CPSC 340: Machine Learning and Data Mining

Gradient Descent

Fall 2017

Admin

- We will have tutorials on non-holiday days this week.

- Assignment 2 is due Friday.
  - 1 late day to hand it in on Monday, 2 for Wednesday.
  - The "imread" function is in PyPlot (not Images.jl), weird error in findMin.jl (fixed in a2.zip).
- Assignment 1 marks are up.
  - If you have questions, see "Assignment 1 Marking Thread" on Piazza.

- Extra office hours:
  - 2 TAs on the Thursday 2-3pm office hours when assignments are due.
  - Extra office hours this Friday at 1-2 (Siyuan at Table 2).
  - Extra instructor office hours on October 19th 4pm (ICICS 246).

- Midterm details:
  - In class October 20th (55 minutes).
  - 1 page double-sided cheat sheet.
  - Previous midterms posted on Piazza.
  - Short-answer questions on "non-bonus" (white) slides.
  - Calculation questions will focus on assignment topics.
  - Topics only appearing in L14 will treated as "bonus".

Last Week: Linear Regression

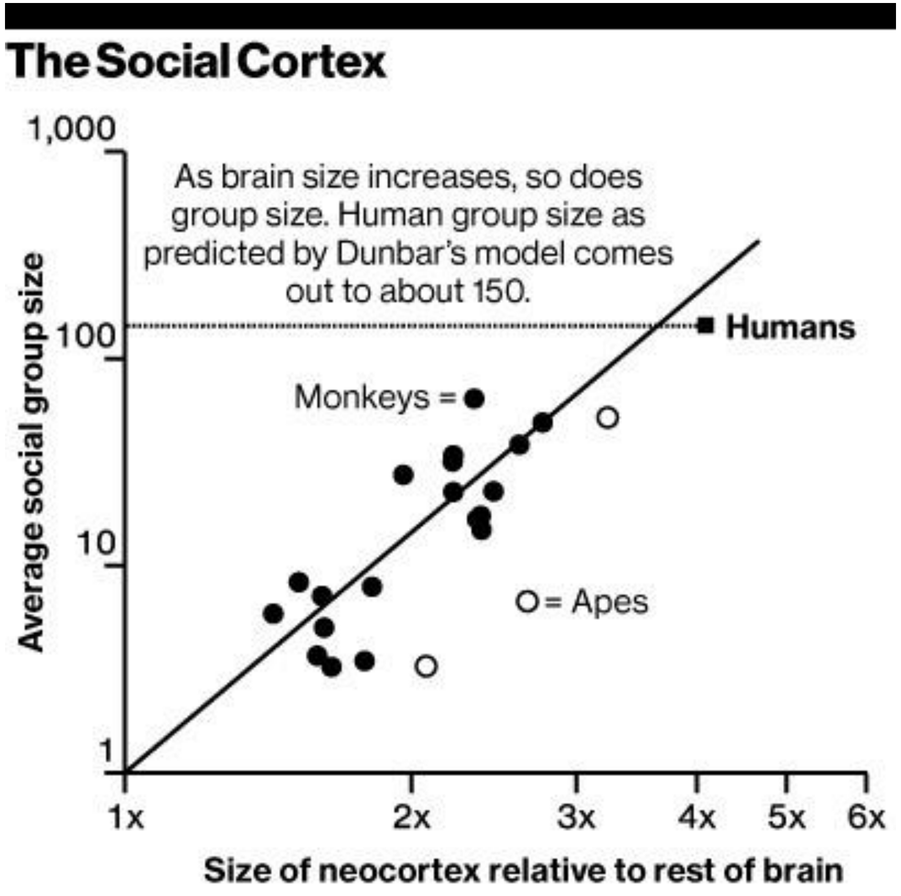
- We discussed linear models:

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id}$$
$$= \sum_{j=1}^{d} w_j x_{ij} = w^T x_i$$

- "Multiply feature x_{ij} by weight w_j, add them to get $\hat{y}_i$".
- We discussed squared error function:

$$f(w) = \frac{1}{2} \sum_{i=1}^{n} (\underbrace{w^T x_i}_{\text{Predicted value}} - \underbrace{y_i}_{\text{True value}})^2$$

- Interactive demo:
  - http://setosa.io/ev/ordinary-least-squares-regression



DATA: THE SOCIAL BRAIN HYPOTHESIS, DUNBAR 1998

To predict on test case $\tilde{x}_i$
use $\hat{y}_i = w^T \tilde{x}_i$

http://www.bloomberg.com/news/articles/2013-01-10/the-dunbar-number-from-the-guru-of-social-networks

Motivation: Large-Scale Least Squares

- Normal equations find 'w' with ∇ f(w) = 0 in O(nd² + d³) time.

$$\underbrace{\underbrace{(X^TX)}_{\substack{O(nd^2)\\ \text{(matrix multiply)}}} w = \underbrace{X^Ty}_{\substack{O(nd)\\ \text{(matrix-vector)}}}}_{}$$

→ Solving a $d \times d$ system is $O(d^3)$

  – Very slow if 'd' is large.

- Alternative when 'd' is large is gradient descent methods.
  – Probably the most important class of algorithms in machine learning.

Gradient Descent for Finding a Local Minimum

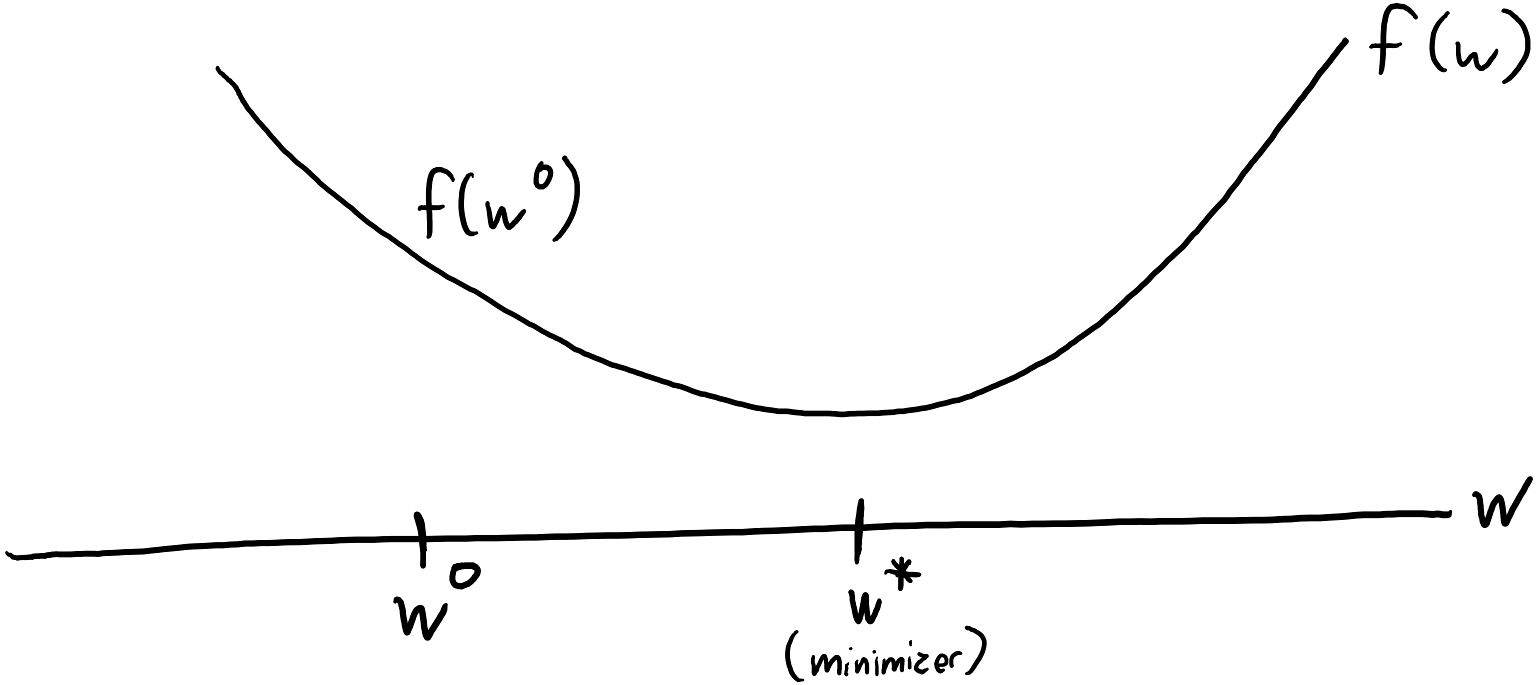
- Gradient descent is an iterative optimization algorithm:
  - It starts with a "guess" w^0.
  - It uses the gradient $\nabla f(w^0)$ to generate a better guess w^1.
  - It uses the gradient $\nabla f(w^1)$ to generate a better guess w^2.
  - It uses the gradient $\nabla f(w^2)$ to generate a better guess w^3.

    …
  - The limit of w^t as 't' goes to ∞ has $\nabla f(w^t) = 0$.

- It converges to the global optimum if 'f' is convex.

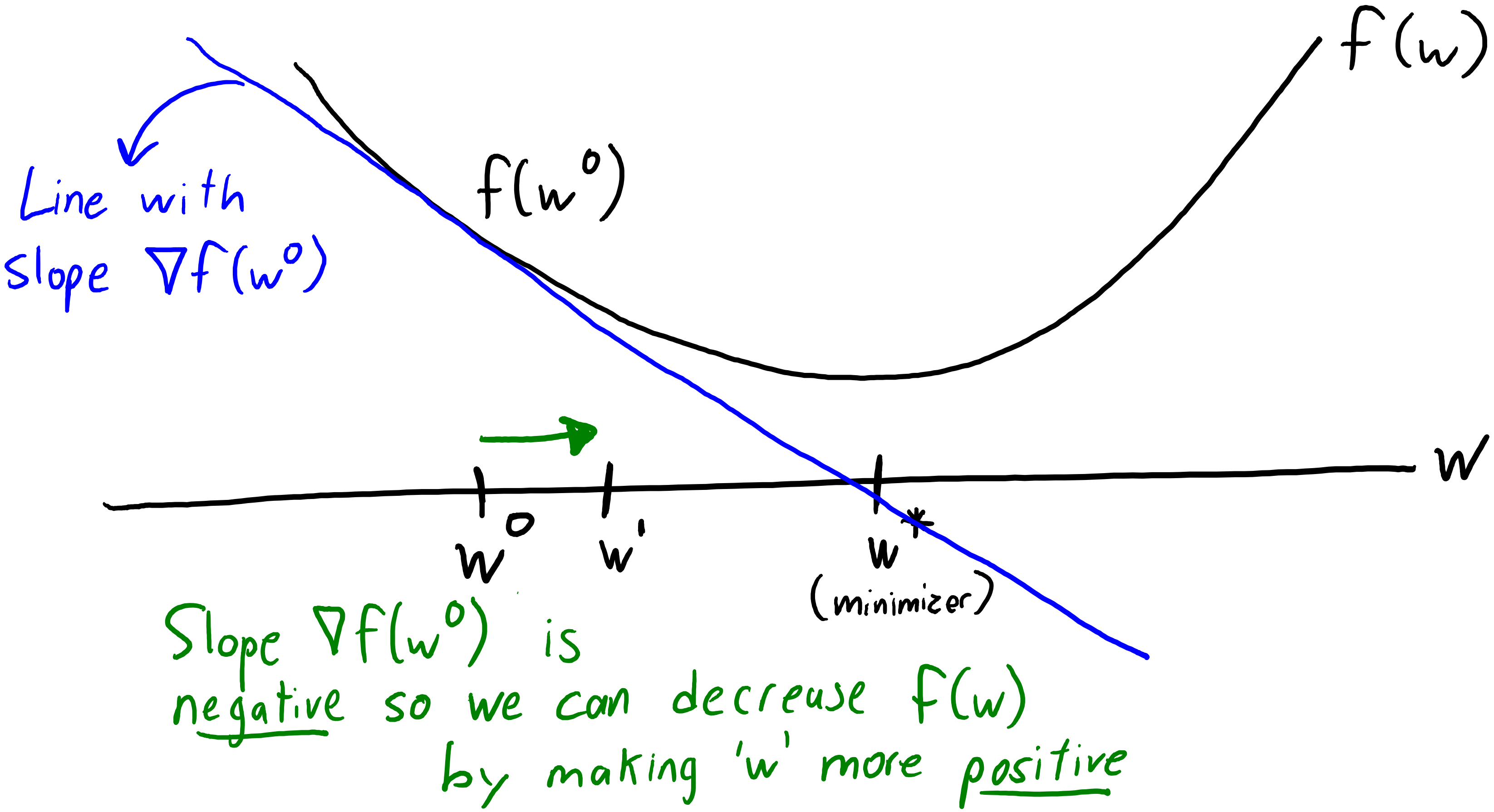
Gradient Descent for Finding a Local Minimum

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



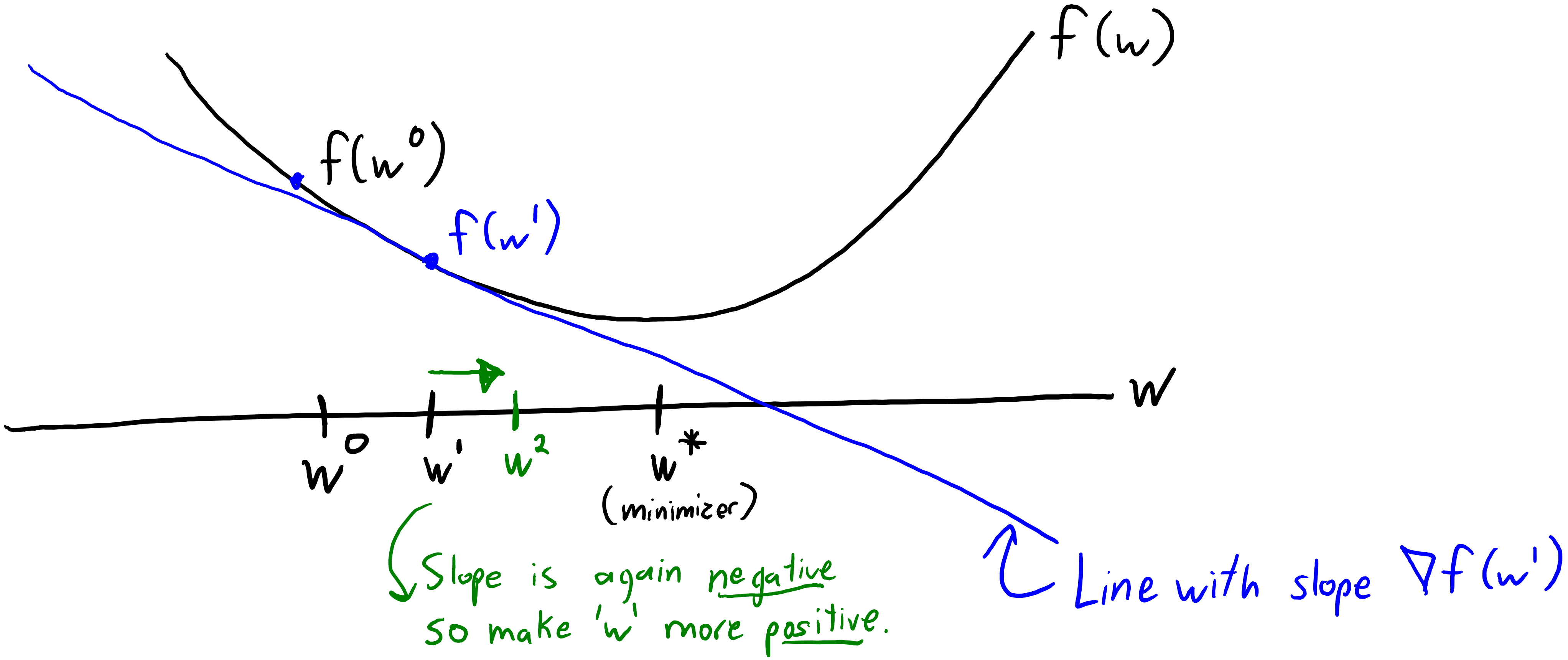
Gradient Descent for Finding a Local Minimum

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



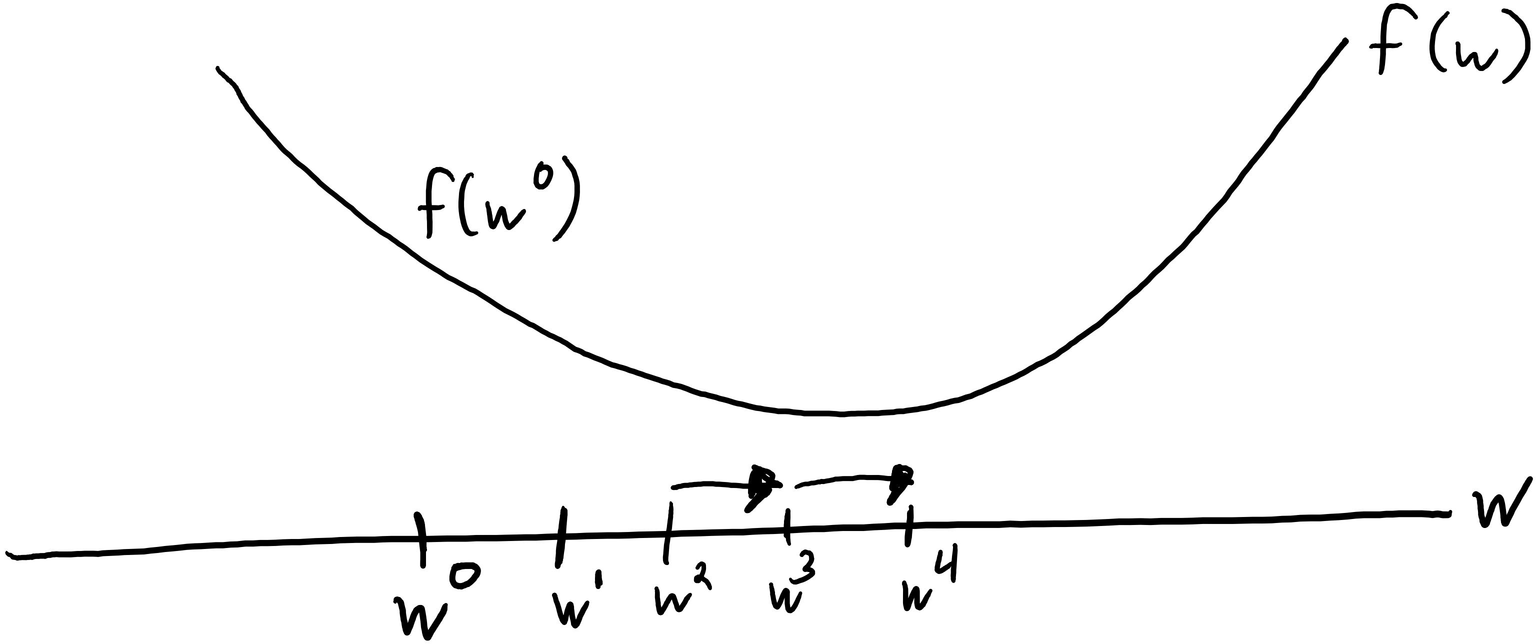
Gradient Descent for Finding a Local Minimum

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



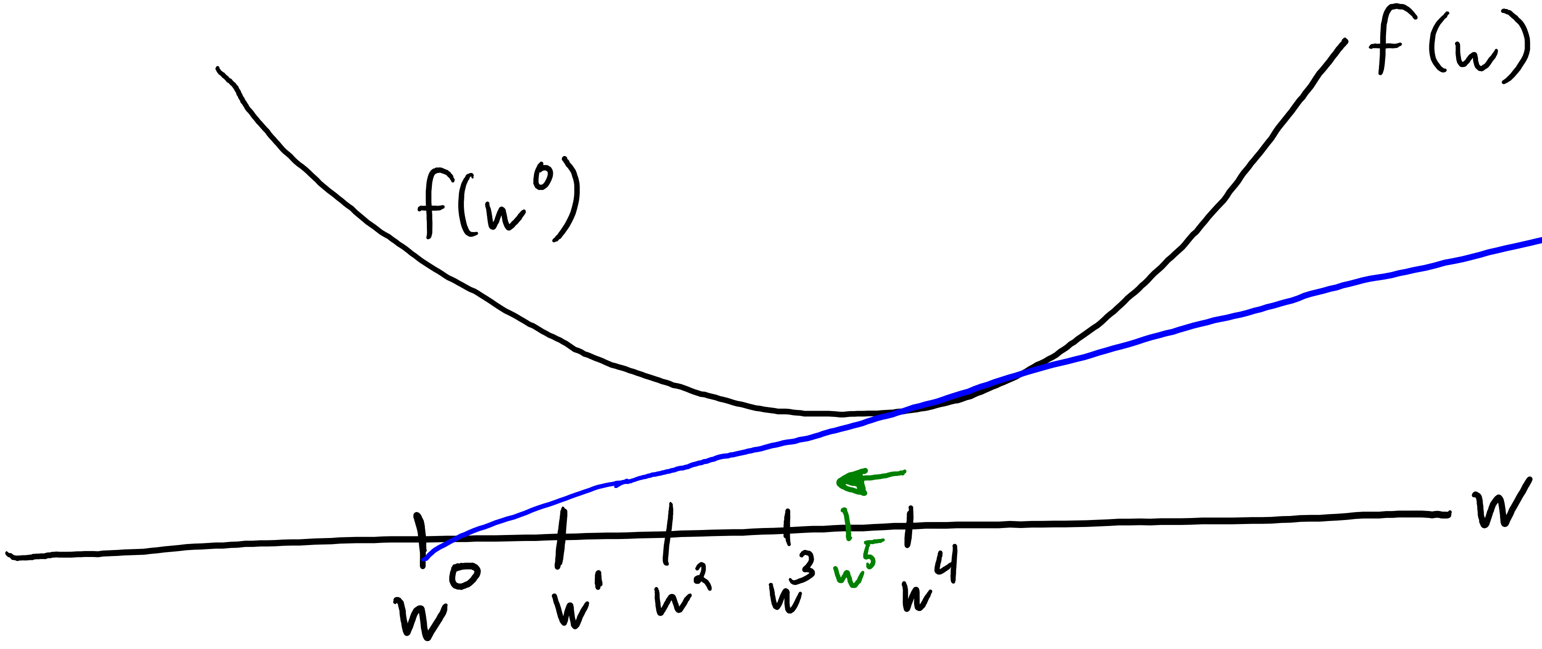
Gradient Descent for Finding a Local Minimum

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



Gradient Descent for Finding a Local Minimum

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



Now the slope $\nabla f(w^4)$ is positive so we move in the negative direction.

Gradient Descent for Finding a Local Minimum

– We start with some initial guess, w^0.

– Generate new guess by moving in the negative gradient direction:

$$w^1 = w^0 - \alpha^0 \nabla f(w^0)$$

- This decreases 'f' if the "step size" α^0 is small enough.
- Usually, we decrease α^0 if it increases 'f' (see "findMin.jl").

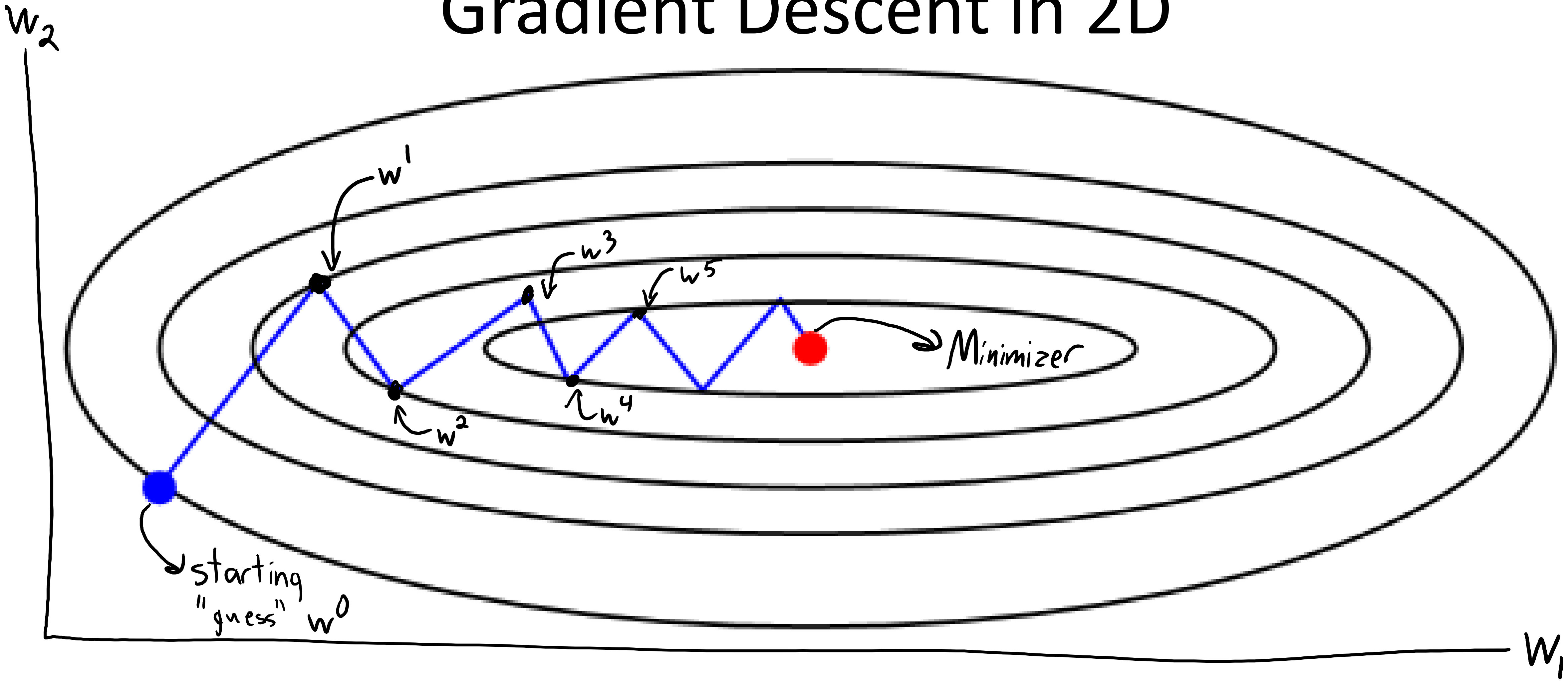
– Repeat to successively refine the guess:

$$w^{t+1} = w^t - \alpha^t \nabla f(w^t) \quad \text{for } t = 1, 2, 3, \dots$$

– Stop if not making progress or $\underbrace{\|\nabla f(w^t)\| \leq \epsilon}_{\text{Approximate local minimum}}$

ϵ → Some small scalar.

Gradient Descent in 2D



- Under weak conditions, algorithm converges to a 'w' with $\nabla f(w) = 0$.
  - 'f' is bounded below, ∇f doesn't change arbitrarily fast, small and constant α^t.

Gradient Descent

- Least squares via normal equations vs. gradient descent:
  - Normal equations cost $O(nd^2 + d^3)$.
  - Gradient descent costs $O(ndt)$ to run for 't' iterations.

Computing $\nabla f(w) = X^TXw - \underbrace{X^Ty}_{O(nd)}$ only costs $O(nd)$.

$$X^TXw = \underbrace{X^T\underbrace{(Xw)}_{O(nd)}}_{O(nd)}$$

  - Gradient descent can be faster when 'd' is very large:
    - If solution is "good enough" for a 't' less than minimum$(d,d^2/n)$.
    - CPSC 540: 't' proportional to "condition number" of X^TX (no direct 'd' dependence).
  - Normal equations only solve linear least squares problems.
    - Gradient descent solves many other problems.

Beyond Gradient Descent

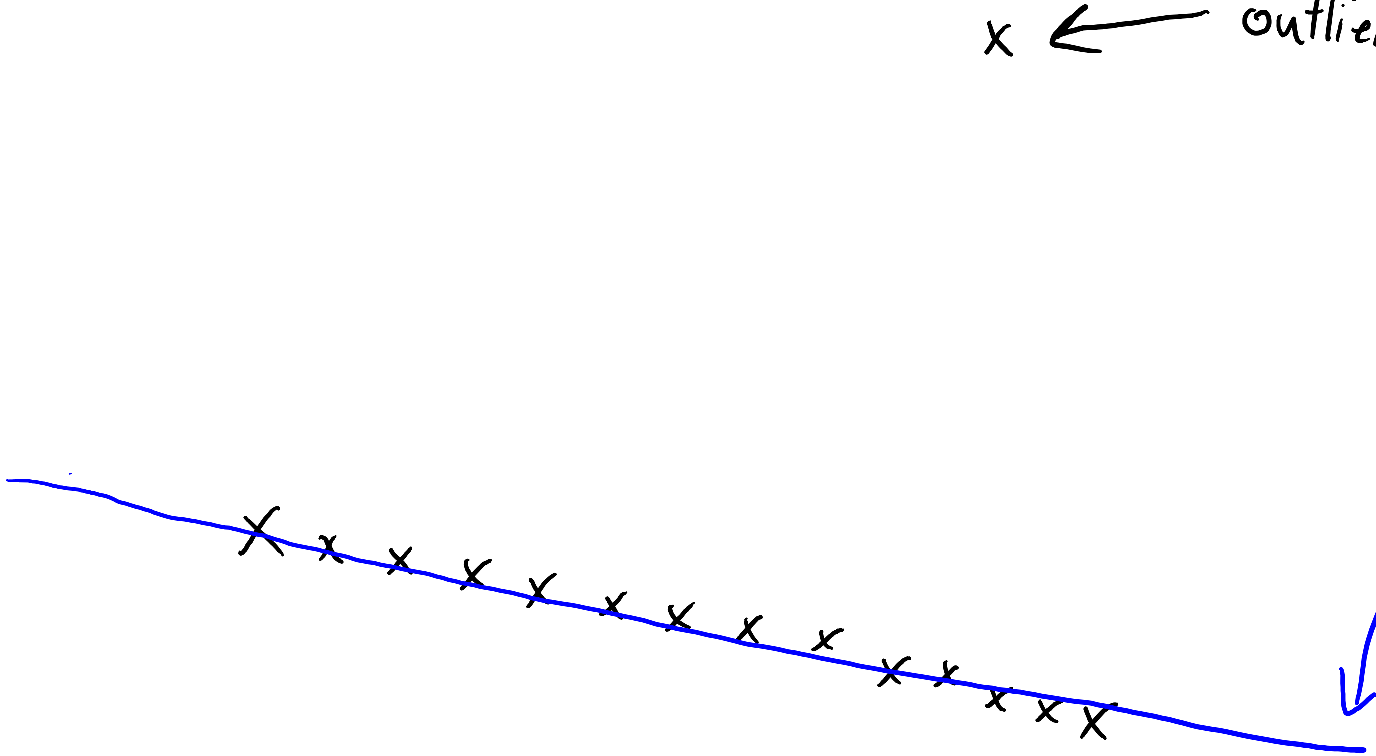
- There are many variations on gradient descent.
  - Methods employing a “line search” to choose the step-size.
  - “Conjugate” gradient and “accelerated” gradient methods.
  - Newton’s method (which uses second derivatives).
  - Quasi-Newton and Hessian-free Newton methods.
  - Stochastic gradient (later in course).

- This course focuses on gradient descent and stochastic gradient:
  - They’re simple and give reasonable solutions to most ML problems.
  - But the above can be faster for some applications.

(pause)

Least Squares with Outliers

- Consider least squares problem with outliers:



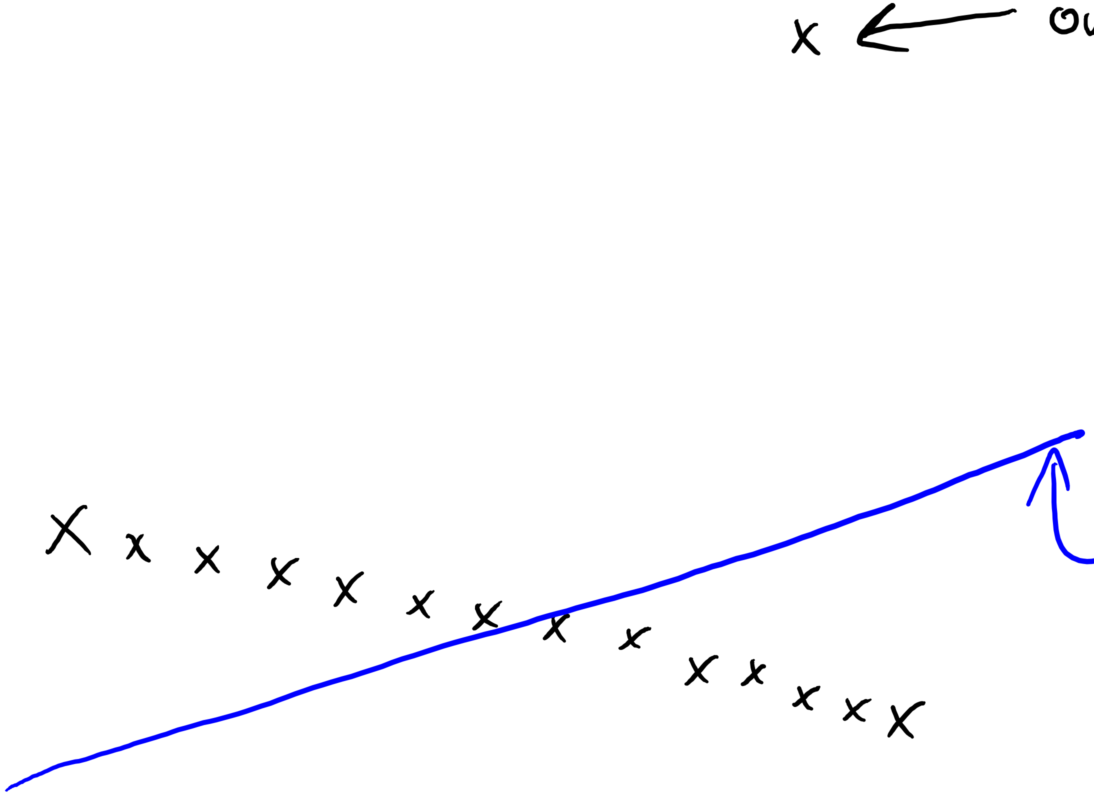
"outlier" that doesn't follow trend

This is what we <u>want</u> least squares to do.

http://setosa.io/ev/ordinary-least-squares-regression

Least Squares with Outliers

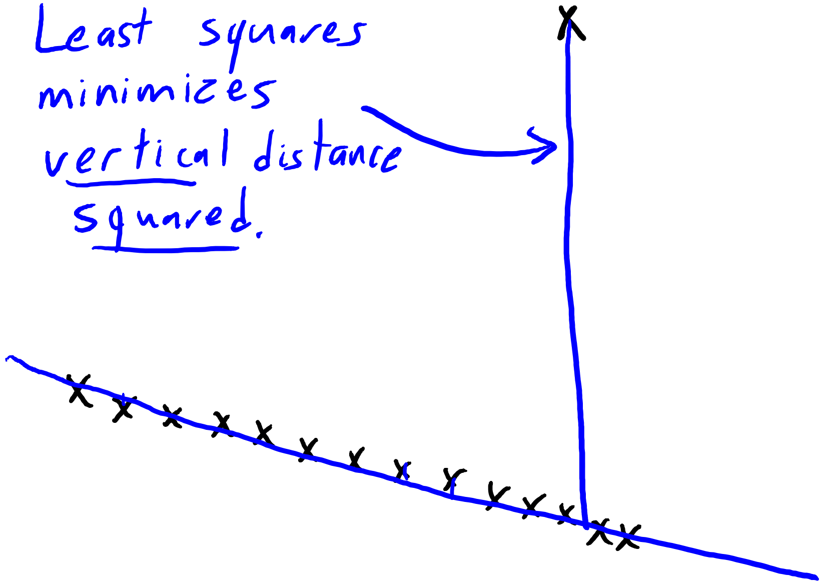
- Consider least squares problem with outliers:

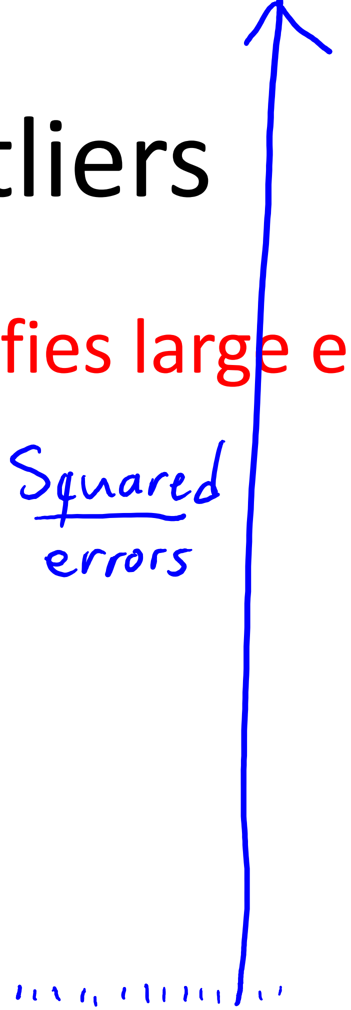


- Least squares is very sensitive to outliers.

Least Squares with Outliers

- Squaring error shrinks small errors, and magnifies large errors:



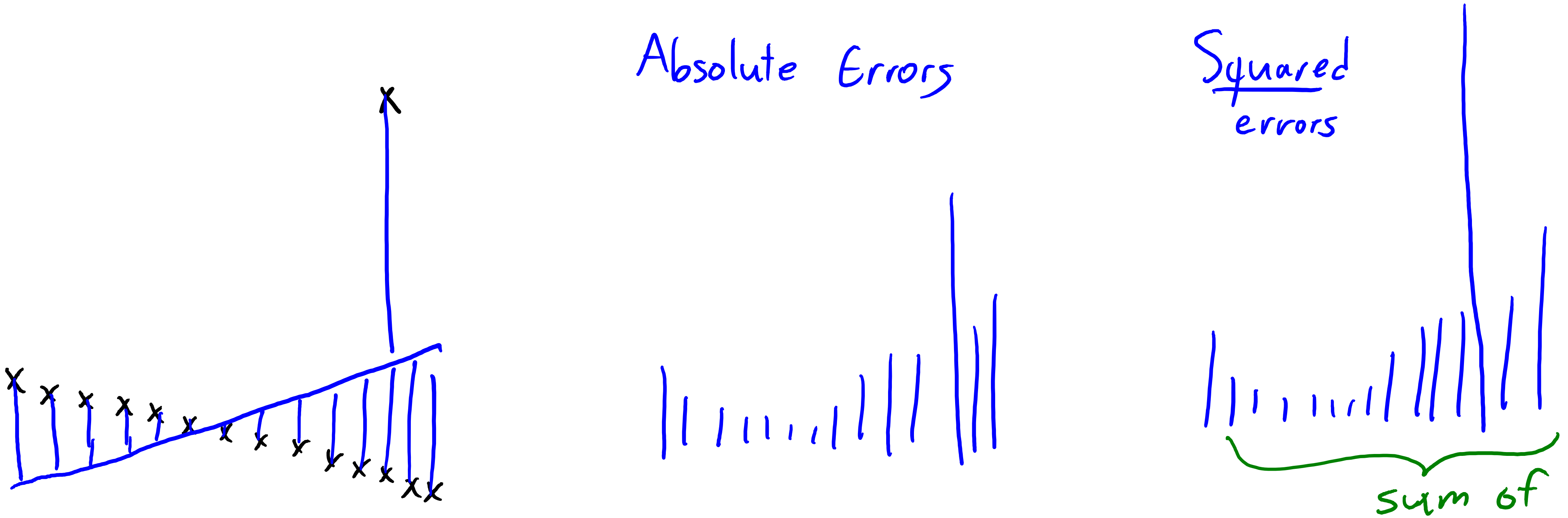


- Outliers (large error) influence 'w' much more than other points.

http://students.brown.edu/seeing-theory/regression/index.html

Least Squares with Outliers

- Squaring error shrinks small errors, and magnifies large errors:



- Outliers (large error) influence 'w' much more than other points.
  - Good if outlier means 'plane crashes', bad if it means 'data entry error'.

sum of these is smaller than for the "correct" line.

Robust Regression

- Robust regression objectives put less focus large errors (outliers).
- For example, use absolute error instead of squared error:

$$f(w) = \sum_{i=1}^{n} |w^T x_i - y_i|$$

- Now decreasing 'small' and 'large' errors is equally important.
- Instead of minimizing L2-norm, minimizes L1-norm of residuals:

Least squares:

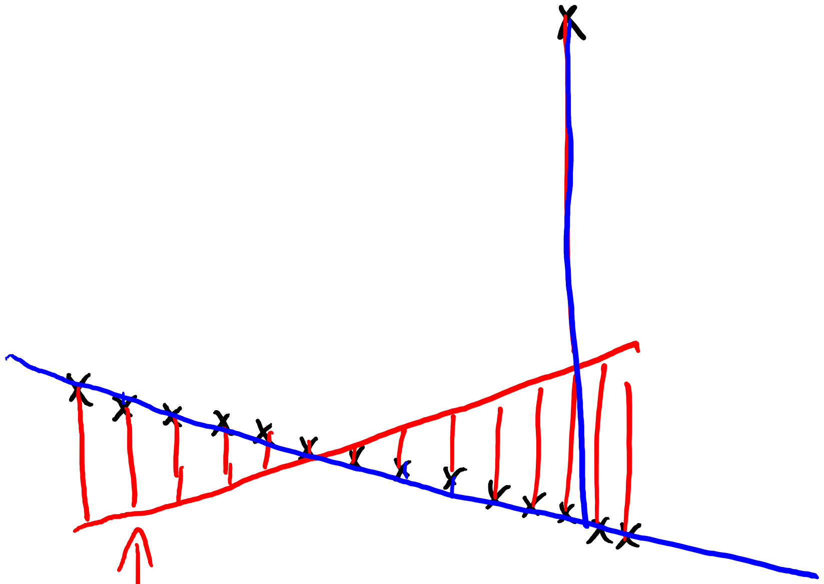
$$f(w) = \frac{1}{2}\|Xw - y\|^2$$

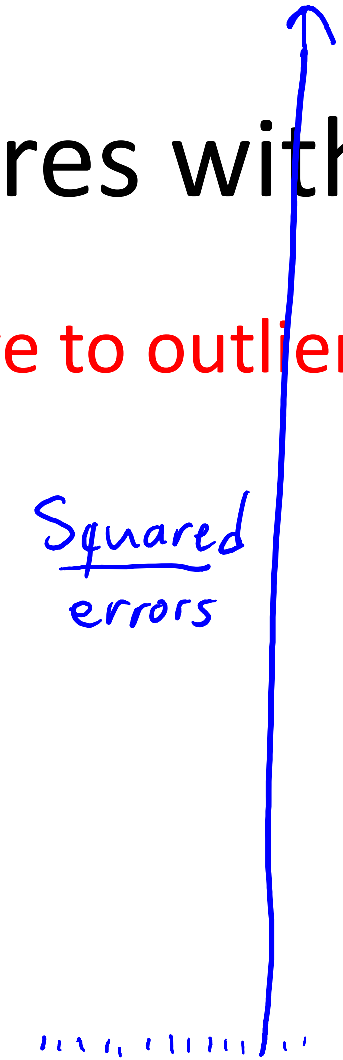
Least absolute error:

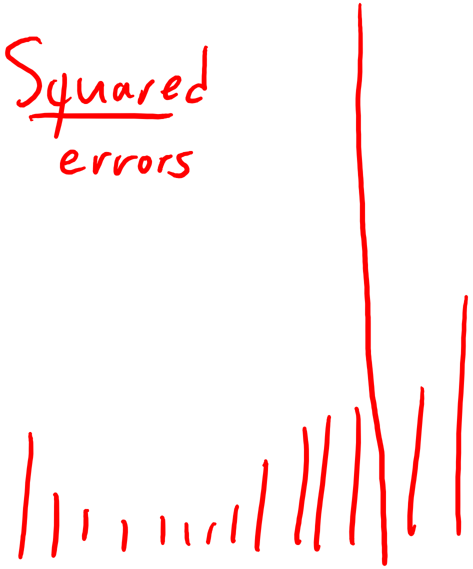
$$f(w) = \|Xw - y\|_1$$

Least Squares with Outliers

- Least squares is very sensitive to outliers.



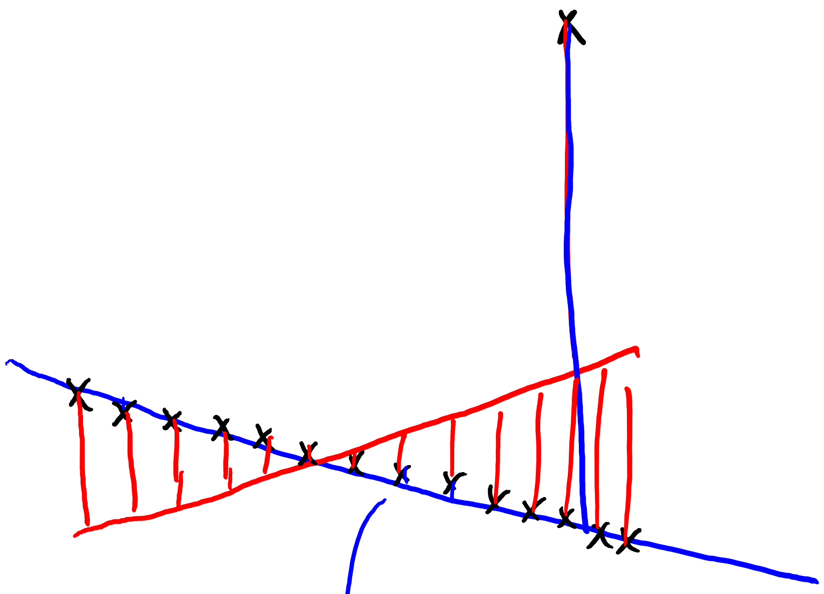


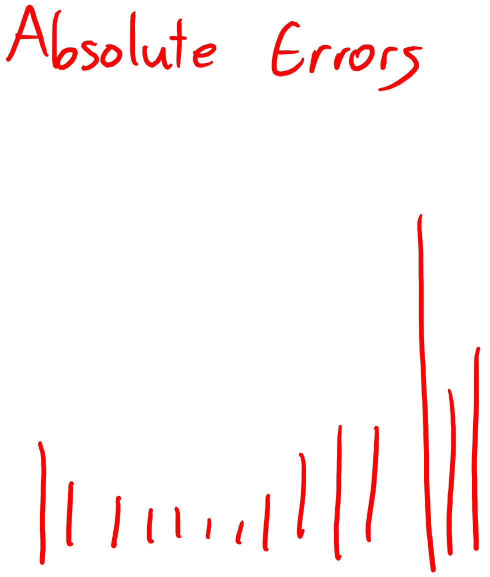


Linear model 'w' minimizing $f(w) = \frac{1}{2}\|Xw - y\|^2$

Least Squares with Outliers

- Absolute error is more robust to outliers:

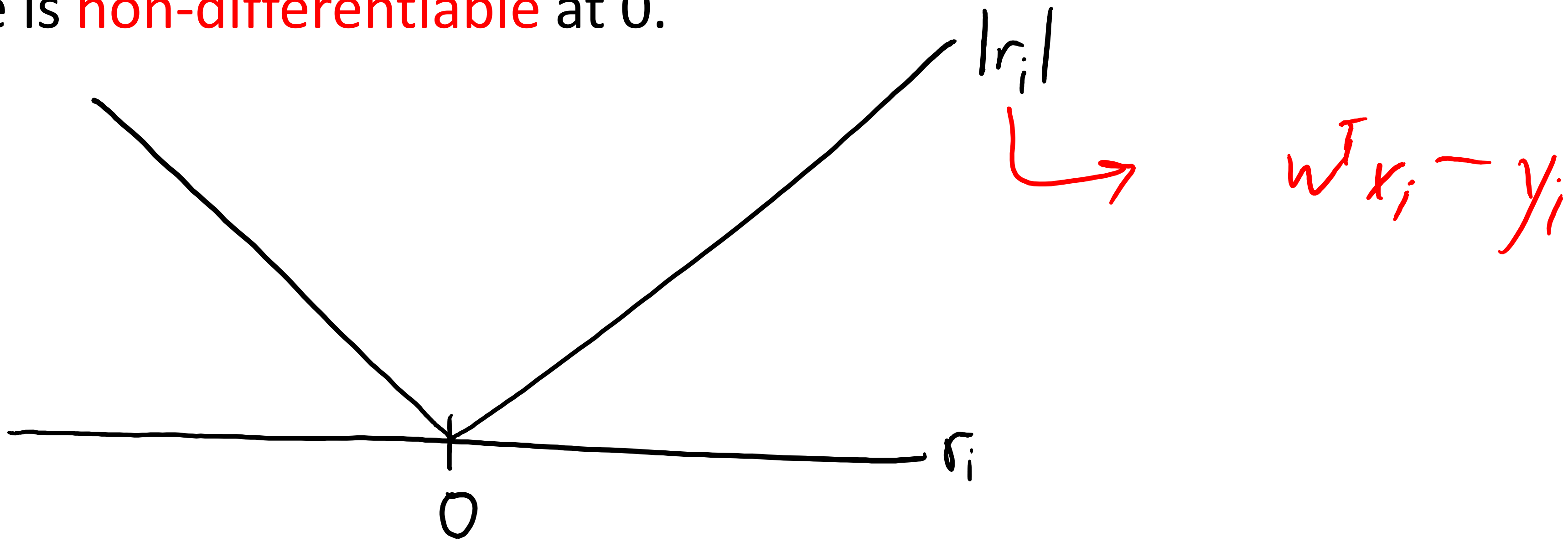




Linear model 'w' minimizing $f(w) = \|Xw - y\|_1 = \sum_{i=1}^{n} |w^T x_i - y_i|$

Regression with the L1-Norm

- Unfortunately, minimizing the absolute error is harder.
  - We don't have "normal equations" for minimizing the L1-norm.
  - Absolute value is non-differentiable at 0.



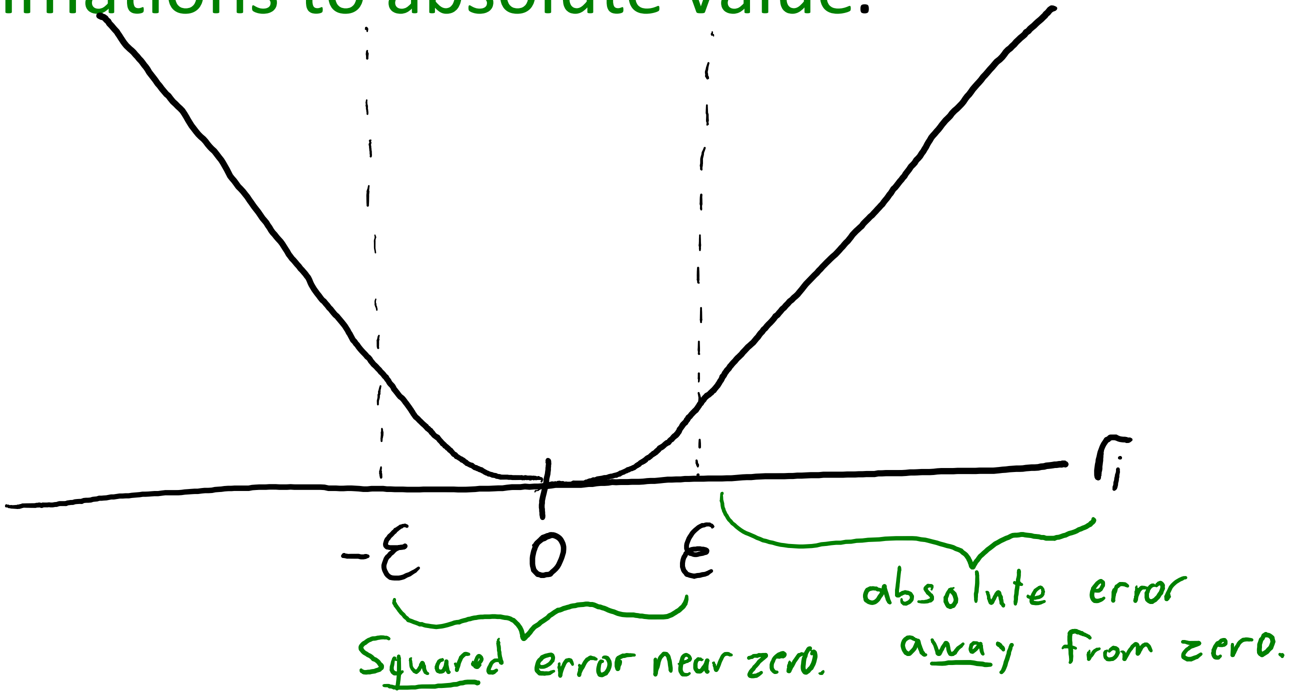
  - Generally, harder to minimize non-smooth than smooth functions.
    - Unlike smooth functions, the gradient may not get smaller near a minimizer.
  - We're going to use a smooth approximation, then apply gradient descent.

Smooth Approximations to the L1-Norm

- There are differentiable approximations to absolute value.
  - Common example is Huber loss:

$$f(w) = \sum_{i=1}^{n} h(w^T x_i - y_i)$$

$$h(r_i) = \begin{cases} \frac{1}{2} r_i^2 & \text{for } |r_i| \leq \varepsilon \\ \varepsilon(|r_i| - \frac{1}{2}\varepsilon) & \text{otherwise} \end{cases}$$



  - Note that 'h' is differentiable: $h'(\varepsilon) = \varepsilon$ and $h'(-\varepsilon) = -\varepsilon$.
  - This 'f' is convex but setting $\nabla f(x) = 0$ does not give a linear system.
  - But we can minimize the Huber loss using gradient descent.

Motivation for Considering Worst Case

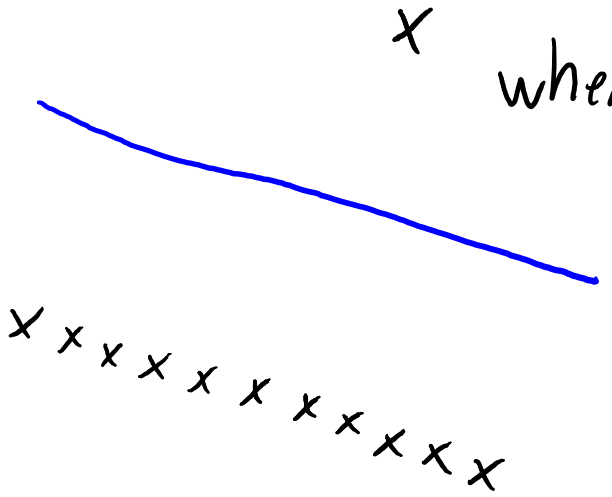
THE PROBLEM WITH AVERAGING STAR RATINGS

https://xkcd.com/937/

“Brittle” Regression

- What if you really care about getting the outliers right?
  - You want best performance on worst training example.
  - For example, if in worst case the plane can crash.
- In this case you could use something like the infinity-norm:

$$f(w) = \|Xw - y\|_\infty \quad \text{where} \quad \|r\|_\infty = \max_i \{|r_i|\}$$



- Very sensitive to outliers (“brittle”), but worst case will be better.

Log-Sum-Exp Function

- As with the L_1-norm, the L_∞-norm is convex but non-smooth:
  - We can again use a smooth approximation and fit it with gradient descent.

- Convex and smooth approximation to max function is log-sum-exp function:

$$\max_i \{z_i\} \approx \log\left(\sum_i \exp(z_i)\right)$$

  - We'll use this several times in the course.
  - Notation alert: when I write "log" I always mean "natural" logarithm: log(e) = 1.

- Intuition behind log-sum-exp:
  - $\sum_i \exp(z_i) \approx \max_i \exp(z_i)$, as largest element is magnified exponentially (if no ties).
    - While $\log(\exp(z_i)) = z_i$.

Summary

- Gradient descent finds stationary point of differentiable function.
  - Finds global optimum if function is convex.
- Robust regression using L1-norm is less sensitive to outliers.
- Brittle regression using Linf-norm is more sensitive to outliers.
- Smooth approximations:
  - Let us apply gradient descent to non-smooth functions.
  - Huber loss is a smooth approximation to absolute value.
  - Log-Sum-Exp is a smooth approximation to maximum.

- Next time:
  - We start our quest to automatically find the right features…

Why use the negative gradient direction?

- For a twice-differentiable 'f', multivariable Taylor expansion gives:

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

for some 'v' between w^{t+1} and w^t.

- If gradient can't change arbitrarily quickly, Hessian is bounded and:

$$f(w^{t+1}) = f(w^t) + \nabla f(w^t)^T (w^{t+1} - w^t) + \underbrace{O(\|w^{t+1} - w^t\|^2)}$$

becomes negigible as w^{t+1} gets close to w^t

  – But which choice of w^{t+1} decreases 'f' the most?

    - As $||w^{t+1}-w^t||$ gets close to zero, the value of w^{t+1} minimizing $f(w^{t+1})$ in this formula converges to $(w^{t+1} – w^t) = - \alpha^t \nabla f(w^t)$ for some scalar α^t.
    - So if we're moving a small amount, the optimal w^{t+1} is: $w^{t+1} = w^t - \alpha_t \nabla f(w^t)$ for some scalar α_t.

Normalized Steps

Question from class: "can we use $w^{t+1} = w^t - \frac{1}{\|\nabla f(w^t)\|} \nabla f(w^t)$"

This will work for a while, but notice that

$$\|w^{t+1} - w^t\| = \left\| \frac{1}{\|\nabla f(w^t)\|} \nabla f(w^t) \right\|$$

$$= \frac{1}{\|\nabla f(w^t)\|} \|\nabla f(w^t)\|$$

$$= 1$$

So the algorithm <u>never converges</u>

Log-Sum-Exp for Brittle Regression

- To use log-sum-exp for brittle regression:

$$\|Xw - y\|_\infty = \max_i \{|w^T x_i - y_i|\}$$

$$= \max_i \{\max\{w^T x_i - y_i, y_i - w^T x_i\}\}$$ since $|z| = \max\{z, -z\}$

$$= \log\left(\sum_{i=1}^n \exp(w^T x_i - y_i) + \sum_{i=1}^n \exp(y_i - w^T x_i)\right)$$ using log-sum-exp to approximate "max" over $2n$ terms.

Log-Sum-Exp Numerical Trick

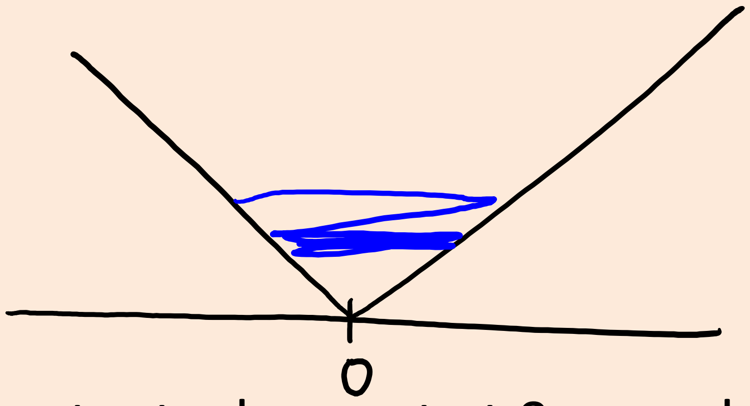
- Numerical problem with log-sum-exp is that $\exp(z_i)$ might overflow.
  - For example, $\exp(100)$ has more than 40 digits.
- Implementation 'trick': Let $\beta = \max_i \{z_i\}$

$$
\begin{aligned}
\log\left(\sum_i \exp(z_i)\right) &= \log\left(\sum_i \exp(z_i - \beta + \beta)\right) \\
&= \log\left(\sum_i \exp(z_i - \beta)\exp(\beta)\right) \\
&= \log\left(\exp(\beta)\sum_i \exp(z_i - \beta)\right) \\
&= \log(\exp(\beta)) + \log\left(\sum_i \exp(z_i - \beta)\right) \\
&= \beta + \log\left(\sum_i \underbrace{\exp(z_i - \beta)}_{\leq 1}\right)
\end{aligned}
$$

≤ 1 so no overflow

Gradient Descent for Non-Smooth?

- "You are unlikely to land on a non-smooth point, so gradient descent should work for non-smooth problems?"
  - Consider just trying to minimize the absolute value function:



  - Norm(gradient) is constant when not at 0, so unless you are lucky enough to hit exactly 0, you will just bounce back and forth forever.
  - We didn't have this problem for smooth functions, since the gradient gets smaller as you approach a minimizer.
  - You could fix this problem by making the step-size slowly go to zero, but you need to do this carefully to make it work, and the algorithm gets much slower.

Gradient Descent for Non-Smooth?

- Counter-example from Bertsekas' "Nonlinear Programming" where gradient descent for a non-smooth convex problem does not converge to a minimum.

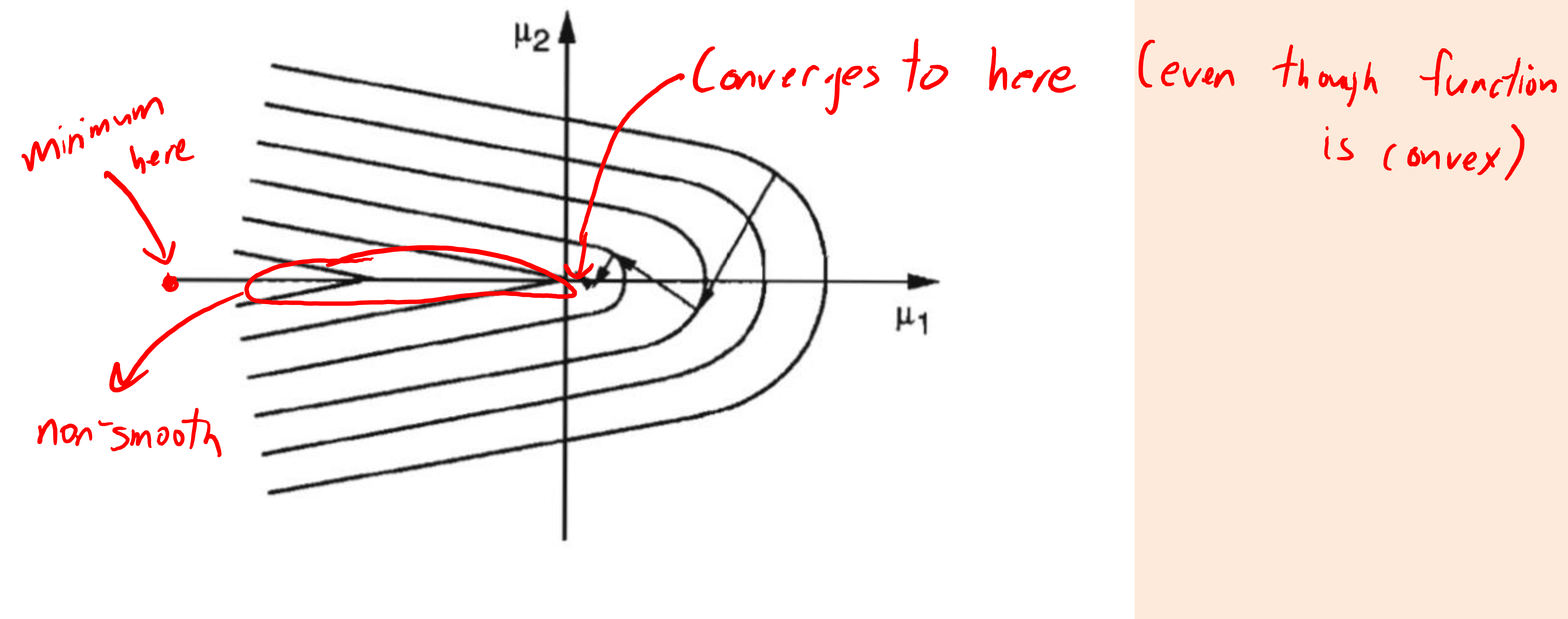
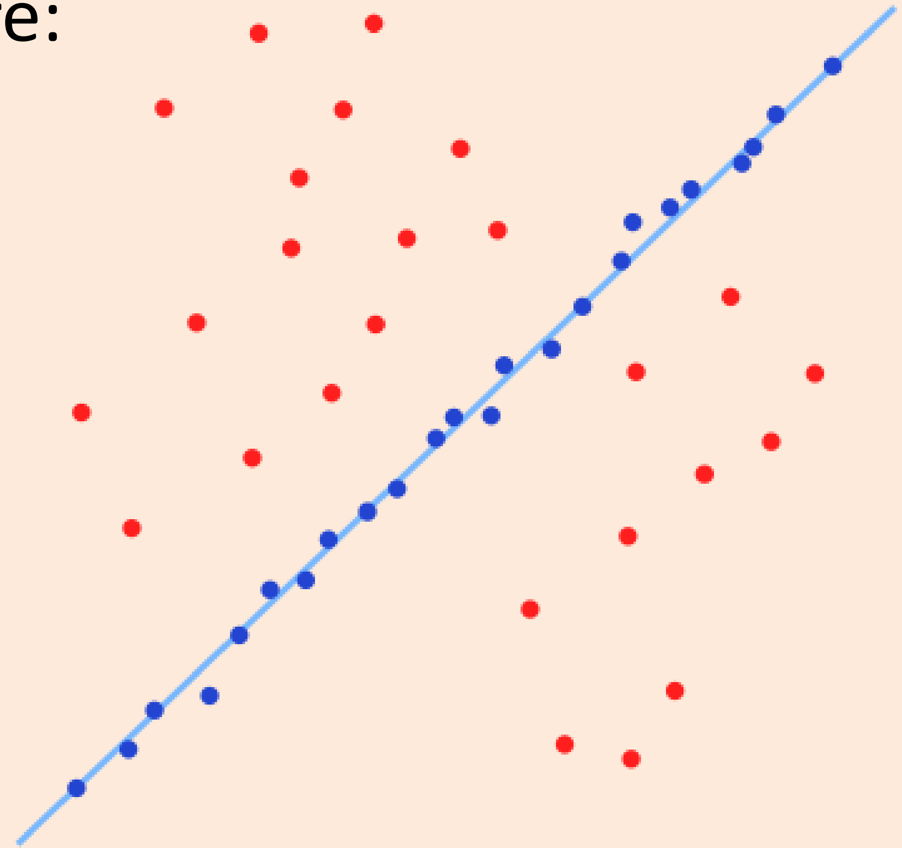


Figure 6.3.8. Contours and steepest ascent path for the function of Exercise 6.3.8.

Random Sample Consensus (RANSAC)

- In computer vision, a widely-used generic framework for robust fitting is random sample consensus (RANSAC).
- This is designed for the scenario where:
  - You have a large number of outliers.
  - Majority of points are “inliers”: it’s really easy to get low error on them.



https://en.wikipedia.org/wiki/Random_sample_consensus

Random Sample Consensus (RANSAC)

- RANSAC:
  - Sample a small number of training examples.
    - Minimum number needed to fit the model.
    - For linear regression with 1 feature, just 2 examples.
  - Fit the model based on the samples.
    - Fit a line to these 2 points.
    - With ‘d’ features, you’ll need ‘d’ examples.
  - Test how many points are fit well based on the model.
  - Repeat until we find a model that fits at least the expected number of “inliers”.
- You might then re-fit based on the estimated “inliers”.