CPSC 540: Machine Learning

Convergence of Gradient Descent

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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.
- Office hours: start today after class.
- Assignment 1 due Friday.
  - 1 late day to hand in Monday, 2 late days for Wednesday.
  - Instructions to hand in assignment on Piazza.
  - If you don't have a CS account, sign up ASAP: `https://www.cs.ubc.ca/getacct`

Last Time: Convex Optimization

- We discussed convex optimization problems.
  - Off-the-shelf solvers are available for solving medium-sized convex problems.

- We discussed ways to show functions are convex:
  - Show that f is below chord for any convex combination of points.
  - f is constructed from operations that preserve convexity.
    - Non-negative scaling, sum, max, composition with affine map.
  - Show that $\nabla^2 f(w)$ is positive semi-definite for all w,

$$\nabla^2 f(w) \succeq 0 \;\; \text{(zero matrix)}$$

- Formally, the notation $A \succeq B$ means that for any vector v we have

$$v^T A v \geq v^T B v,$$

and this is called a "generalized inequality".
  - It defines an "ordering" among some matrices, but not all matrices can be compared.

Strict Convexity and Positive-Definite Matrices

- We say that a C^2 function is strictly convex iff for all w we have

$$\nabla^2 f(w) \succ 0,$$

meaning that the Hessian is positive definite everywhere.

- Equivalent definitions of a positive definite matrix A:
  1. The eigevalues of A are all positive.
  2. $v^\top Av > 0$ for all $v \neq 0$.

- Why do we care about strict convexity?
  - Positive-definite matrices are invertible, so $[\nabla^2 f(w)]^{-1}$ exists.
  - There can be at most one global optimum (so it's unique, if one exists).

Strict Convexity and L2-Regularized Least Squares

- In L2-regularized least squares, the Hessian matrix is

$$\nabla^2 f(w) = (X^\top X + \lambda I).$$

- This matrix is positive-definite,

$$v^\top (X^\top X + \lambda I) v = \underbrace{\|Xv\|^2}_{\geq 0} + \underbrace{\lambda \|v\|^2}_{>0} > 0,$$

  which follows from properties of norms:
  - Both terms are non-negative because they're norms.
  - Second term $\|v\|$ is positive because $v \neq 0$ and $\lambda > 0$.

- This implies that:
  - The matrix $(X^\top X + \lambda I)$ is invertible.
  - The solution is unique.

Cost of L2-Regularizd Least Squares

- Two strategies from 340 for L2-regularized least squares:
  1. Closed-form solution,
  $$w = (X^TX + \lambda I)^{-1}(X^Ty),$$
  which costs $O(nd^2 + d^3)$.
     - This is fine for $d = 5000$, but may be too slow for $d = 1,000,000$.
  2. Run t iterations of gradient descent,
  $$w^{k+1} = w^k - \alpha_k \underbrace{(X^T(Xw^k - y) + \lambda w^k)}_{\nabla f(w^k)},$$
  which costs $O(ndt)$.
     - I'm using t as total number of iterations, and k as iteration number.

- Gradient descent is faster if t is not too big:
  - If we only do $t < \max\{d, d^2/n\}$ iterations.

Cost of Logistic Regression

- Gradient descent can also be applied to other models like logistic regression,

$$f(w) = \sum_{i=1}^{n} \log(1 + \exp(-y^i w^T x^i)),$$

which we can't formulate as a linear system or linear program.

  - Setting $\nabla f(w) = 0$ gives a system of transcendental equations.

- But this objective function is convex and differentiable.
  - So gradient descent converges to a global optimum.

- Alternately, another common approach is Newton's method.
  - Requires computing Hessian $\nabla^2 f(w^k)$, and known as "IRLS" in statistics.

Digression: Logistic Regression Gradient and Hessian

- With some tedious manipulations, gradient for logistic regression is

$$\nabla f(w) = X^T r.$$

where vector r has $r_i = -y^i h(-y^i w^T x^i)$ and h is the sigmoid function.

- We know the gradient has this form from the multivariate chain rule.
  - Functions for the form $f(Xw)$ always have $\nabla f(w) = X^T r$ (see bonus slide).

- With some more tedious manipulations we get

$$\nabla^2 f(w) = X^T D X.$$

where D is a diagonal matrix with $d_{ii} = h(y_i w^T x^i) h(-y^i w^T x^i)$.
  - The $f(Xw)$ structure leads to a $X^T DX$ Hessian structure.
  - For other problems D may not be diagonal.

Cost of Logistic Regression

- Gradient descent costs $O(nd)$ per iteration to compute Xw^k and X^Tr^k.
- Newton costs $O(nd^2 + d^3)$ per iteration to compute and invert $\nabla^2 f(w^k)$.

- Newton typically requires substantially fewer iterations.

- But for datasets with very large d, gradient descent might be faster.
  - If $t < \max\{d, d^2/n\}$ then we should use the "slow" algorithm with fast iterations.

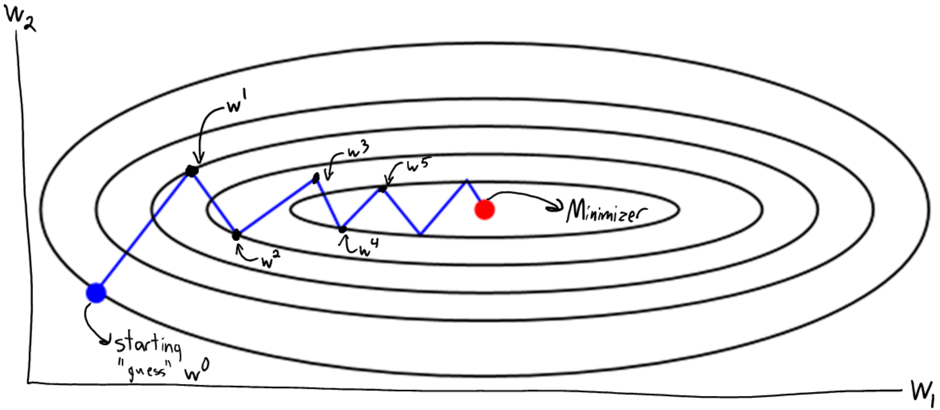
- So, how many iterations t of gradient descent do we need?

Outline

Gradient Descent for Finding a Local Minimum

- A typical gradient descent algorithm:
  - Start with some initial guess, w^0.
  - Generate new guess w^1 by moving in the negative gradient direction:
    $$w^1 = w^0 - \alpha_0 \nabla f(w^0),$$
    where α_0 is the step size.
  - Repeat to successively refine the guess:
    $$w^{k+1} = w^k - \alpha_k \nabla f(w^k), \quad \text{for } k = 1, 2, 3, \dots$$
    where we might use a different step-size α_k on each iteration.
  - Stop if $\|\nabla f(w^k)\| \leq \epsilon$.
    - In practice, you also stop if you detect that you aren't making progress.

Gradient Descent in 2D



Lipschitz Contuity of the Gradient

- Let's first show a basic property:
  - If the step-size α_t is small enough, then gradient descent decreases f.
- We'll analyze gradient descent assuming gradient of f is Lipschitz continuous.
  - There exists an L such that for *all* w and v we have
$$\|\nabla f(w) - \nabla f(v)\| \leq L\|w - v\|.$$
  - "Gradient can't change arbitrarily fast".
- This is a fairly weak assumption: it's true in almost all ML models.
  - Least squares, logistic regression, neural networks with sigmoid activations, etc.

Lipschitz Contuity of the Gradient

- For C^2 functions, Lipschitz continuity of the gradient is equivalent to

$$\nabla^2 f(w) \preceq LI,$$

  for all w.
- Equivalently: "singular values of the Hessian are bounded above by L".
  - For least squares, minimum L is the maximum eigenvalue of $X^T X$.
- This means we can bound quadratic forms involving the Hessian using

$$\begin{aligned} d^T \nabla^2 f(u) d &\leq d^T (LI) d \\ &= L d^T d \\ &= L\|d\|^2. \end{aligned}$$

Descent Lemma

- For a C^2 function, a variation on the multivariate Taylor expansion is that

$$f(v) = \underbrace{f(w) + \nabla f(w)^T(v-w)}_{\text{tangent hyper-plane}} + \underbrace{\frac{1}{2}(v-w)^T\nabla^2 f(u)(v-w)}_{\text{quadratic form}},$$

for any w and v (with u being some convex combination of w and v).

- Lipschitz continuity implies the green term is at most $L\|v-w\|^2$,

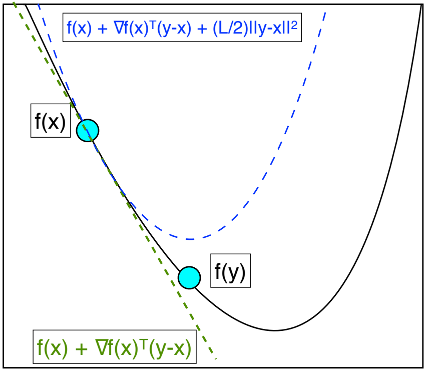
$$f(v) \leq f(w) + \nabla f(w)^T(v-w) + \frac{L}{2}\|v-w\|^2,$$

which is called the descent lemma.

- The descent lemma also holds for C^1 functions (bonus slide).

Descent Lemma

- The descent lemma gives us a convex quadratic upper bound on f:



- This bound is minimized by a gradient descent step from w with $\alpha_k = 1/L$.

Gradient Descent decreases f for $\alpha_k = 1/L$

- So let's consider doing gradient descent with a step-size of $\alpha_k = 1/L$,

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

- If we substitle w^{k+1} and w^k into the descent lemma we get

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

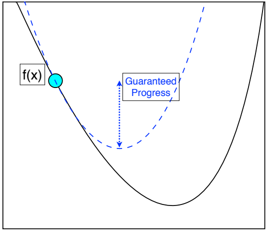
- Now if we use that $(w^{k+1} - w^k) = -\frac{1}{L}\nabla f(w^k)$ in gradient descent,

$$\begin{aligned} f(w^{k+1}) &\leq f(w^k) - \frac{1}{L}\nabla f(w^k)^T\nabla f(w^k) + \frac{L}{2}\|\frac{1}{L}\nabla f(w^k)\|^2 \\ &= f(w^k) - \frac{1}{L}\|\nabla f(w^k)\|^2 + \frac{1}{2L}\|\nabla f(w^k)\|^2 \\ &= f(w^k) - \frac{1}{2L}\|\nabla f(w^k)\|^2. \end{aligned}$$

Implication of Lipschitz Continuity

- We've derived a bound on guaranteed progress when using $\alpha_k = 1/L$.

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



- If gradient is non-zero, $\alpha_k = 1/L$ is guaranteed to decrease objective.
- Amount we decrease grows with the size of the gradient.
- Same argument shows that any $\alpha_k < 2/L$ will decrease f.

Choosing the Step-Size in Practice

- In practice, you should never use $\alpha_k = 1/L$.
  - L is usually expensive to compute, and this step-size is really small.
    - You only need a step-size this small in the worst case.
- One practical option is to approximate L:
  - Start with a small guess for $\hat{L}$ (like $\hat{L} = 1$).
  - Before you take your step, check if the progress bound is satisfied:

$$f(\underbrace{w^k - (1/\hat{L})\nabla f(w^k)}_{\text{potential } w^{k+1}}) \leq f(w^k) - \frac{1}{2\hat{L}}\|\nabla f(w^k)\|^2.$$

  - Double $\hat{L}$ if it's not satisfied, and test the inequality again.
- Worst case: eventually have $L \leq \hat{L} < 2L$ and you decrease f at every iteration.
- Good case: $\hat{L} << L$ and you are making way more progress than using $1/L$.

Choosing the Step-Size in Practice

- An approach that usually works better is a backtracking line-search:
  - Start each iteration with a large step-size α.
    - So even if we took small steps in the past, be optimistic that we're not in worst case.
  - Decrease α until if Armijo condition is satisfied (this is what *findMin.jl* does),

$$f(\underbrace{w^k - \alpha \nabla f(w^k)}_{\text{potential } w^{k+1}}) \leq f(w^k) - \alpha\gamma\|\nabla f(w^k)\|^2 \quad \text{for} \quad \gamma \in (0, 1/2],$$

  often we choose γ to be very small like $\gamma = 10^{-4}$.
    - We would rather take a small decrease instead of trying many α values.

- Good codes use clever tricks to initialize and decrease the α values.
  - Usually only try 1 value per iteration.
- Even more fancy line-search: Wolfe conditions (makes sure α is not too small).
  - Good reference on these tricks: Nocedal and Wright's Numerical Optimization book.

Outline

Convergence Rate of Gradient Descent

- In 340, we claimed that $\nabla f(w^k)$ converges to zero as k goes to ∞.
  - For convex functions, this means it converges to a global optimum.
  - However, we may not have $\nabla f(w^k) = 0$ for any finite k.
- Instead, we're usually happy with $\|\nabla f(w^k)\| \leq \epsilon$ for some small ϵ.
  - Given an ϵ, how many iterations does it take for this to happen?
- We'll first answer this question only assuming that
  1. Gradient ∇f is Lipschitz continuous (as before).
  2. Step-size $\alpha_k = 1/L$ (this is only to make things simpler).
  3. Function f can't go below a certain value f^* ("bounded below").
- Most ML objectives f are bounded below (like the squared error being at least 0).
  - We're not assuming convexity (argument will work for any smooth problem).

Convergence Rate of Gradient Descent

- Key ideas:
  1. We start at some $f(w^0)$, and at each step we decrease f by at least $\frac{1}{2L}\|\nabla f(w^k)\|^2$.
  2. But we can't decrease $f(w^k)$ below f^*.
  3. So $\|\nabla f(w^k)\|^2$ must be going to zero "fast enough".
- Let's start with our guaranteed progress bound,

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

- Since we want to bound $\|\nabla f(w^k)\|$, let's rearrange as

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

Convergence Rate of Gradient Descent

- So for each iteration k, we have

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

- Let's sum up the squared norms of all the gradients up to iteration t,

$$\sum_{k=1}^{t} \|\nabla f(w^{k-1})\|^2 \leq 2L \sum_{k=1}^{t}[f(w^{k-1}) - f(w^k)].$$

- Now we use two tricks:
  1. On the left, use that all $\|\nabla f(w^{k-1})\|$ are at least as big as their minimum.
  2. On the right, use that this is a telescoping sum:

$$\begin{aligned}\sum_{k=1}^{t}[f(w^{k-1}) - f(w^k)] &= f(w^0) - \underbrace{f(w^1) + f(w^1)}_{0} - \underbrace{f(w^2) + f(w^2)}_{0} - \dots f(w^t) \\ &= f(w^0) - f(w^t).\end{aligned}$$

Convergence Rate of Gradient Descent

- With these substitutions we have

$$\sum_{k=1}^{t} \underbrace{\min_{j \in \{0,\dots,t-1\}} \{\|\nabla f(w^j)\|^2\}}_{\text{no dependence on } k} \leq 2L[f(w^0) - f(w^t)].$$

- Now using that $f(w^t) \geq f^*$ we get

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

and finally that

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

so if we run for t iterations, we'll find $\underbrace{\text{least one } k}_{\text{the minimum}}$ with $\|\nabla f(w^k)\|^2 = O(1/t)$.

Convergence Rate of Gradient Descent

- Our "error on iteration t" bound:

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

- We want to know when the norm is below ϵ, which is guaranteed if:

$$\frac{2L[f(w^0) - f^*]}{t} \leq \epsilon.$$

- Solving for t gives that this is guaranteed for every t where

$$t \geq \frac{2L[f(w^0) - f^*]}{\epsilon},$$

so gradient descent requires $t = O(1/\epsilon)$ iterations to achieve $\|\nabla f(w^k)\|^2 \leq \epsilon$.

Summary

- Gradient descent can be suitable for solving high-dimensional problems.
- Guaranteed progress bound if gradient is Lipschitz, based on norm of gradient.
- Practical step size strategies based on the progress bound.
- Error on iteration t of $O(1/t)$ for functions that are bounded below.
  - Implies that we need $t = O(1/\epsilon)$ iterations to have $\|\nabla f(x^k)\| \leq \epsilon$.

- Next time: didn't I say that regularization makes gradient descent go faster?

Strictly-Convex Functions

- A function is strictly-convex if the convexity definitions hold strictly:

$$f(\theta w + (1-\theta)v) < \theta f(w) + (1-\theta)f(v), \quad 0 < \theta < 1 \qquad (C^0)$$

$$f(v) > f(w) + \nabla f(w)^\top (v - w) \qquad (C^1)$$

$$\nabla^2 f(w) \succ 0 \qquad (C^2)$$

- Function is always strictly below any chord, strictly above any tangent, and curved upwards in every direction.

- Strictly-convex function have at most one global minimum:
  - w and v can't both be global minima if $w \neq v$:
    it would imply convex combinations u of w and v would have $f(u)$ below the global minimum.

Checking Derivative Code

- Gradient descent codes require you to write objective/gradient code.
  - This tends to be error-prone, although automatic differentiation codes are helping.

- Make sure to check your derivative code:
  - Numerical approximation to partial derivative:

$$\nabla_i f(x) \approx \frac{f(x + \delta e_i) - f(x)}{\delta}$$

  - For large-scale problems you can check a random direction d:

$$\nabla f(x)^T d \approx \frac{f(x + \delta d) - f(x)}{\delta}$$

  - If the left side coming from your code is very different from the right side, there is likely a bug.

Multivariate Chain Rule

- If $g : \mathbb{R}^d \mapsto \mathbb{R}^n$ and $f : \mathbb{R}^n \mapsto \mathbb{R}$, then $h(x) = f(g(x))$ has gradient

$$\nabla h(x) = \nabla g(x)^T \nabla f(g(x)),$$

  where $\nabla g(x)$ is the Jacobian (since g is multi-output).
- If g is an affine map $x \mapsto Ax + b$ so that $h(x) = f(Ax + b)$ then we obtain

$$\nabla h(x) = A^T \nabla f(Ax + b).$$

- Further, for the Hessian we have

$$\nabla^2 h(x) = A^T \nabla^2 f(Ax + b)A.$$

Convexity of Logistic Regression

- Logistic regression Hessian is

$$\nabla^2 f(w) = X^T D X.$$

  where D is a diagonal matrix with $d_{ii} = h(y_i w^T x^i) h(-y^i w^T x^i)$.

- Since the sigmoid function is non-negative, we can compute $D^{\frac{1}{2}}$, and

$$v^T X^T D X v = v^T X^T D^{\frac{1}{2}} D^{\frac{1}{2}} X v = (D^{\frac{1}{2}} X v)^T (D^{\frac{1}{2}} X v) = \|X D^{\frac{1}{2}} v\|^2 \geq 0,$$

  so $X^T D X$ is positive semidefinite and logistic regression is convex.
  - It becomes strictly convex if you add L2-regularization, making solution unique.

Lipschitz Continuity of Logistic Regression Gradient

- Logistic regression Hessian is

$$\begin{aligned}\nabla^2 f(w) &= \sum_{i=1}^n \underbrace{h(y_i w^T x^i)h(-y^i w^T x^i)}_{d_{ii}} x^i(x^i)^T \\ &\preceq 0.25 \sum_{i=1}^n x^i(x^i)^T \\ &= 0.25 X^T X.\end{aligned}$$

- In the second line we use that $h(\alpha) \in (0,1)$ and $h(-\alpha) = 1 - \alpha$.
  - This means that $d_{ii} \leq 0.25$.

- So for logistic regression, we can take $L = \frac{1}{4}\max\{\text{eig}(X^T X)\}$.

Why the gradient descent iteration?

- For a C^2 function, a variation on the multivariate Taylor expansion is that

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

  for any w and v (with u being some convex combination of w and v).

- If w and v are very close to each other, then we have

$$f(v) = f(w) + \nabla f(w)^T(v-w) + O(\|v-w\|^2),$$

  and the last term becomes negligible.

- Ignoring the last term, for a fixed $\|v-w\|$ I can minimize $f(v)$ by choosing $(v-w) \propto -\nabla f(w)$.
  - So if we're moving a small amount the optimal choice is gradient descent.

Descent Lemma for C^1 Functions

- Let ∇f be L-Lipschitz continuous, and define $g(\alpha) = f(x + \alpha z)$ for a scalar α.

$$f(y) = f(x) + \int_0^1 \nabla f(x + \alpha(y - x))^T (y - x) d\alpha \quad \text{(fund. thm. calc.)}$$

$$\text{(}\pm\text{ const.)} = f(x) + \nabla f(x)^T (y - x) + \int_0^1 (\nabla f(x + \alpha(y - x)) - \nabla f(x))^T (y - x) d\alpha$$

$$\text{(CS ineq.)} \leq f(x) + \nabla f(x)^T (y - x) + \int_0^1 \|\nabla f(x + \alpha(y - x)) - \nabla f(x)\| \|y - x\| d\alpha$$

$$\text{(Lipschitz)} \leq f(x) + \nabla f(x)^T (y - x) + \int_0^1 L\|x + \alpha(y - x) - x\| \|y - x\| d\alpha$$

$$\text{(homog.)} = f(x) + \nabla f(x)^T (y - x) + \int_0^1 L\alpha \|y - x\|^2 d\alpha$$

$$\left(\int_0^1 \alpha = \frac{1}{2}\right) = f(x) + \nabla f(x)^T (y - x) + \frac{L}{2}\|y - x\|^2.$$

Equivalent Conditions to Lipschitz Continuity of Gradient

- We said that Lipschitz continuity of the gradient

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

  is equivalent for C^2 functions to having

$$\nabla^2 f(w) \preceq LI.$$

- There are a lot of other equivalent definitions, see here:
  - `http://xingyuzhou.org/blog/notes/Lipschitz-gradient`.