CPSC 540: Machine Learning

Rates of Convergence

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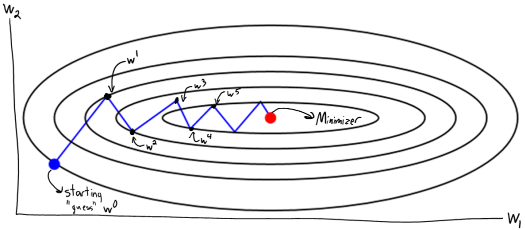
Winter 2019

Admin

- Audditting/registration forms:
  - Submit them at end of class, pick them up end of next class.
  - I need your prereq form before I'll sign registration forms.
  - I wrote comments on the back of some forms.
- Assignment 1 due tonight at midnight (Vancouver time).
  - 1 late day to hand in Monday, 2 late days for Wednesday.
- No tutorial Monday: we'll have them on the 2 weeks before assignmets are due.

Last Time: Gradient Descent

- Gradient descent:
  - Iterative method for finding stationary point ($\nabla f(w) = 0$) of differentiable function.
  - For convex functions if converges to a global minimum (if one exists).



Start with w^0, apply

$$w^{k+1} = w^k - \alpha_k \nabla f(w^k),$$

for step-size α_k.

- Cost of algorithm scales linearly with number of variables d.
  - Costs $O(ndt)$ for t iterations for least squares and logistic regression.
  - For $t < d$, faster than $O(nd^2 + d^3)$ of normal equations or Newton's method.

Last Time: Convergence Rate of Gradient Descent

- We discussed gradient descent,

$$w^{k+1} = w^k - \alpha_k \nabla f(w^k).$$

  assuming that the gradient was Lipschitz continuous (weak assumption),

$$\|\nabla f(w) - \nabla f(v)\| \leq L\|w - v\|,$$

- We showed that setting $\alpha_k = 1/L$ gives a progress bound of

$$f(w^{k+1}) \leq f(w^k) - \frac{1}{2L}\|\nabla f(w^k)\|^2,$$

- We discussed practical α_k values that give similar bounds.
  - "Try a big step-size, and decrease it if isn't satisfying a progress bound."

Discussion of $O(1/t)$ and $O(1/\epsilon)$ Results

- We showed that after t iterations, there will be a k such that

$$\|\nabla f(w^k)\|^2 = O(1/t).$$

- If we want to have a k with $\|\nabla f(w^k)\|^2 \leq \epsilon$, number of iterations we need is

$$t = O(1/\epsilon).$$

- So if computing gradient costs $O(nd)$, total cost of gradient descent is $O(nd/\epsilon)$.
  - $O(nd)$ per iteration and $O(1/\epsilon)$ iterations.
- This also be shown for practical step-size strategies from last time.
  - Just changes constants.

Discussion of $O(1/t)$ and $O(1/\epsilon)$ Results

- Our precise "error on iteration t" result was

$$\min_{k=0,1,\dots,t-1}\{\|\nabla f(w^k)\|^2\} \leq \frac{2L[f(w^0) - f^*]}{t}.$$

- This is a non-asymptotic result:
  - It holds on iteration 1, there is no "limit as $t \to \infty$" as in classic results.
  - But if t goes to ∞, argument can be modified to show that $\nabla f(w^t)$ goes to zero.

- This convergence rate is dimension-independent:
  - It does not directly depend on dimension d.
  - Though L might grow as dimension increases.

- Consider least squares with a fixed L and $f(w^0)$, and an accuracy ϵ:
  - There is dimension d beyond which gradient descent is faster than normal equations.

Discussion of $O(1/t)$ and $O(1/\epsilon)$ Results

- We showed that after t iterations, there is always a k such that

$$\min_{k=0,1,\dots,t-1}\{\|\nabla f(w^k)\|^2\} \leq \frac{2L[f(w^0) - f^*]}{t}.$$

- It isn't necessarily the last iteration t that achieves this.
  - But iteration t does have the lowest value of $f(w^k)$.

- For real ML problems optimization bounds like this are often very loose.
  - In practice gradient descent converges much faster.
  - So there is a practical and theoretical component to research.

- This does not imply that gradient descent finds global minimum.
  - We could be minimizing an NP-hard function with bad local optima.

Faster Convergence to Global Optimum?

- What about finding the global optimum of a non-convex function?
- Fastest possible algorithms requires $O(1/\epsilon^d)$ iterations for Lipschitz-continuous f.
  - This is actually achieved by by picking w^k values randomly (or by "grid search").
  - You **can't** beat this with simulated annealing, genetic algorithms, Bayesian optim,...
- Without some assumption like Lipschitz f, getting within ϵ of f^* is impossible.
  - Due to real numbers being uncountable.
  - "Math with Bad Drawings" sketch of proof here.
- These issues are discussed in post-lecture bonus slides.

Convergence Rate for Convex Functions

- For convex functions we can get to a global optimum much faster.
- This is because $\nabla f(w) = 0$ implies w is a global optimum.
  - So gradient descent will converge to a global optimum.
- Using a similar proof (with telescoping sum), for convex f

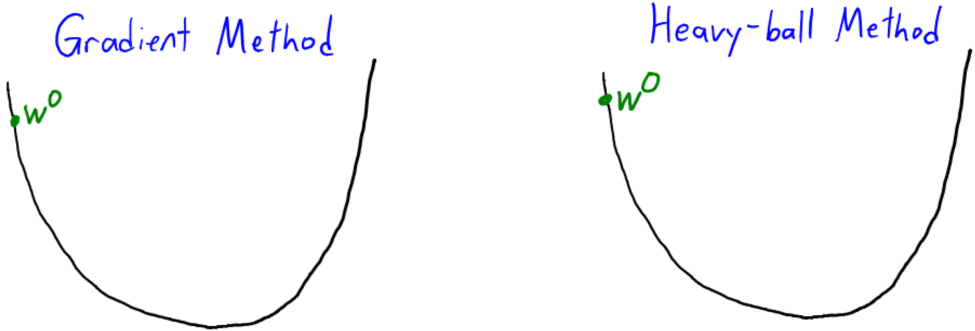
$$f(w^t) - f(w^*) = O(1/t),$$

  if there exists a global optimum w^* and ∇f is Lipschitz.
  - So we need $O(1/\epsilon)$ iterations to get ϵ-close to global optimum, not $O(1/\epsilon^d)$.

Faster Convergence to Global Optimum?

- Is $O(1/\epsilon)$ the best we can do for convex functions?
- No, there are algorithms that only need $O(1/\sqrt{\epsilon})$.
  - This is optimal for any algorithm based only on functions and gradients.
    - And restricting to dimension-independent rates.
- First algorithm to achieve this: Nesterov's accelerated gradient method.
  - A variation on what's known as the "heavy ball' method (or "momentum").

Heavy-Ball Method Method



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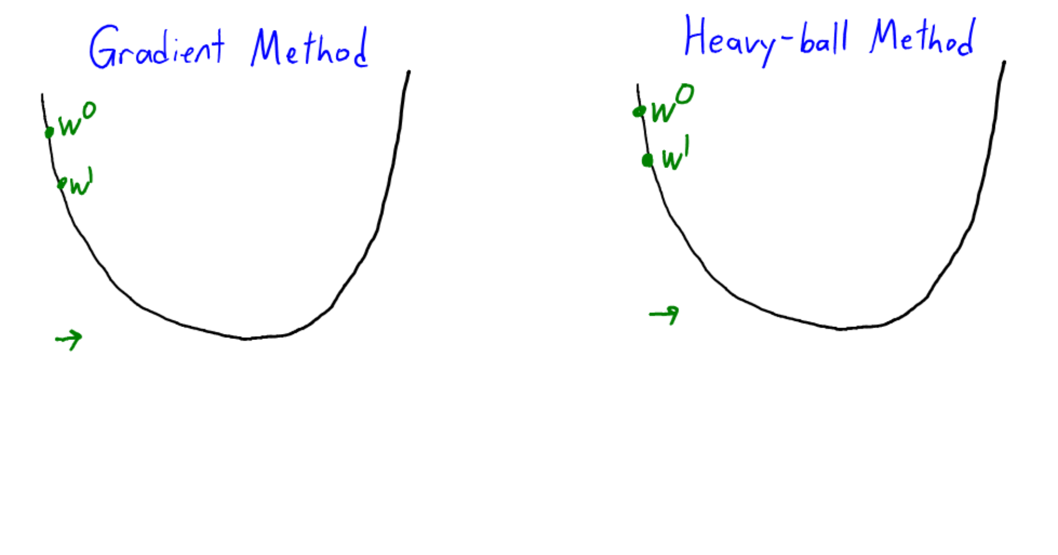

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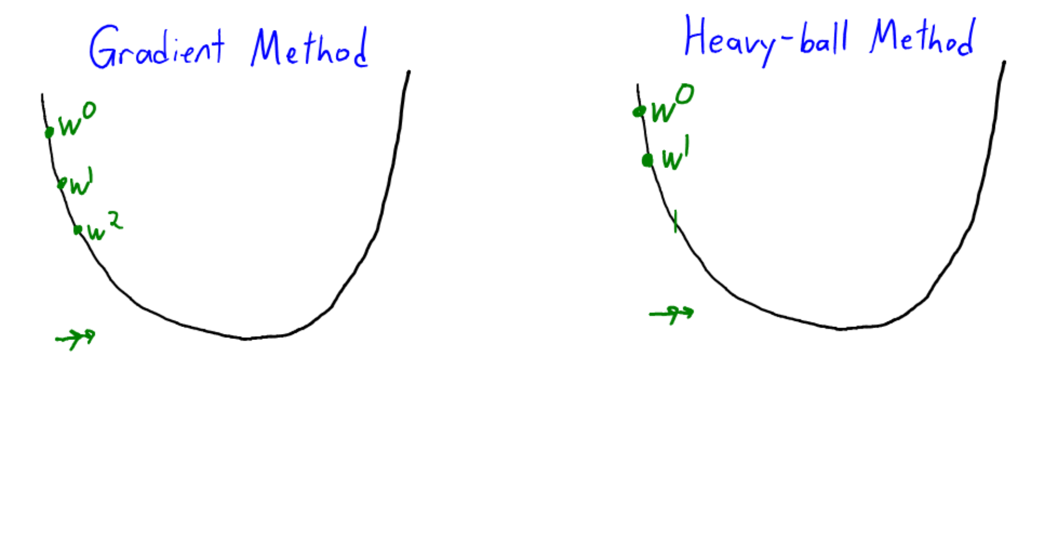

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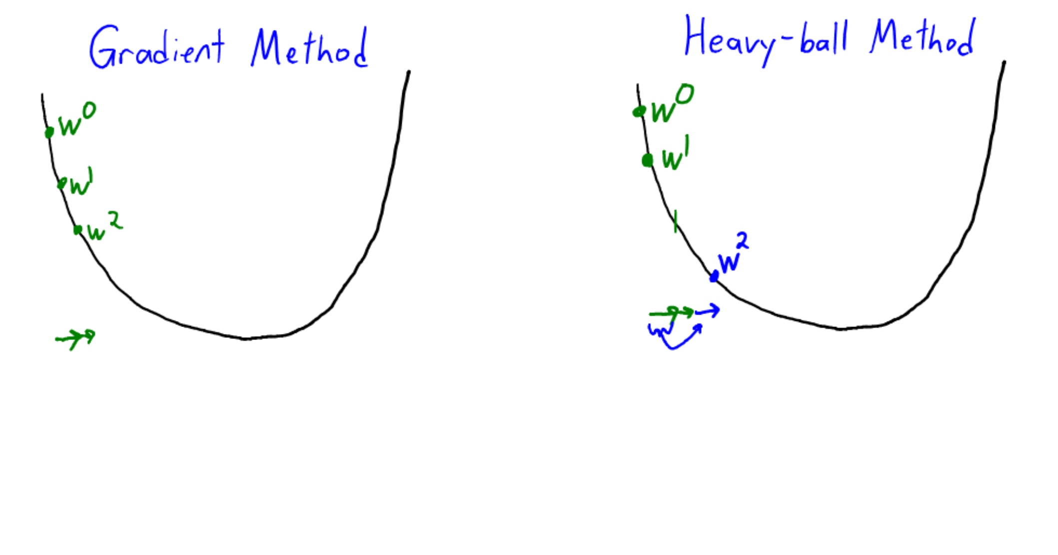

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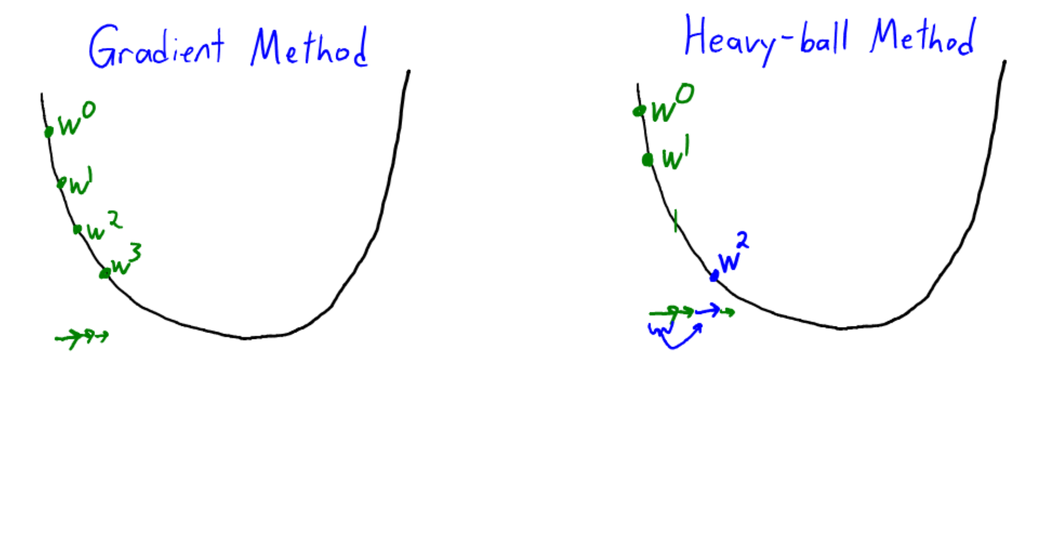

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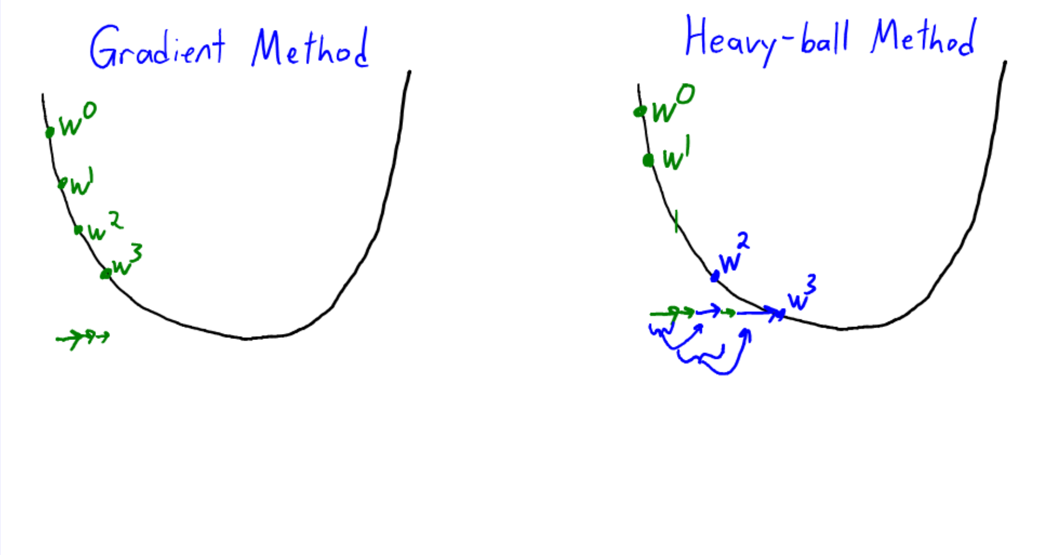

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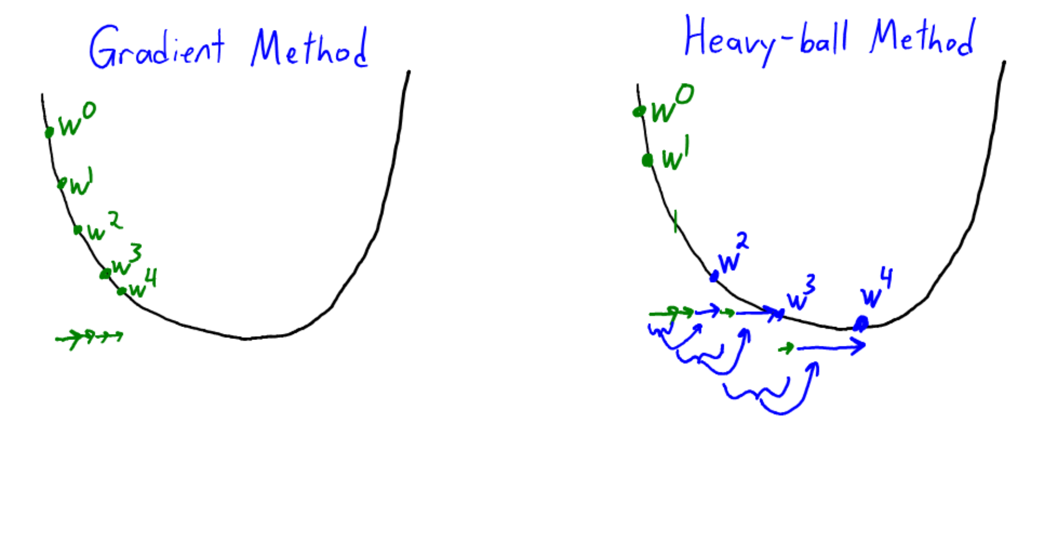

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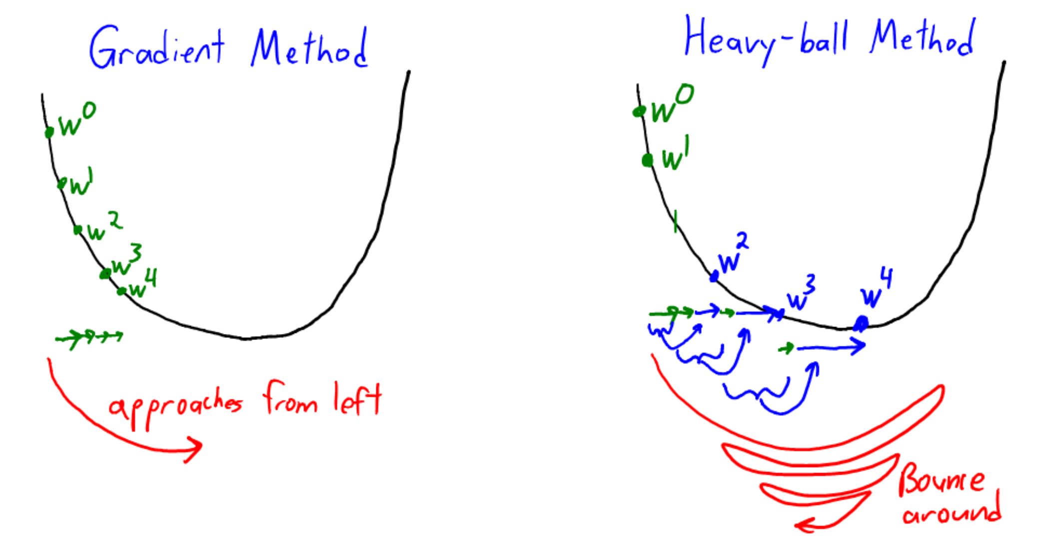


Heavy-Ball, Momentum, CG, and Accelerated Gradient

- The heavy-ball method (called momentum in neural network papers) is

$$w^{k+1} = w^k - \alpha_k \nabla f(w^k) + \beta_k (w^k - w^{k-1}).$$

- For strictly-convex quadratics, achieves faster rate (for appropriate α_k and β_k).
  - With the optimal α_k and β_k, we obtain conjugate gradient.

- Variation is Nesterov's accelerated gradient method,

$$\begin{aligned} w^{k+1} &= v^k - \alpha_k \nabla f(v^k), \\ v^{k+1} &= w^k + \beta_k (w^{k+1} - w^k), \end{aligned}$$

- Has an error of $O(1/t^2)$ after t iterations instead of $O(1/t)$ for convex functions.
  - So it only needs $O(1/\sqrt{\epsilon})$ iterations to get within ϵ of global opt.
  - Can use $\alpha_k = 1/L$ and $\beta_k = \frac{k-1}{k+2}$ to achieve this.

Iteration Complexity

- Iteration complexity: smallest t such that algorithm guarantees ϵ-solution.
- Think of $\log(1/\epsilon)$ as "number of digits of accuracy" you want.
  - We want iteration complexity to grow slowly with $1/\epsilon$.
- Is $O(1/\epsilon)$ a good iteration complexity?
- Not really, if you need 10 iterations for a "digit "of accuracy then:
  - You might need 100 for 2 digits.
  - You might need 1000 for 3 digits.
  - You might need 10000 for 4 digits.
- We would normally call this exponential time.

Rates of Convergence

- A way to measure rate of convergence is by limit of the ratio of successive errors,

$$\lim_{k\to\infty} \frac{f(w^{k+1}) - f(w^*)}{f(w^k) - f(w^*)} = \rho.$$

- Different ρ values of give us different rates of convergence:
  1. If $\rho = 1$ we call it a sublinear rate.
  2. If $\rho \in (0,1)$ we call it a linear rate.
  3. If $\rho = 0$ we call it a superlinear rate.

- Having $f(w^t) - f(w^*) = O(1/t)$ gives sublinear convergence rate:
  - “The longer you run the algorithm, the less progress it makes”.

Sub/Superlinear Convergence vs. Sub/Superlinear Cost

- As a computer scientist, what would we ideally want?
  - Sublinear rate is bad, we don't want $O(1/t)$ ("exponential" time: $O(1/\epsilon)$ iterations).
  - Linear rate is ok, we're ok with $O(\rho^t)$ ("polynomial" time: $O(\log(1/\epsilon))$ iterations).
  - Superlinear rate is great, amazing to have $O(\rho^{2^t})$ ("constant": $O(\log(\log(1/\epsilon)))$).
- Notice that terminology is backwards compared to computational cost:
  - Superlinear cost is bad, we don't want $O(d^3)$.
  - Linear cost is ok, having $O(d)$ is ok.
  - Sublinear cost is great, having $O(\log(d))$ is great.
- Ideal algorithm: superlinear convergence and sublinear iteration cost.

Outline

1 Rates of Convergence

2 Linear Convergence of Gradient Descent

Polyak-Łojasiewicz (PL) Inequality

- For least squares, we have linear cost but we only showed sublinear rate.
- For many "nice" functions f, gradient descent actually has a linear rate.
- For example, for functions satisfying the Polyak-Łojasiewicz (PL) inequality,

$$\frac{1}{2}\|\nabla f(w)\|^2 \geq \mu(f(w) - f^*),$$

  for all w and some $\mu > 0$.
  - "Gradient grows as a quadratic function as we increase f".

Linear Convergence under the PL Inequality

- Recall our guaranteed progress bound

$$f(w^{k+1}) \leq f(w^k) - \frac{1}{2L}\|\nabla f(w^k)\|^2.$$

- Under the PL inequality we have $-\|\nabla f(w^k)\|^2 \leq -2\mu(f(w^k) - f^*)$, so

$$f(w^{k+1}) \leq f(w^k) - \frac{\mu}{L}(f(w^k) - f^*).$$

- Let's subtract f^* from both sides,

$$f(w^{k+1}) - f^* \leq f(w^k) - f^* - \frac{\mu}{L}(f(w^k) - f^*),$$

  and factorizing the right side gives

$$f(w^{k+1}) - f^* \leq \left(1 - \frac{\mu}{L}\right)(f(w^k) - f^*).$$

Linear Convergence under the PL Inequality

- Applying this recursively:

$$\begin{aligned} f(w^k) - f^* &\leq \left(1 - \frac{\mu}{L}\right)[f(w^{k-1}) - f(w^*)] \\ &\leq \left(1 - \frac{\mu}{L}\right)\left[\left(1 - \frac{\mu}{L}\right)[f(w^{k-2}) - f^*]\right] \\ &= \left(1 - \frac{\mu}{L}\right)^2 [f(w^{k-2}) - f^*] \\ &\leq \left(1 - \frac{\mu}{L}\right)^3 [f(w^{k-3}) - f^*] \\ &\leq \left(1 - \frac{\mu}{L}\right)^k [f(w^0) - f^*] \end{aligned}$$

- We'll always have $0 < \mu \leq L$ so we have $(1 - \mu/L) < 1$.
    - So PL implies a linear convergence rate: $f(w^k) - f^* = O(\rho^k)$ for $\rho < 1$.

Linear Convergence under the PL Inequality

- We've shown that

$$f(w^k) - f^* \leq \left(1 - \frac{\mu}{L}\right)^k [f(w^0) - f^*]$$

- By using the inequality that

$$(1 - \gamma) \leq \exp(-\gamma),$$

  we have that

$$f(w^k) - f^* \leq \exp\left(-k\frac{\mu}{L}\right)[f(w^0) - f^*],$$

  which is why linear convergence is sometimes called "exponential convergence".

- We'll have $f(w^t) - f^* \leq \epsilon$ for any t where

$$t \geq \frac{L}{\mu}\log((f(w^0) - f^*)/\epsilon) = O(\log(1/\epsilon)).$$

Discussion of Linear Convergence under the PL Inequality

- PL is satisfied for many standard convex models like least squares (bonus).
  - So cost of least squares is $O(nd\log(1/\epsilon))$.
- PL is also satisfied for some non-convex functions like $w^2 + 3\sin^2(w)$.
  - It's satisfied for PCA on a certain "Riemann manifold".
  - But it's not satisfied for many models, like neural networks.
- The PL constant μ might be terrible.
  - For least squares μ is the smallest non-zero eigenvalue of the Hessian

.

- It may be hard to show that a function satisfies PL.
  - But regularizing a convex function gives a PL function with non-trivial μ...

Strong Convexity

- We say that a function f is strongly convex if the function

$$f(w) - \frac{\mu}{2}\|w\|^2,$$

is a convex function for some $\mu > 0$.
  - "If you 'un-regularize' by μ then it's still convex."

- For C^2 functions this is equivalent to assuming that

$$\nabla^2 f(w) \succeq \mu I,$$

that the eigenvalues of the Hessian are at least μ everywhere.

- Two nice properties of strongly-convex functions:
  - A unique solution exists.
  - C^1 strongly-convex functions satisfy the PL inequality.

Strong Convexity Implies PL Inequality

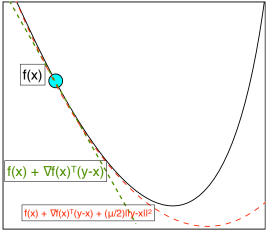
- As before, from Taylor's theorem we have for C^2 functions that

$$f(v) = f(w) + \nabla f(w)^\top (v - w) + \frac{1}{2}(v - w)^\top \nabla^2 f(u)(v - w).$$

- By strong-convexity, $d^\top \nabla^2 f(u) d \geq \mu \|d\|^2$ for any d and u.

$$f(v) \geq f(w) + \nabla f(w)^\top (v - w) + \frac{\mu}{2}\|v - w\|^2$$

- Treating right side as function of v, we get a quadratic lower bound on f.



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$$f(v) \geq f(w) + \nabla f(w)^\top (v - w) + \frac{\mu}{2}\|v - w\|^2.$$

- Treating right side as function of v, we get a quadratic lower bound on f.

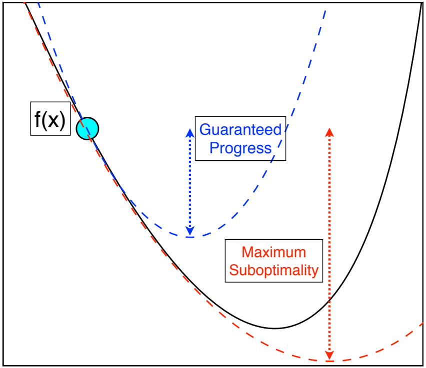
- Minimize both sides in terms of v gives

$$f^* \geq f(w) - \frac{1}{2\mu}\|\nabla f(w)\|^2,$$

which is the PL inequality (bonus slides show for C^1 functions).

Combining Lipschitz Continuity and Strong Convexity

- Lipschitz continuity of gradient gives guaranteed progress.
- Strong convexity of functions gives maximum sub-optimality.



- Progress on each iteration will be at least a fixed fraction of the sub-optimality.

Effect of Regularization on Convergence Rate

- We said that f is strongly convex if the function

$$f(w) - \frac{\mu}{2}\|w\|^2,$$

  is a convex function for some $\mu > 0$.
  - For a C^2 univariate function, equivalent to $f''(w) \geq \mu$.

- If we have a convex loss f, adding L2-regularization makes it strongly-convex,

$$f(w) + \frac{\lambda}{2}\|w\|^2,$$

  with μ being at least λ.

- So adding L2-regularization can improve rate from sublinear to linear.
  - Go from exponential $O(1/\epsilon)$ to polynomial $O(\log(1/\epsilon))$ iterations.
  - And guarantees a unique solution.

Effect of Regularization on Convergence Rate

- Our convergence rate under PL was

$$f(w^k) - f^* \leq \underbrace{\left(1 - \frac{\mu}{L}\right)^k}_{\rho^k}[f(w^0) - f^*].$$

- For L2-regularized least squares we have

$$\frac{L}{\mu} = \frac{\max\{\text{eig}(X^\top X)\} + \lambda}{\min\{\text{eig}(X^\top X)\} + \lambda}.$$

- So as λ gets larger ρ gets closer to 0 and we converge faster.

- The number $\frac{L}{\mu}$ is called the condition number of f.
  - For least squares, it's the "matrix condition number" of $\nabla^2 f(w)$.

Summary

- Sublinear/linear/superlinear convergence measure speed of convergence.
- Polyak-Łojasiewicz inequality leads to linear convergence of gradient descent.
  - Only needs $O(\log(1/\epsilon))$ iterations to get within ϵ of global optimum.
- Strongly-convex differentiable functions functions satisfy PL-inequality.
  - Adding L2-regularization makes gradient descent go faster.

- Next time: why does L1-regularization set variables to 0?

First-Order Oracle Model of Computation

- Should we be happy with an algorithm that takes $O(\log(1/\epsilon))$ iterations?
  - Is it possible that algorithms *exist* that solve the problem faster?
- To answer questions like this, need a class of functions.
  - For example, strongly-convex with Lipschitz-continuous gradient.
- We also need a model of computation: what operations are allowed?
- We will typically use a first-order oracle model of computation:
  - On iteration k, algorithm choose an x^k and receives $f(x^k)$ and $\nabla f(x^k)$.
  - To choose x^k, algorithm can do anything that doesn't involve f.
- Common variation is zero-order oracle where algorithm only receives $f(x^k)$.

Complexity of Minimizing Real-Valued Functions

- Consider minimizing real-valued functions over the unit hyper-cube,

$$\min_{x \in [0,1]^d} f(x).$$

- You can use any algorithm you want.

  (simulated annealing, gradient descent + random restarts, genetic algorithms, Bayesian optimization,...)
- How many zero-order oracle calls t before we can guarantee $f(x^t) - f(x^*) \leq \epsilon$?
  - Impossible!
- Given any algorithm, we can construct an f where $f(x^k) - f(x^*) > \epsilon$ forever.
  - Make $f(x) = 0$ except at x^* where $f(x) = -\epsilon - 2^{\text{whatever}}$.

    (the x^* is algorithm-specific)
- To say anything in oracle model we need assumptions on f.

Complexity of Minimizing Lipschitz-Continuous Functions

- One of the simplest assumptions is that f is Lipschitz-continuous,

$$|f(x) - f(y)| \leq L\|x - y\|.$$

- Function can't change arbitrarily fast as you change x.

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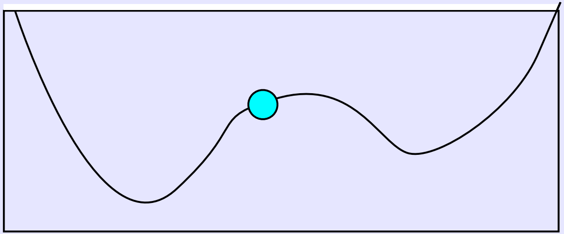

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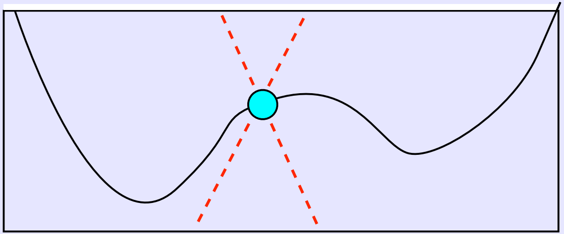

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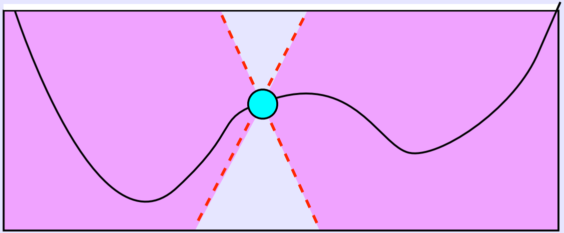

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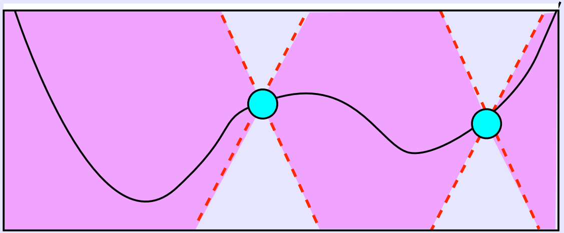

Complexity of Minimizing Lipschitz-Continuous Functions

- One of the simplest assumptions is that f is Lipschitz-continuous,

$$|f(x) - f(y)| \leq L\|x - y\|.$$

- Function can't change arbitrarily fast as you change x.

- Under only this assumption, any algorithm requires at least $\Omega(1/\epsilon^d)$ iterations.
- An optimal $O(1/\epsilon^d)$ worst-case rate is achieved by a grid-based search method.

- You can also achieve optimal rate in expectation by random guesses.
  - Lipschitz-continuity implies there is a ball of ϵ-optimal solutions around x^*.
  - The radius of the ball is $\Omega(\epsilon)$ so its area is $\Omega(\epsilon^d)$.
  - If we succeed with probability $\Omega(\epsilon^d)$, we expect to need $O(1/\epsilon^d)$ trials.

(mean of geometric random variable)

Complexity of Minimizing Convex Functions

- Life gets better if we assume convexity.
  - We'll consider first-order oracles and rates with no dependence on d.

- Subgradient methods (next week) can minimize convex functions in $O(1/\epsilon^2)$.
  - This is optimal in dimension-independent setting.

- If the gradient is Lipschitz continuous, gradient descent requires $O(1/\epsilon)$.
  - With Nesterov's algorithm, this improves to $O(1/\sqrt{\epsilon})$ which is optimal.
  - Here we don't yet have strong-convexity.

- What about the CPSC 340 approach of smoothing non-smooth functions?
  - Gradient descent still requires $O(1/\epsilon^2)$ in terms of solving original problem.
  - Nesterov improves to $O(1/\epsilon)$ in terms of original problem.

Why is $\mu \leq L$?

- The descent lemma for functions with L-Lipschitz ∇f is that

$$f(v) \leq f(w) + \nabla f(w)^\top (v - w) + \frac{L}{2}\|v - w\|^2.$$

- Minimizing both sides in terms of v (by taking the gradient and setting to 0 and observing that it's convex) gives

$$f^* \leq f(w) - \frac{1}{2L}\|\nabla f(w)\|^2.$$

- So with PL and Lipschitz we have

$$\frac{1}{2\mu}\|\nabla f(w)\|^2 \geq f(w) - f^* \geq \frac{1}{2L}\|\nabla f(w)\|^2,$$

which implies $\mu \leq L$.

C^1 Strongly-Convex Functions satisfy PL

- If $g(x) = f(x) - \frac{\mu}{2}\|x\|^2$ is convex then from C^1 definition of convexity

$$g(y) \geq g(x) + \nabla g(x)^\top (y - x)$$

or that

$$f(y) - \frac{\mu}{2}\|y\|^2 \geq f(x) - \frac{\mu}{2}\|x\|^2 + (\nabla f(x) - \mu x)^\top (y - x),$$

which gives

$$\begin{aligned} f(y) &\geq f(x) + \nabla f(x)^\top (y - x) + \frac{\mu}{2}\|y\|^2 - \mu x^\top y + \frac{\mu}{2}\|x\|^2 \\ &= f(x) + \nabla f(x)^\top (y - x) + \frac{\mu}{2}\|y - x\|^2, \quad \text{(complete square)} \end{aligned}$$

the inequality we used to show C^2 strongly-convex function f satisfies PL.

Linear Convergence without Strong-Convexity

- The least squares problem is convex but not strongly convex.
  - We could add a regularizer to make it strongly-convex.
  - But if we really want the MLE, are we stuck with sub-linear rates?

- Many conditions give linear rates that are weaker than strong-convexity:
  - 1963: Polyak-Łojasiewicz (PL).
  - 1993: Error bounds.
  - 2000: Quadratic growth.
  - 2013-2015: essential strong-convexity, weak strong convexity, restricted secant inequality, restricted strong convexity, optimal strong convexity, semi-strong convexity.
- Least squares satisfies all of the above.

- Do we need to study any of the newer ones?
  - No! All of the above imply PL except for QG.
  - But with only QG gradient descent may not find optimal solution.

PL Inequality for Least Squares

- Least squares can be written as $f(x) = g(Ax)$ for a σ-strongly-convex g and matrix A, we'll show that the PL inequality is satisfied for this type of function.
- The function is minimized at some $f(y^*)$ with $y^* = Ax$ for some x, let's use $\mathcal{X}^* = \{x | Ax = y^*\}$ as the set of minimizers. We'll use x_p as the "projection" (defined next lecture) of x onto $\mathcal{X}^*$.

$$
\begin{aligned}
f^* = f(x_p) &\geq f(x) + \langle \nabla f(x), x_p - x \rangle + \frac{\sigma}{2} ||A(x_p - x)||^2 \\
&\geq f(x) + \langle \nabla f(x), x_p - x \rangle + \frac{\sigma\theta(A)}{2} ||x_p - x||^2 \\
&\geq f(x) + \min_y \left[\langle \nabla f(x), y - x \rangle + \frac{\sigma\theta(A)}{2} ||y - x||^2 \right] \\
&= f(x) - \frac{1}{2\theta(A)\sigma} ||\nabla f(x)||^2.
\end{aligned}
$$

- The first line uses strong-convexity of g, the second line uses the "Hoffman bound" which relies on $\mathcal{X}^*$ being a polyhedral set defined in this particular way to give a constant $\theta(A)$ depending on A that holds for all x (in this case it's the smallest non-zero singular value of A), and the third line uses that x_p is a particular y in the min.

Linear Convergence for “Locally-Nice” Functions

- For linear convergence it’s sufficient to have

$$L[f(x^{t+1}) - f(x^t)] \geq \frac{1}{2}\|\nabla f(x^t)\|^2 \geq \mu[f(x^t) - f^*],$$

for all x^t for some L and μ with $L \geq \mu > 0$.

(technically, we could even get rid of the connection to the gradient)

- Notice that this only needs to hold for all x^t, not for all possible x.
  - We could get linear rate for “nasty” function if the iterations stay in a “nice” region.
  - We can get lucky and converge faster than the global L/μ would suggest.

- Arguments like this give linear rates for some non-convex problems like PCA.

Convergence of Iterates

- Under strong-convexity, you can also show that the iterations converge linearly.
- With a step-size of $1/L$ you can show that

$$\|w^{k+1} - w^*\| \leq \left(1 - \frac{\mu}{L}\right) \|w^k - w^*\|.$$

- If you use a step-size of $2/(\mu + L)$ this improves to

$$\|w^{k+1} - w^*\| \leq \left(\frac{L - \mu}{L + \mu}\right) \|w^k - w^*\|.$$

- Under PL, the solution w^* is not unique.
  - You can show linear convergence of $\|w^k - w_p^k\|$, where w_p^k is closest solution.

Improved Rates on Non-Convex Functions

- We showed that we require $O(1/\epsilon)$ iterations for gradient descent to get norm of gradient below ϵ in the non-convex setting.
- Is it possible to improve on this with a gradient-based method?
- Yes, in 2016 it was shown that a gradient method can improve this to $O(1/\epsilon^{3/4})$:
  - Combination of acceleration and trying to estimate a "local" μ value.