CS7301: Advanced Topics in Optimization for Machine Learning

Lecture 5.1: Second Order Methods Cont., Barzelia Borwein GD and Conjugate Gradient Method

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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 $B_{k-l} = I$:

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

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- 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

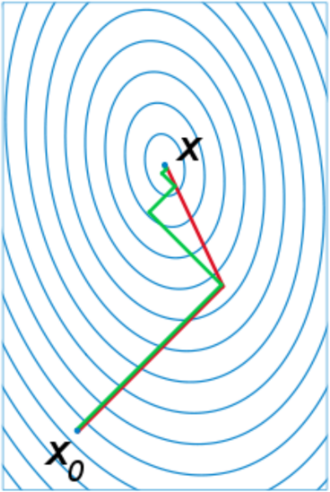
A comparison of

* 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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- Hestenes–Stiefel conjugate gradient update is equivalent to LBFGS with $l = 1$!
- 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!

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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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- BB Gradient Descent: Choose $\alpha_t \nabla f(x_t)$ such that it approximates $H_t^{-1} \nabla f(x_t)$

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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!