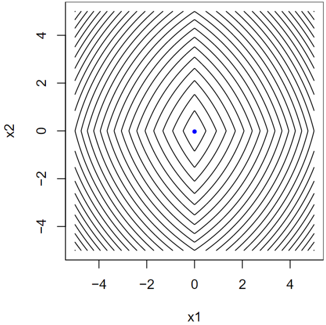


A: No! Look at the above counterexample

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 ... ? (Nonsmooth part here called separable)

Optimality Conditions: Seperable Functions





A: Yes! Proof: for any y,

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

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

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  3. Slight Improvement for Steepest CD: $(1 - \frac{\sigma}{dL})^k(f(x_0) - f_*)$
  4. Similar bound for exact coordinate minimization. Method of choice if the coordinate wise minimization can be solved exactly!

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- Extensions: Accelerated Coordinate Minimization also possible!