CS7301: Advanced Topics in Optimization for Machine Learning

Lecture 4.1: Newton, Quasi Newton and Second Order Methods

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February 12, 2021

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

Outline of this Lecture

- Newton's Algorithm
- Newton vs Quasi Newton Methods
- Barzilai-Borwein GD
- BFGS
- Conjugate Gradient Family
- LBFGS
- Understanding how these Algorithms perform in practice!

Newton Methods

- Recall unconstrained convex minimization:

$$\min_{x \in \mathrm{dom}(f)} \quad f(x)$$

- Newtons Method:

$$x_{t+1} = x_t - \nabla^2 f(x_t)^{-1} \nabla f(x_t)$$

- Requires the convex function to be twice differentiable.
- Recall GD was:

$$x_{t+1} = x_t - \alpha_t \nabla f(x_t)$$

Newton vs Gradient Descent

- Recall Gradient Descent step could be seen as solving the optimization problem:

$$x_{t+1} = \text{argmin}_x f(x_t) + \nabla f(x_t)^T (x - x_t) + \frac{1}{2\alpha_t} ||x - x_t||^2$$

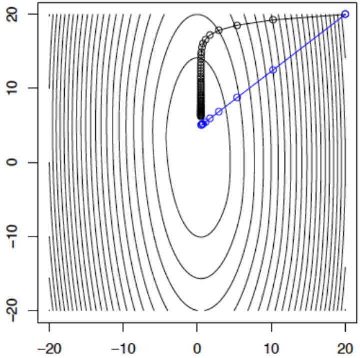
- Newton step can be seen as solving:

$$x_{t+1} = \text{argmin}_x f(x_t) + \nabla f(x_t)^T (x - x_t) + \frac{1}{2} (x - x_t)^T \nabla^2 f(x_t)(x - x_t)$$

- No need to step size in Newton.

Newton vs Gradient Descent

For $f(x) = (10x_1^2 + x_2^2)/2 + 5\log(1 + e^{-x_1-x_2})$, compare gradient descent (black) to Newton's method (blue), where both take steps of roughly same length



Newtons method for finding the roots - I

Goal: $\phi : \mathbb{R} \to \mathbb{R}$

$$\phi(x^*) = 0$$

$$x^* = ?$$

Linear Approximation (1st order Taylor approx):

$$\underbrace{\phi(\underbrace{x + \Delta x}_{x^*})}_{\phi(x^*) = 0} = \phi(x) + \phi'(x)\Delta x + o(|\Delta x|)$$

Therefore,

$$0 \approx \phi(x) + \phi'(x)\Delta x$$

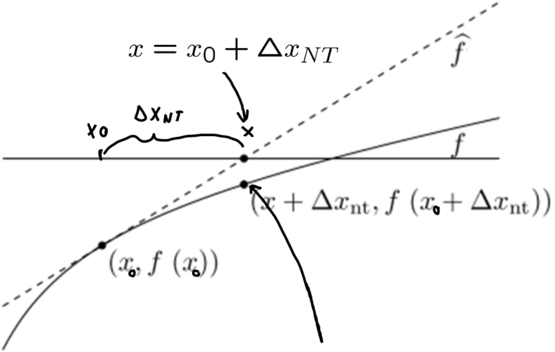
$$x^* - x = \Delta x = -\frac{\phi(x)}{\phi'(x)}$$

$$x_{k+1} = x_k - \frac{\phi(x)}{\phi'(x)}$$

Newtons method for finding the roots - II

Goal: finding a root

$$\hat{f}(x) = f(x_0) + f'(x_0)(x - x_0)$$



In the next step we will linearize here in *x*

Newtons method for finding the roots - Multivariate Functions

This can be generalized to multivariate functions

$F : \mathbb{R}^n \to \mathbb{R}^m$

$$0_m = F(x^*) = F(x + \Delta x) = F(x) + \underbrace{\nabla F(x)}_{\mathbb{R}^{m \times n}} \underbrace{\Delta x}_{\mathbb{R}^n} + o(|\Delta x|)$$

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Therefore,

$$0_m = F(x) + \nabla F(x) \Delta x$$

$$\Delta x = -[\nabla F(x)]^{-1} F(x)$$

[Pseudo inverse if there is no inverse]

$\Delta x = x_{k+1} - x_k$, and thus

$$\underset{\mathbb{R}^n}{x_{k+1}} = \underset{\mathbb{R}^n}{x_k} - \underset{\mathbb{R}^{n \times m}}{[\nabla F(x_k)]^{-1}} \underset{\mathbb{R}^m}{F(x_k)}$$

Newtons method for finding the roots $\Rightarrow$ Optimization Algorithm

Newton's method for solving the optimization problem:

$$\min_x f(x)$$

is the same as Newton's method for finding the root of

$$\nabla f(x) = 0$$

History: The work of Newton (1685) and Raphson (1690) originally focused on finding roots for Polynomials. Simpson (1740) applied this idea to general nonlinear equations and optimization.

Local Convergence

- Under suitable conditions and starting close enough to the global minimum, Newton's method will reach ϵ close to the the minimum in $\log\log(1/\epsilon)$ iterations!
- This is faster than anything we have seen so far (even strongly convex and smooth functions!)
- However this holds only if we are close to the minima (hence local convergence). Global convergence from any starting point is unknown for Newton's method.
- Local convergence is characterized by bounded inverse Hessians: There exists μ s.t. $||\nabla^2 f(x)^{-1}|| \leq \frac{1}{\mu}$ and Lipschitz continuous Hessians.

Local Convergence Theorem

Theorem

Let f be convex with a unique global minium x^*. Suppose there is a ball X with center x^* such that:

1. *There exists a real number μ s.t $||\nabla^2 f(x)^{-1}|| \leq \frac{1}{\mu}$*
2. *There exists a real number B s.t.*

$$||\nabla^2 f(x) - \nabla^2 f(y)|| \leq B||x - y||$$

Then for $x_t \in X$ and x_{t+1} resulting from the Newton step, we have

$$||x_{t+1} - x^*|| \leq \frac{B}{2\mu}||x_t - x^*||^2$$

Local Convergence Theorem

- If we assume that
$$||x_0 - x_*|| \leq \frac{\mu}{B}$$
and given the assumptions of the local convergence:
- The Newton method yields:
$$||x_T - x^*|| \leq \frac{\mu}{B}(\frac{1}{2})^{2^T - 1}$$
- This is called superlinear convergence (convergence rate of $\log\log(1/\epsilon)$ iterations)!
- Intuitive reason: Once the Hessian is bounded, the function is almost quadratic, which ensures Newton's algorithm convergences very fast!

Local vs Global Convergence

- What about global convergence, i.e. if we start from any x_0?
- Global convergence of Newton was not known until recently (Sai Praneeth Karimireddy, Sebastian U. Stich, Martin Jaggi, Arxiv 2018).
- They only show linear global convergence (recall we had superlinear local convergence above).
- They also show it under the assumption that the Hessians are *stable*.

Pros and Cons of Newton's Method

- Pros: Much faster than anything we have seen so far!
- Pros: Even in practice, converges in very few iterations
- Pros: Affine Invariance and Robustness
- Cons: Requires computing the Hessian and inverting or solving a linear system (since we can solve $H_t(\Delta x) = -\nabla f(x_t)$ for the next step). Both are roughly $O(d^3)$!
- In many cases, d (number of features) is large and each step can be prohibitive!

Affine Invariance of Newtons method

Important property Newton's method: affine invariance.

Assume $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable and $A \in \mathbb{R}^{n\times n}$ is nonsingular. Let $g(y) := f(Ay)$.

Newton step for g starting from y is

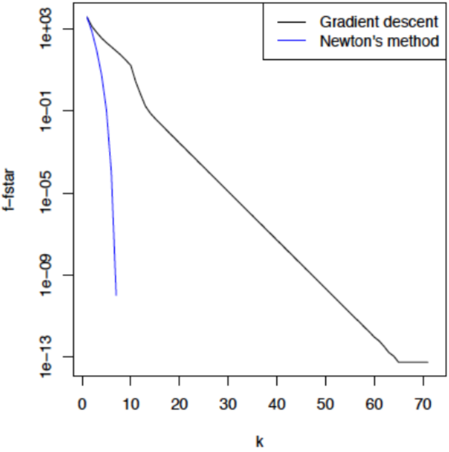
$$y^+ = y - \left(\nabla^2 g(y)\right)^{-1} \nabla g(y).$$

It turns out that the Newton step for f starting from $x = Ay$ is $x^+ = Ay^+$.

Therefore progress is independent of problem scaling. By contrast, this is not true of gradient descent.

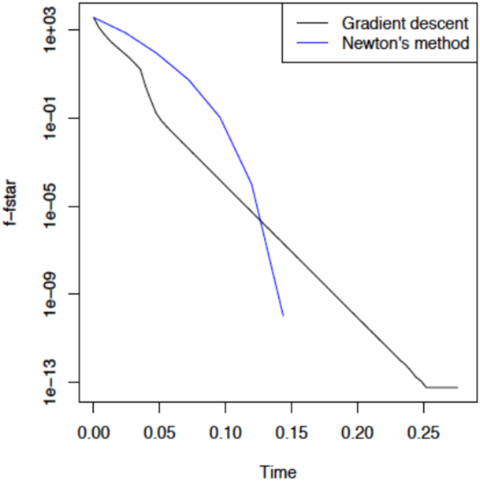
Newton vs Gradient: Empirically

Logistic Regression example with $n = 500, p = 100$. Compare GD with Newtons method.



Newton vs Gradient: Empirically

Same as earlier, just x-axis being total time instead of number of iterations (since iteration complexity is $O(d^3)$ for Newton and $O(d)$ for GD!



Secant Method

- Lets start with 1 dimension.
- Approximate the double derivative

$$f''(x_t) \approx H_t = \frac{f'(x_t) - f'(x_{t-1})}{x_t - x_{t-1}}$$

- This implies $f'(x_t) - f'(x_{t-1}) = H_t(x_t - x_{t-1})$
- Secant method: $x_{t+1} = x_t - H_t^{-1} f'(x_t)$
- In higher dimensions, the Matrix H_t must satisfy $\nabla f(x_t) - \nabla f(x_{t-1}) = H_t(x_t - x_{t-1})$
- This is called the secant conditions. When $d > 1$, this is an under-determined linear system and can infinitely many symmetric solutions.

History of Quasi Newton Methods

- In the mid 1950s, William Davidon was a mathematician/physicist at Argonne National Lab
- He was using coordinate descent on an optimization problem and his computer kept crashing before finishing
- He figured out a way to accelerate the computation, leading to the first quasi-Newton method (soon Fletcher and Powell followed up on his work)
- Although Davidon's contribution was a major breakthrough in optimization, his original paper was rejected (for dubious notation and no convergence analysis)
- In 1991, after more than 30 years, his paper was published in the first issue of the SIAM Journal on Optimization
- In addition to his remarkable work in optimization, Davidon was a peace activist (see the book "The Burglary")

History of Quasi Newton Methods

- Davidon's original paper:
- William C Davidon, Variable Metric Method for Minimization, Technical Report, ANL, 1959
- Davidon's 1991 publication:
- William C Davidon, Variable Metric Method for Minimization, SIAM Journal of Optimization, 1(1), 1-17, 1991 (**This is one of the best journals on optimization**).

Quasi newton Template

Let $x_0 \in \mathbb{R}^d, B_0 \succ 0$. For $k = 1, 2, \cdots$, repeat:

- Define s_{k-1} as the descent step.
- Solve $B_{k-1} s_{k-1} = -\nabla f(x_{k-1})$
- Update $x_k = x_{k-1} + \alpha_k s_{k-1}$
- Compute B_k from B_{k-1}

Different Quasi Newton methods implement step three differently. Also it makes sense to update B_k^{-1} directly from B_{k-1}^{-1}.

Also, a reasonable requirement for B_k is the secant method discussed earlier: $\nabla f(x_k) = \nabla f(x_{k-1}) + B_k s_{k-1}$.

Additionally, we want a) B_k to be symmetric, b) B_k to be close to B_{k-1} and c) $B_{k-1} \succ 0 \Rightarrow B_k \succ 0$.

Symmetric Rank-One Update

- Easiest choice is a rank one update of the kind:

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

- Denote $y_{k-1} = \nabla f(x_k) - \nabla f(x_{k-1})$.
- The secant condition is $B_k s_{k-1} = y_{k-1}$ and this implies:

$$a(u^T s_{k-1})u = y_{k-1} - B_{k-1}s_{k-1}$$

.

- Define $u = y_{k-1} - B_{k-1}s_{k-1}$. Then solving for the above, we get: $a = 1/(y_{k-1} - B_{k-1}s_{k-1})^T s_{k-1}$ which leads:

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

Symmetric Rank-One Update

- This is great! But we still need to solve for s_k: $B_k s_k = -\nabla f(x_k)$. Recall that we obtain $x_k = x_{k-1} + \alpha_k s_{k-1}$
- Fortunately, we can propogate inverses using the Sherman-Morrison formula:
$$(A + uu^T)^{-1} = \frac{A^{-1} - A^{-1}uu^T A^{-1}}{1 + v^T A^{-1} u}$$
- Symmetric Rank One Update is cheap(er) since now it is $O(d^2)$ in compute and memory!
- However, the key shortcomming is it does not preserve the positive definiteness!

Broyden-Fletcher-Goldfarb-Shanno (BFGS) update

- BFGS update is a rank two update:

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

- Key idea is to use the Secant rule and then define $u = y_{k-1}$ and $v = B_k s_{k-1}$.
- We then get the BFGS update:

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

- Similar to SR1 update, we can propogate the Inverse Matrices and the resulting update is $O(d^2)$ in time and memory!
- BFGS update also preserves the positive definiteness!

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- Recall BFGS update:

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- BFGS Inverse Update:

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

Positive Definiteness of BFGS

- If $y_{k-1}^T s_{k-1} > 0$, BFGS updates preserve positive definiteness of B_k
- If f is strictly convex, then the above condition holds.
- Intuition of the Positive Definiteness. Use the inverse formula and compute $v^T B_{k+1}^{-1} v$ and show that it is non-negative if $B_k \succ 0$.
- From the inverse update formula:

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

- Easy to now see that B_{k+1} is positive definite if B_k is positive definite!

Davidon-Fletcher-Powell (DFP) update

- We have the rank two update:

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

- Recall in BFGS, we set: $u = y_{k-1}$ and $v = B_k s_{k-1}$.
- We can optionally also set $u = s_{k-1}$ and $v = B_k y_{k-1}$. We get an update analogous to BFGS but with s_{k-1} and y_{k-1} exchanged!

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

- DFP update also preserves the positive definiteness!
- In practice, BFGS often outperforms DFP!

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- Global Convergence: If f is strongly convex, BFGS with backtracking line search convergences from any x_0
- Superlinear local convergence: Under similar assumptions to the Newton's method, BFGS convergences locally at a superlinear rate!
- Empirically BFGS vs Newton: BFGS converges to the same error rate in only a constant number of iterations more than Newton, while being $O(n)$ faster in each iteration! numerical stability, a *Square root BFGS update* is often used where H_k is factored as $H_k = L_k L_k^T$. The complexity is the same, but in certain cases this can be numerically more stable.

Another Interesting view of BFGS!

- The BFGS update can be seen as solving the following optimization problem:

$$\text{minimize } tr(B_k^{-1}X) - \log\det(B_k^{-1}X) - n \tag{1}$$

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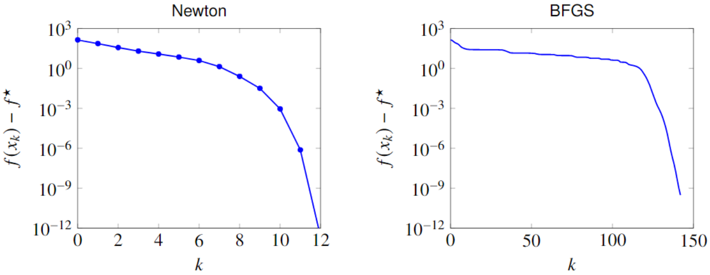
- BFGS update is a least change secant update!
- This can be seen from the KKT conditions of optimality!

Example

$$\text{minimize} \quad c^T x - \sum_{i=1}^{m} \log(b_i - a_i^T x)$$

$n = 100$, $m = 500$



- cost per Newton iteration: $O(n^3)$ plus computing $\nabla^2 f(x)$
- cost per BFGS iteration: $O(n^2)$

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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

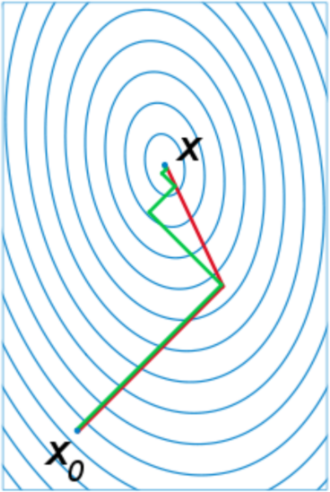
A comparison of

* 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:

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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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$$x_{t+1} = x_t - \alpha_t \nabla f(x_t)$$

. Pros: Simple! Cons: No second order information at all!

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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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where $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = \nabla f(x_k) - \nabla f(x_{k-1}$

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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!

Next Few Lectures

- Conditional Gradient Descent (Frank Wolfe) for Constrained Optimization
- Coordinate Descent
- Stochastic Gradient Descent and Family
- Duality (Legrange Duality and Fenchel Duality)
- After Spring Break, we will start Discrete (Submodular) Optimization.