CPSC 540: Machine Learning

Gradient Descent, Newton-like Methods

Mark Schmidt

University of British Columbia

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Admin

- Auditting/registration forms:
    - Submit them in class/help-session/tutorial this week.
    - Pick them up in the next class/help-session/tutorial.
    - Add/drop deadline is Tuesday.
- Tutorials: start this Friday (4:00 in DMP 110).
- Assignment 1 due January 16.
    - 1 late day to hand it in January 18.
    - 2 late days to hand it in January 23.

Last Time: MAP Estimation

- We showed that the loss plus regularizer framework

$$f(w) = \underbrace{\sum_{i=1}^{n} f_i(w)}_{\text{data-fitting term}} + \underbrace{\lambda g(w)}_{\text{regularizer}},$$

can arise from the MAP estimation principle applied to IID data,

$$w^* \in \underset{w \in \mathbb{R}^d}{\text{argmax}} \underbrace{p(w|y,X)}_{\text{posterior}} \equiv \underset{w \in \mathbb{R}^d}{\text{argmin}} - \underbrace{\sum_{i=1}^{n} \log p(y^i|x^i, w)}_{\text{log-likelihood}} - \underbrace{\log p(w)}_{\text{log-prior}}.$$

- Most common models arise from particular assumptions:
  - Gaussian likelihood $\rightarrow$ squared error.
  - Gaussian prior $\rightarrow$ L2-regularization.
  - Laplace likelihood $\rightarrow$ absolute error.
  - Sigmoid likelihood $\rightarrow$ logistic loss.

Last Time: Gaussian-Gaussian Model and L2-Regularized Least Squares

- Least squares corresponds to MLE under the assumption,

$$y^i \sim \mathcal{N}(w^T x^i, \sigma^2),$$

  where σ^2 is irrelevant.
- Why does σ^2 not affect sensitivity to outliers?
  - Scales all residuals by the same quantity (unlike switching norms).
- If we use a different σ_i^2 for each example, the σ_i^2 values would be relevant.
  - Leads to weighted least squares

- L2-regularized least squares corresponds to the assumption

$$y^i \sim \mathcal{N}(w^T x^i, \sigma^2), \quad w_j \sim \mathcal{N}(0, 1/\lambda),$$

  with $\sigma^2 = 1$.
- Here changing σ^2 changes solution, but it's equivalent to changing λ.

Last Time: Converting Absolute/Max Problems to Smooth/Constrained

- We turned non-smooth problems involving absolute values and maxes like

$$\underset{w\in\mathbb{R}^d}{\text{argmin}}\ \|Xw-y\|_1+\lambda\|w\|_1,$$

into smooth problems with linear constraints,

$$\underset{w\in\mathbb{R}^d, r\in\mathbb{R}^n, v\in\mathbb{R}^d}{\text{argmin}}\quad 1^Tr+\lambda 1^Tv, \quad \text{with} \quad r\geq Xw-y,\ r\geq y-Xw,\ v\geq w,\ v\geq -w.$$

- This is a linear objective and linear constraints: linear program.
- If we had an L2-regularizer or a squared error we would get a quadratic program.

Convex Sets and Functions

- Software like CVX can minimize many convex functions over convex sets.
  - Key property: all local minima are global minima for convex problems.

- We discussed proving sets are convex:
  - Show that for w for $v \in \mathcal{C}$, any convex combination u is in $\mathcal{C}$.
  - Show that the set is an intersection of convex sets.

- We discussed proving functions are convex:
  - Show that for w for $v \in \mathcal{C}$, $f(u)$ is below chord for any convex combination u.
  - Show that $\nabla^2 f(w)$ is positive semi-definite for all w.
  - Show that f is convex functions and operations that preserve convexity:
    - Non-negative scaling, sum, max, composition with affine map.

Strictly-Convex Functions

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

$$f(\theta w + (1-\theta)v) < \theta f(w) + (1-\theta)f(v), \quad 0 < \theta < 1 \qquad \text{(general)}$$

$$f(v) > f(w) + \nabla f(w)^T(v - w) \qquad \text{(differentiable)}$$

$$\nabla^2 f(w) \succ 0 \qquad \text{(twice-differentiable)}$$

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

- L2-regularized least squares has unique solution since we showed $\nabla^2 f(w) \succ 0$.

Outline

Gradient Descent

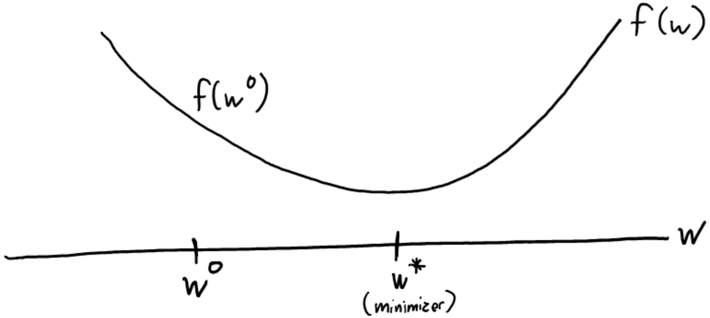
- Most ML objective functions can't be written as a linear system/program.
- But many of them yield differentiable and convex objective functions.
  - An example is logistic regression.

- We can minimize these functions using gradient descent:
  - Algorithm for finding a stationary point of a differentiable function.

- Gradient descent is an iterative optimization algorithm:
  - It starts with a "guess" w^0.
  - It uses w^0 to generate a better guess w^1.
  - It uses w^1 to generate a better guess w^2.
  - ...
  - The limit of w^t as t goes to ∞ has $\nabla f(w^t) = 0$.

Gradient Descent for Finding a Local Minimum

- Gradient descent is based on a simple observation:
  - Given parameters w, the direction of largest instantaneous decrease is $-\nabla f(w)$.



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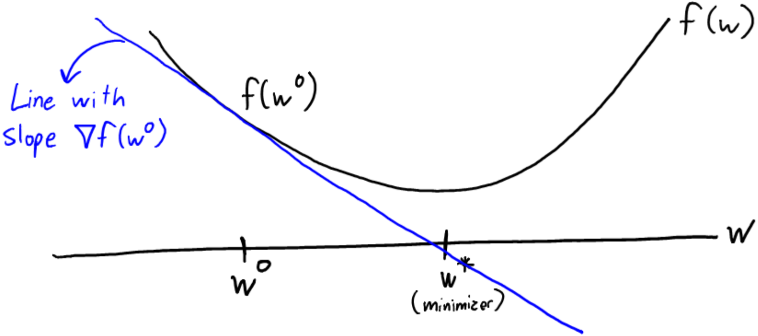

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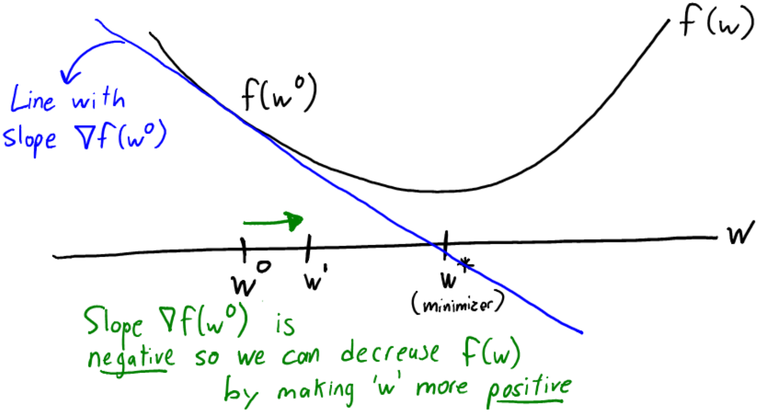

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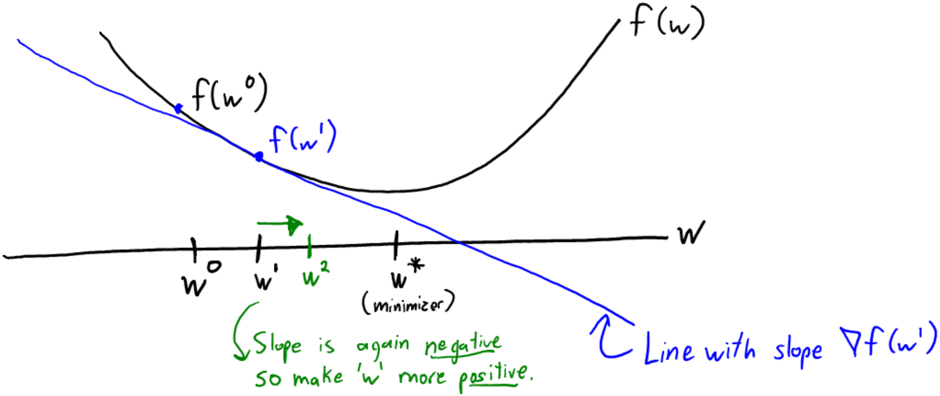

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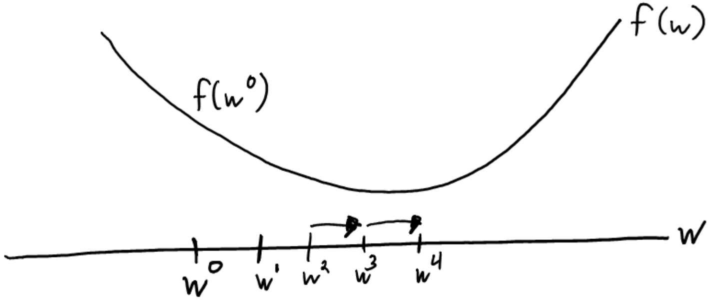

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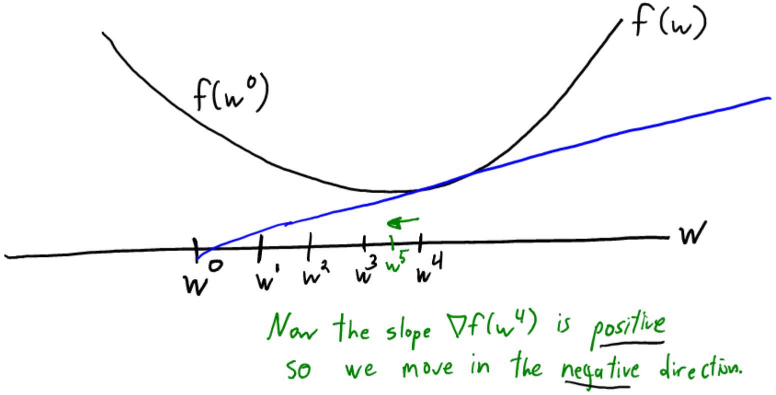
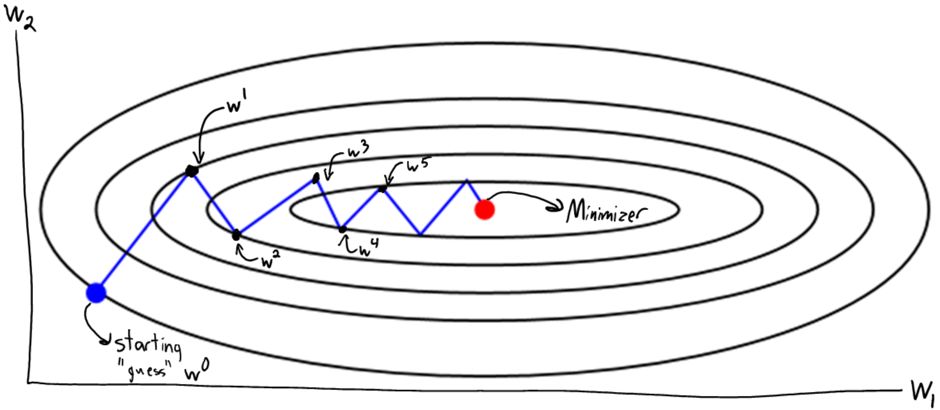


Gradient Descent for Finding a Local Minimum

- 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:
    $$w^{t+1} = w^t - \alpha_t \nabla f(w^t), \quad \text{for } t = 1, 2, 3, \dots$$
  - Stop if not making progress $\|\nabla f(w^t)\|$ is small.
- If α_t is small enough and $\nabla f(w^t) \neq 0$, guaranteed to decrease f.
- Under weak conditions, procedure converges to a stationary point.
  - If f is convex, converges to a global minimum.

Gradient Descent in 2D



Digression: Cost of L2-Regularizd Least Squares

- We've shown that L2-regularized least squares has the solution

$$w = (X^TX + \lambda I)^{-1}(X^Ty).$$

- With basic matrix multiplication, cost is dominated by:
  - $O(nd^2)$ to form X^TX.
  - $O(d^3)$ to solve the linear system.
    - Use "Cholesky" factorization because it's positive-definite.

- This is fine for $d = 5000$, but too slow for $d = 1,000,000$.

Cost of L2-Regularizd Least Squares

- Would it make any sense to use gradient descent instead?
- The gradient descent iteration would be

$$w^{t+1} = w^t - \alpha_t \nabla f(w^t), \quad \text{where} \quad \nabla f(w^t) = X^T(Xw) - X^T y,$$

  and the cost of each iteration is $O(nd)$, due to the multiplications by X and X^T.
- So t iterations of gradient descent cost $O(ndt)$.
- Gradient descent can be faster if t is not too big:
  - $O(ndt)$ is less than $O(nd^2 + d^3)$ when $(t < \max\{d, d^2/n\})$.

Iteration Complexity

- How many iterations of gradient descent do we need?

- Let w^* be the optimal solution and ϵ be the accuracy that we want.
- We want to know the smallest number of iteration t that guarantees

$$f(w^t) - f(w^*) \leq \epsilon,$$

which is called the iteration complexity.

- Think of $1/\epsilon$ as "number of digits of accuracy" I want.
  - We want to grow slowly with $1/\epsilon$.

Strong-Smoothness and Strong-Convexity Assumptions

- We'll assume f is twice-differentiable and satisfies two assumptions on $\nabla^2 f(w)$:
    - Strong smoothness means that eigenvalues of $\nabla^2 f(w)$ are at most a $L < \infty$
    - Strong convexity means that the eigenvalues of $\nabla^2 f(w)$ are at least $\mu > 0$.
- We denote these assumptions by

$$\mu I \preceq \nabla^2 f(w) \preceq LI, \quad \forall w.$$

- Equivalently, for all w and v we have

$$\mu \|v\|^2 \leq v^T \nabla^2 f(w) v \leq L\|v\|^2.$$

- Note that strong-convexity $\Rightarrow$ strict-convexity $\Rightarrow$ convexity:

$$\nabla^2 f(w) \succeq \mu I \succ 0 \succeq 0.$$

    - Strongly-convex functions on closed convex sets have exactly 1 minimizer.
- For L2-regularized least squares we have (see bonus slide).

$$L = \max\{\text{eig}(X^T X)\} + \lambda, \quad \mu = \min\{\text{eig}(X^T X)\} + \lambda,$$

- We'll use different notation for optimization algorithms:
  - For optimization algorithms our variables will be x instead of w.
- So the the gradient descent iteration will be

$$x^{t+1} = x^t - \alpha_t \nabla f(x^t).$$

Convergence Rate of Gradient Descent

- For our first result we're assuming:
  - Function f is L-strongly smooth and μ-strongly convex,
$$\mu I \preceq \nabla^2 f(x) \preceq LI.$$
  - We use a step-size of $\alpha_t = 1/L$ (makes proof easier).
- We'll show that gradient descent has a linear convergence rate,
$$f(x^t) - f(x^*) = O(\rho^t) \quad \text{for} \quad \rho < 1.$$
  which is sometimes called "geometric" or "exponential" convergence rate.
- Implies that iteration complexity is $t = O(\log(1/\epsilon))$ iterations (see bonus slide).
  - This is good! We're growing with logarithm of "digits of accuracy".

Implication of Strong-Smoothness

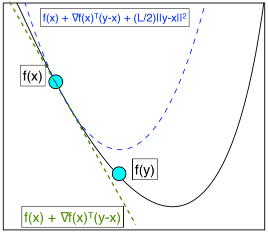
- From Taylor's theorem, for any x and y there is a z such that

$$f(y) = f(x) + \nabla f(x)^T(y-x) + \frac{1}{2}(y-x)^T\nabla^2 f(z)(y-x)$$

- By strong-smoothness, $v^T\nabla^2 f(z)v \leq L\|v\|^2$ for any v and z.

$$f(y) \leq f(x) + \nabla f(x)^T(y-x) + \frac{L}{2}\|y-x\|^2$$

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



Implication of Strong-Smoothness

- The quadratic upper-bound from strong-smoothness at x^t is:

$$f(y) \leq f(x^t) + \nabla f(x^t)^T (y - x^t) + \frac{L}{2}\|y - x^t\|^2$$

- If we set x^{t+1} to minimize the right side in terms of y, we get

$$x^{t+1} = x^t - \frac{1}{L}\nabla f(x^t),$$

so gradient descent with $\alpha_t = 1/L$ minimizes this quadratic upper bound.

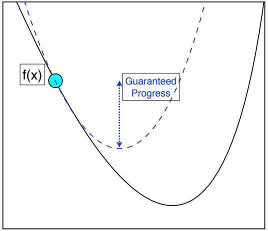
- Plugging in x^{t+1} gives:

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

Implication of Strong-Smoothness

- We've derived a bound on guaranteed progress at iteration t:

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



- If gradient is non-zero, guaranteed to decrease objective.
- Amount we decrease grows with the size of the gradient.
- This bound holds for any strongly-smooth function (including non-convex).

Implication of Strong-Convexity

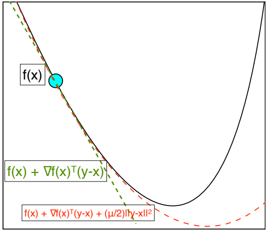
- From Taylor's theorem, for any x and y there is a z such that

$$f(y) = f(x) + \nabla f(x)^T(y-x) + \frac{1}{2}(y-x)^T \nabla^2 f(z)(y-x)$$

- By strong-convexity, $v^T \nabla^2 f(z) v \geq \mu \|v\|^2$ for any v and z.

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

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



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

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

- Minimize both sides in terms of y gives

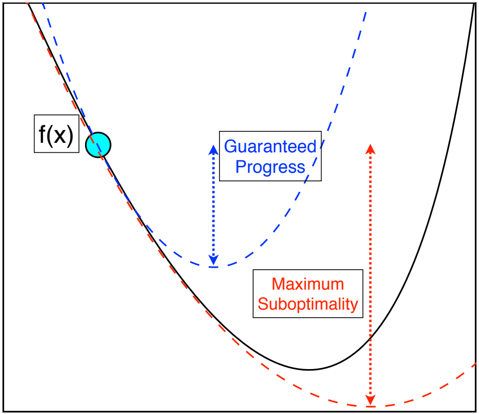
$$f(x^*) \geq f(x) - \frac{1}{2\mu}\|\nabla f(x)\|^2.$$

- This upper bounds how far where we are from the solution.

Combining Strong-Smoothness and Strong-Convexity

- Given x^t, we have bounds on $f(x^{t+1})$ and $f(x^*)$:

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



Combining Strong-Smoothness and Strong-Convexity

- Our bound on guaranteed progress:

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

- Re-arranging our bound on "distance to go":

$$-\frac{1}{2}\|\nabla f(x^t)\|^2 \leq -\mu[f(x^t) - f(x^*)].$$

- Use "distance to go" bound in guaranteed progress bound:

$$f(x^{t+1}) \leq f(x^t) - \frac{1}{L}\left(\mu[f(x^t) - f(x^*)]\right).$$

- Subtract $f(x^*)$ from both sides and factor:

$$\begin{aligned} f(x^{t+1}) - f(x^*) &\leq f(x^t) - f(x^*) - \frac{\mu}{L}[f(x^t) - f(x^*)] \\ &= \left(1 - \frac{\mu}{L}\right)[f(x^t) - f(x^*)]. \end{aligned}$$

Combining Strong-Smoothness and Strong-Convexity

- We've shown that

$$f(x^t) - f(x^*) \leq \left(1 - \frac{\mu}{L}\right)[f(x^{t-1}) - f(x^*)].$$

- Applying this recursively:

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

- Since $\mu \leq L$, we have $(1 - \mu/L) < 1$, and we've shown linear convergence rate:
  - We have $f(x^t) - f(x^*) = O(\rho^t)$ with $\rho = (1 - \mu/L)$.

Discussion of Linear Convergence Rate

- We've shown that gradient descent under certain settings has

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

- This is a non-asymptotic linear convergence rate:
  - It holds on iteration 1, there is no "limit as $t \to \infty$" as in classic results.

- The number L/μ is called the condition number of f.
  - For least squares it's the "matrix condition number" of the Hessian,

$$L/\mu = \text{cond}(\nabla^2 f(w)) = \text{cond}(X^T X).$$

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

- Consider a fixed condition number and accuracy ϵ:
  - There is a dimension d beyond which gradient descent is faster than linear algebra.

Outline

Gradient Descent for Logistic Regression

- Is gradient descent useful beyond least squares?
  - Yes: these types of methods tends to work well for a variety of models.

- For example, logistic regression is among most-used models,

$$f(w) = \sum_{i=1}^{n} \log(1 + \exp(-y^i w^T x^i)) + \frac{\lambda}{2}\|w\|^2.$$

- We can't even 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.
- Let's compute the cost of minimizing f with gradient descent.

Gradient Descent for Logistic Regression

- To apply gradient descent, we'll need the gradient.
- Can we write logistic loss,

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

  in matrix notation?
- A "Matlab-y" way:

$$f(w) = 1^T \log(1 + \exp(-YXw)),$$

  where we're using "element-wise" versions of $\log$ and $\exp$ function.

Gradient Descent for Logistic Regression

- To write in matrix notation without defining new operators we can use

$$f(w) = 1^T v + \frac{\lambda}{2}\|w\|^2$$

where $v_i = \log(1 + \exp(-y^i w^T x^i))$.

- With some tedious manipulations we get

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

where $r_i = -y^i \sigma(-y^i w^T x^i)$.

- We know 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).

Gradient Descent for Logistic Regression

- The gradient has the form

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

  where $r_i = -y^i \sigma(-y^i w^T x^i)$.

- The cost of computing the gradient is dominated by:
  1. Computing Xw to get the n values $w^T x^i$.
  2. Computing $X^T r$ to get the gradient.

- These are matrix-vector multiplications, so the cost is $O(nd)$.
  - So iteration cost is the same as least squares.

Gradient Descent for Logistic Regression

- With some more tedious manipulations we get

$$\nabla^2 f(w) = X^T D X + \lambda I$$

where D is a diagonal matrix with $d_{ii} = \sigma(y_i w^T x^i)\sigma(-y^i w^T x^i)$.
  - The $f(Ax)$ structure leads to a $X^T D X$ Hessian structure.

- This implies the function is strongly-smooth and strongly-convex with

$$L = \frac{1}{4}\max\{\text{eig}(X^T X)\} + \lambda, \quad \mu = \lambda.$$

(1/4 is the maximum value of d_{ii} and the minimum converges to 0.)

Gradient Descent and Logistic Regression

- Condition number L/μ forL2-regularized least squares was

$$\frac{\max\{\text{eig}(X^TX)\}+\lambda}{\min\{\text{eig}(X^TX)\}+\lambda},$$

while for logistic regression it is

$$\frac{\frac{1}{4}\max\{\text{eig}(X^TX)\}+\lambda}{\lambda}.$$

- So number of iterations for logistic regression is similar to least squares.
- Also, in both cases number of iterations gets smaller as λ increases.

- For fixed condition number, total cost is $O(nd\log(1/\epsilon))$.
- Common approach in many software packages is called IRLS:
  - A Newton-like method that takes $O(nd^2 + d^3)$ per iteration.

Outline

Gradient Method: Practical Issues

- In practice, you should never use $\alpha = 1/L$.
  - Often you don't know L, or it's expensive to compute.
  - The "local" L may be much smaller than the "global" L.
  - You might also get a "lucky" direction that makes much more progress.
    - In practice, you can often take much bigger steps.
- One practical option is an adaptive step-size:
  - Start with a small guess for L (like $L = 1$).
  - Double L if the progress inequality in the proof is not satisfied:

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

  - This often gives you a much smaller L: gives bigger steps and faster progress.
  - But with this strategy, step-size never increases.

Gradient Method: Practical Issues

- In practice, you should never use $\alpha = 1/L$.
  - Often you don't know L, or it's expensive to compute.
  - Even if you did, the "local" L may be much smaller than the "global" L.
  - You might also get a "lucky" direction that makes much more progress.
    - In practice, you can often take much bigger steps.
- Another practical option is a backtracking line-search:
  - On *each* iteration, start with a large step-size α.
  - Decrease α if the Armijo condition is not satisfied,

$$f(x^{t+1}) \leq f(x^t) - \alpha\gamma\|\nabla f(x^t)\|^2 \quad \text{for} \quad \gamma \in (0, 1/2].$$

(often $\gamma = 10^{-4}$)

  - Tends to work well if you use interpolation to select initial/decreasing α values.
    - Good codes often only need around 1 value of α per iteration.
  - Even more fancy line-search: Wolfe conditions (make sure α is not too small).

Gradient Method: Practical Issues

- Gradient descent codes require you to write objective/gradient code:

```
function [nll,g,H] = objective(w,X,y,lambda)
yXw = y.*(X*w);

% Function value
nll = sum(log(1+exp(-yXw))) + (lambda/2)*(w'*w);

% Gradient
sigmoid = 1./(1+exp(-yXw));
g = -X'*(y.*(1-sigmoid)) + lambda*w;
```

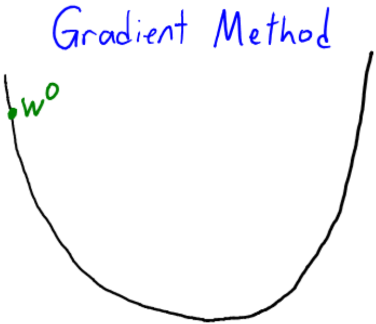
- Make sure to check your derivative code:
  - Numerical approximation to partial derivative:

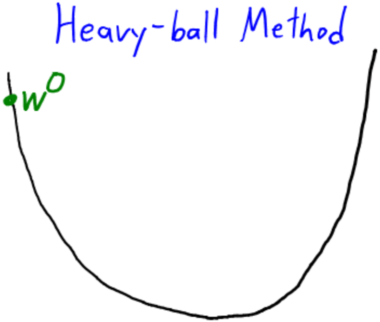
$$\nabla_i f(x) \approx \frac{f(x+\delta e_i) - f(x)}{\delta}$$

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

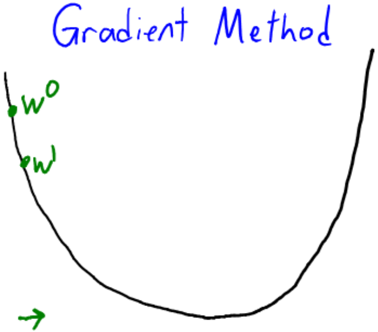
$$\nabla f(x)^T d \approx \frac{f(x+\delta d) - f(x)}{\delta}$$

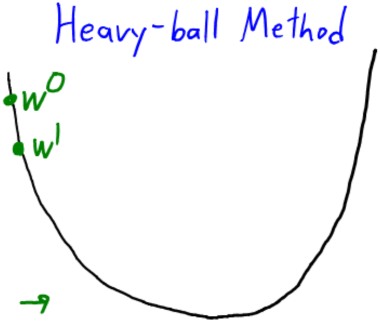
Heavy-Ball Method Method





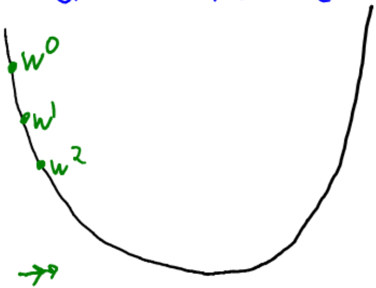
Heavy-Ball Method Method



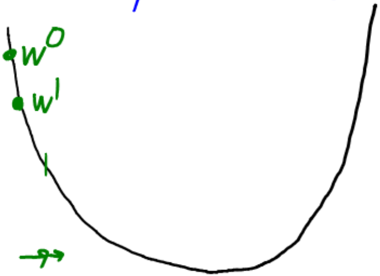


Heavy-Ball Method Method

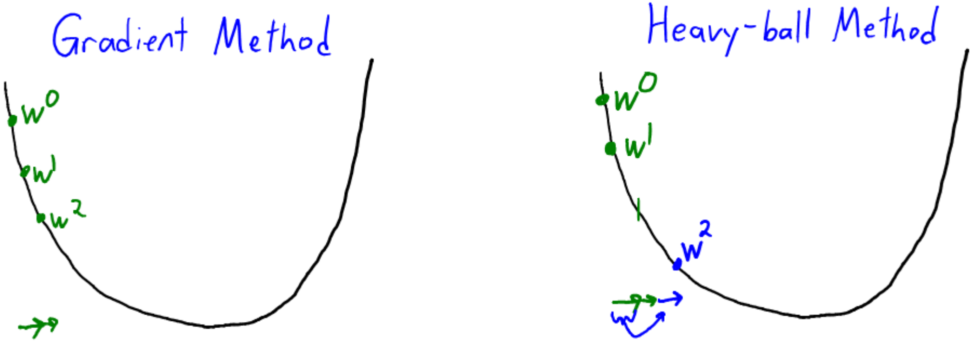
Gradient Method



Heavy-ball Method



Heavy-Ball Method Method



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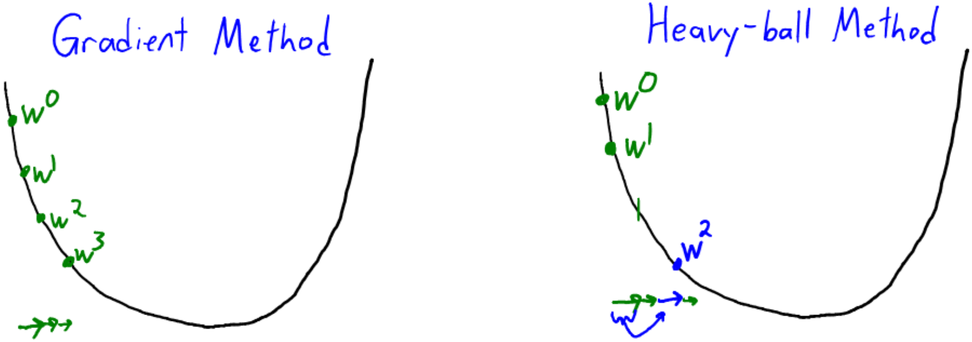

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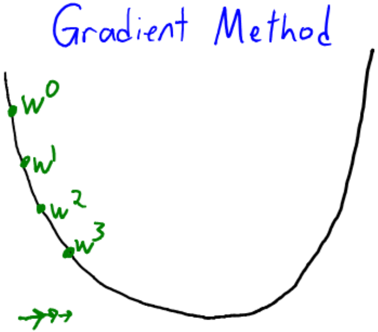

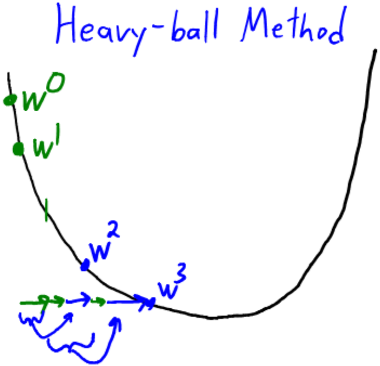

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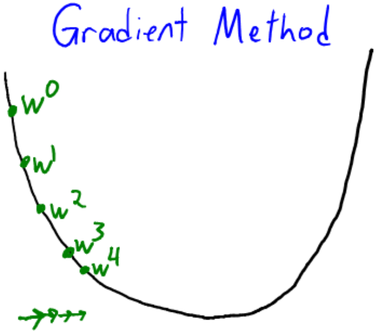
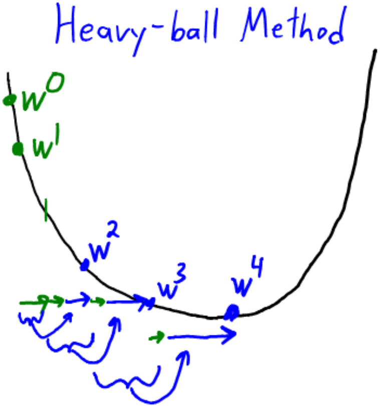
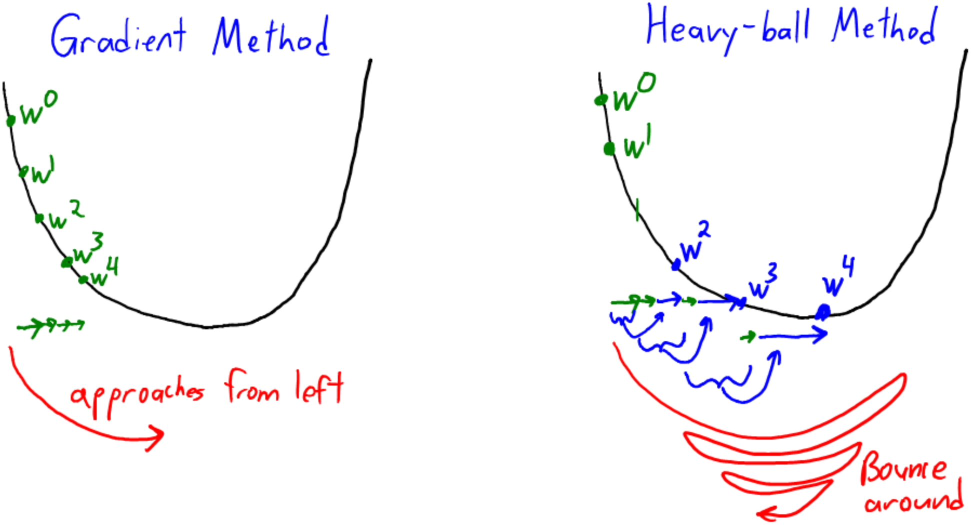




Heavy-Ball Method Method



Heavy-Ball Method and Variations

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

$$x^{t+1} = x^t - \alpha_t \nabla f(x^t) + \beta_t (x^t - x^{t-1}).$$

- Faster rate for strictly-convex quadratic functions with appropriate α_t and β_t.
  - Depends on $\sqrt{L/\mu}$ instead of L/μ.
  - With the optimal α_t and β_t, we obtain conjugate gradient.
    - "Optimal" rate for strongly-convex quadratics in "high-dimensional setting".

- Variation is Nesterov's accelerated gradient method for strongly-smooth f,

$$\begin{aligned} x^{t+1} &= y^t - \alpha_t \nabla f(y^t), \\ y^{t+1} &= x^t + \beta_t (x^{t+1} - x^t), \end{aligned}$$

- Rate depends on $\sqrt{L/\mu}$ for strongly-convex f for appropriate α_t and β_t.

Newton's Method

- Newton's method is a second-order strategy.

  (also called IRLS for functions of the form $f(Ax)$)

- Modern form uses the update

$$x^{t+1} = x^t - \alpha_t d^t,$$

  where d^t is a solution to the system

$$\nabla^2 f(x^t) d^t = \nabla f(x^t).$$

  (Assumes $\nabla^2 f(x^t) \succ 0$)

- Equivalent to minimizing the quadratic approximation:

$$f(y) \approx f(x^t) + \nabla f(x^t)^T (y - x^t) + \frac{1}{2\alpha_t}(y - x^t)\nabla^2 f(x^t)(y - x^t).$$

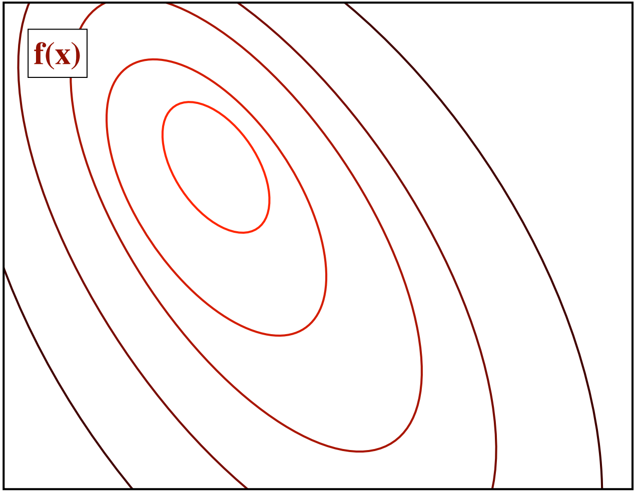
- We can generalize the Armijo condition to

$$f(x^{t+1}) \leq f(x^t) + \gamma\alpha\nabla f(x^t)^T d^t.$$

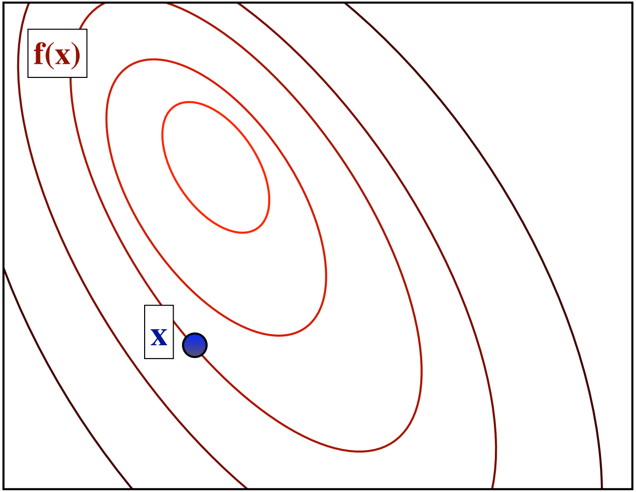
- Has a natural step length of $\alpha = 1$.

  (always accepted when close to a minimizer)

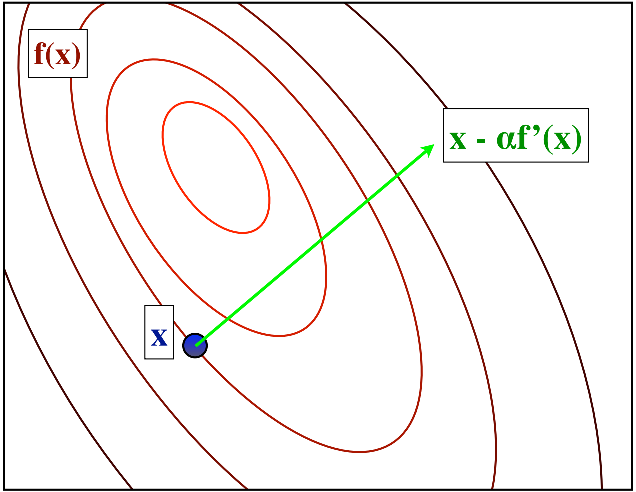
Newton's Method



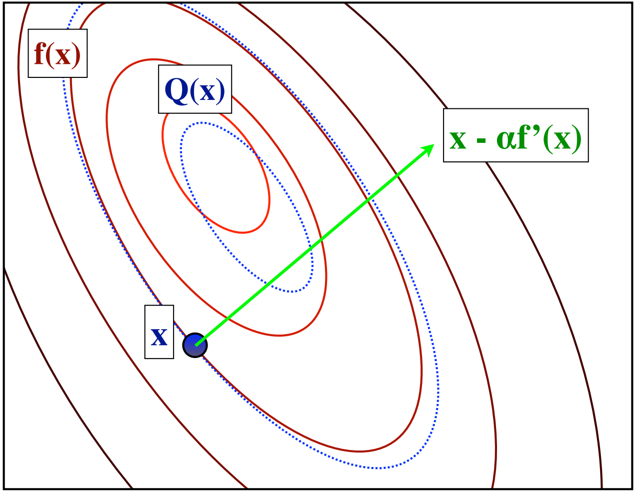
Newton's Method



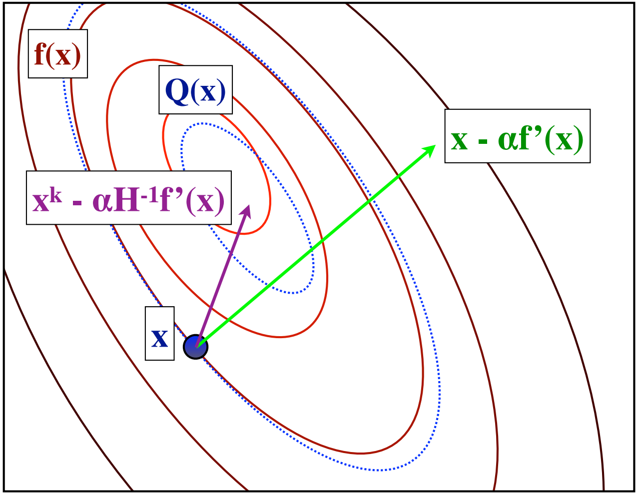
Newton's Method



Newton's Method



Newton's Method



Convergence Rate of Newton's Method

- If $\mu I \preceq \nabla^2 f(x) \preceq LI$ and $\nabla^2 f(x)$ is Lipschitz-continuous, then close to x^* Newton's method has local superlinear convergence:

$$f(x^{t+1}) - f(x^*) \leq \rho_t[f(x^t) - f(x^*)],$$

  with $\lim_{t \to \infty} \rho_t = 0$.
- Converges very fast, use it if you can!
- But Newton's method is expensive if dimension d is large:
  - Requires solving $\nabla^2 f(x^t)d^t = \nabla f(x^t)$.
- "Cubic regularization" of Newton's method gives global convergence rates.

Practical Approximations to Newton's Method

- Practical Newton-like methods (that can be applied to large-scale problems):
  1. Diagonal approximation:
     - Approximate Hessian by a diagonal matrix D (cheap to store/invert).
     - A common choice is $d_{ii} = \nabla^2_{ii} f(x^t)$.
     - This sometimes helps, often doesn't.
  2. Limited-memory quasi-Newton approximation:
     - Approximates Hessian by a diagonal plus low-rank approximation B^t,
       $$B^t = D + UV^T,$$
       which supports fast multiplication/inversion.
     - Based on "quasi-Newton" equations which use differences in gradient values.
       $$(\nabla f(x^t) - \nabla f(x^{t-1})) = B^t(x^t - x^{t-1}).$$
     - A common choice is L-BFGS.

Practical Approximations to Newton's Method

- Practical Newton-like methods (that can be applied to large-scale problems):
  1. Barzilai-Borwein approximation:
     - Approximates Hessian by the identity matrix (as in gradient descent).
     - But chooses step-size based on least squares solution to quasi-Newton equations.

$$\alpha_t = -\alpha_t \frac{v^T \nabla f(w)}{\|v\|^2}, \quad \text{where} \quad v = \nabla f(x^t) - \nabla f(x^{t-1}).$$

     - Works better than it deserves to (*findMind.m* from CPSC 340).
     - We don't understand why it works so well.
  2. Hessian-free Newton:
     - Uses conjugate gradient to approximately solve Newton system.
     - Requires Hessian-vector products, but these cost same as gradient.
     - If you're lazy, you can numerically approximate them using

$$\nabla^2 f(x^t) d \approx \frac{\nabla f(x^t + \delta d) - \nabla f(x^t)}{\delta}.$$

     - If f is analytic, can compute exactly by evaluating gradient with complex numbers.

(look up "complex-step derivative")

- A related appraoch to the above is non-linear conjugate gradient.

Numerical Comparison with minFunc

Result after 25 evaluations of limited-memory solvers on 2D rosenbrock:

x1 = 0.0000, x2 = 0.0000 (starting point)
x1 = 1.0000, x2 = 1.0000 (optimal solution)

x1 = 0.3654, x2 = 0.1230 (minFunc with gradient descent)
x1 = 0.8756, x2 = 0.7661 (minFunc with Barzilai-Borwein)
x1 = 0.5840, x2 = 0.3169 (minFunc with Hessian-free Newton)
x1 = 0.7478, x2 = 0.5559 (minFunc with preconditioned Hessian-free Newton)
x1 = 1.0010, x2 = 1.0020 (minFunc with non-linear conjugate gradient)
x1 = 1.0000, x2 = 1.0000 (minFunc with limited-memory BFGS - default)

Summary

- Gradient descent is findins stationary point of differentiable f.
- Iteration complexity measures number of terations to reach accuracy ϵ.
- Linear convergence rate is achieve by gradident descent.
- Faster first-order methods like Nesterov and Newton-like methods.

- Next time: is using L1-regularization as easy as using L2-regularization?

Bonus Slide: Constants for Least Squares

- Consider least squares: $f(x) = \frac{1}{2}\|Ax - b\|^2$

What are 'L' and 'μ' such that $\mu I \preceq \nabla^2 f(x) \preceq LI$?

Note that $\nabla^2 f(x) = A^TA$, and since it's symmetric we can use spectral decomposition:

$$A^TA = \sum_{j=1}^{d} \lambda_j q_j q_j^T \text{ where } q_j^T q_j = 1 \text{ and } q_i^T q_j = 0 \text{ for } i \neq j. \quad (\text{Assume } \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d)$$

We can write any y as linear combination of orthogonal basis, $y = \alpha_1 q_1 + \alpha_2 q_2 + \cdots + \alpha_d q_d$.

So we have $y^T \nabla^2 f(x) y = y^T A^T A y = y^T \left(\sum_{j=1}^{d} \lambda_j q_j q_j^T\right) y = \sum_{j=1}^{d} \lambda_j \underbrace{y^T q_j}_{=\alpha_j} \underbrace{q_j^T y} = \sum_{j=1}^{d} \lambda_j \alpha_j^2$

Note that we can assume $\|y\| = 1$ or $y^T y = \sum_{j=1}^{d} \alpha_j^2 = 1$.

So $y^T \nabla^2 f(x) y$ is maximized when $\alpha_1^2 = 1$ and minimized when $\alpha_d^2 = 1$, giving $L = \lambda_1 = \max(\text{eig}(A^TA))$ and $\mu = \lambda_n = \min(\text{eig}(A^TA))$

Bonus Slide: Rates vs. Number of Iterations

- If we have
$$f(w^t) - f(w^*) = \epsilon = O(\rho^t),$$
this means $\epsilon \leq \kappa\rho^t$ for some κ for large t or
$$\log(\epsilon) \leq \log(\kappa\rho^t) = \log(\kappa) + t\log(\rho),$$
or
$$t \geq \log(\epsilon)/\log(\rho) - \text{constant},$$
or that it holds for any
$$t \geq O(\log(1/\epsilon)) \quad \text{since} \quad \rho < 1.$$
- Often ρ has the form $(1 - 1/\kappa)$, so if we use $(1 - 1/\kappa) \leq \exp(-\kappa)$ we get
$$t \geq O(\kappa\log(1/\epsilon)).$$

Bonus Slide: Multivariate Chain Rule in Matrix Notation

- 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

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

Bonus Slide: Convergence of Gradient Descent

- We can show convergence of gradient descent without strong convexity.