CPSC 340: Machine Learning and Data Mining

Gradient Descent

Fall 2018

Last Time: Change of Basis

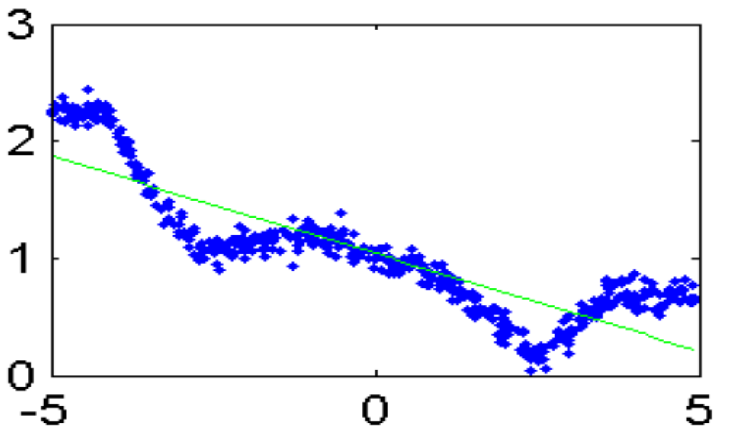
- Last time we discussed change of basis:
  - E.g., polynomial basis:

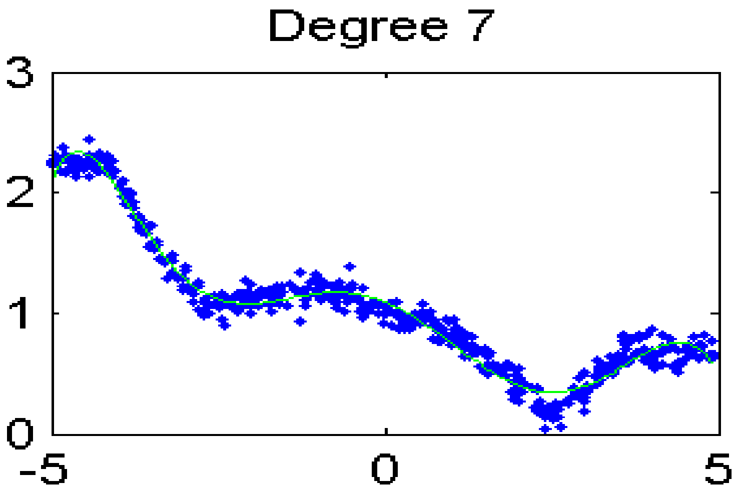
$$\text{Replace } X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \text{ with } Z = \begin{bmatrix} 1 & x_1 & (x_1)^2 & \cdots & (x_1)^p \\ 1 & x_2 & (x_2)^2 & \cdots & (x_2)^p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & (x_n)^2 & \cdots & (x_n)^p \end{bmatrix}$$

  - You can fit non-linear models with linear regression.

$$\hat{y}_i = v^T z_i = w_0 + w_1 x_i + w_2 x_i^2 + w_3 x_i^3 + \cdots + w_p x_i^p$$

  - Just treat 'Z' as your data, then fit linear model.





Optimization Terminology

- When we minimize or maximize a function we call it "optimization".
  - In least squares, we want to solve the "optimization problem":

$$\min_{w \in \mathbb{R}^d} \frac{1}{2} \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

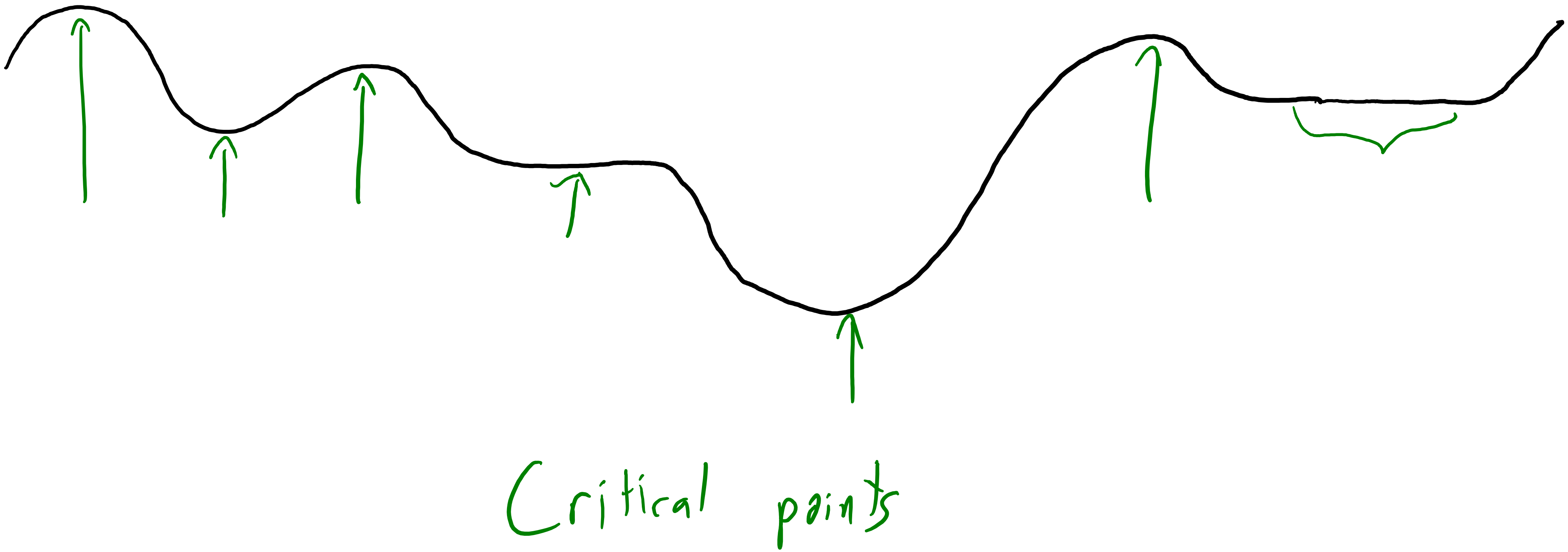
  - The function being optimized is called the "objective".
    - Also sometimes called "loss" or "cost", but these have different meanings in ML.
  - The set over which we search for an optimum is called the domain.
  - Often, instead of the minimum objective value, you want a minimizer.
    - A set of parameters 'w' that achieves the minimum value.

Discrete vs. Continuous Optimization

- We have seen examples of continuous optimization:
  - Least squares:
    - Domain is the real-valued set of parameters ‘w’.
    - Objective is the sum of the squared training errors.
- We have seen examples of discrete optimization:
  - Fitting decision stumps:
    - Domain is the finite set of unique rules.
    - Objective is the number of classification errors (or infogain).
- We have also seen a mixture of discrete and continuous:
  - K-means: clusters are discrete and means are continuous.

Stationary/Critical Points

- A ‘w’ with $\nabla f(w) = 0$ is called a stationary point or critical point.
  - The slope is zero so the tangent plane is “flat”.



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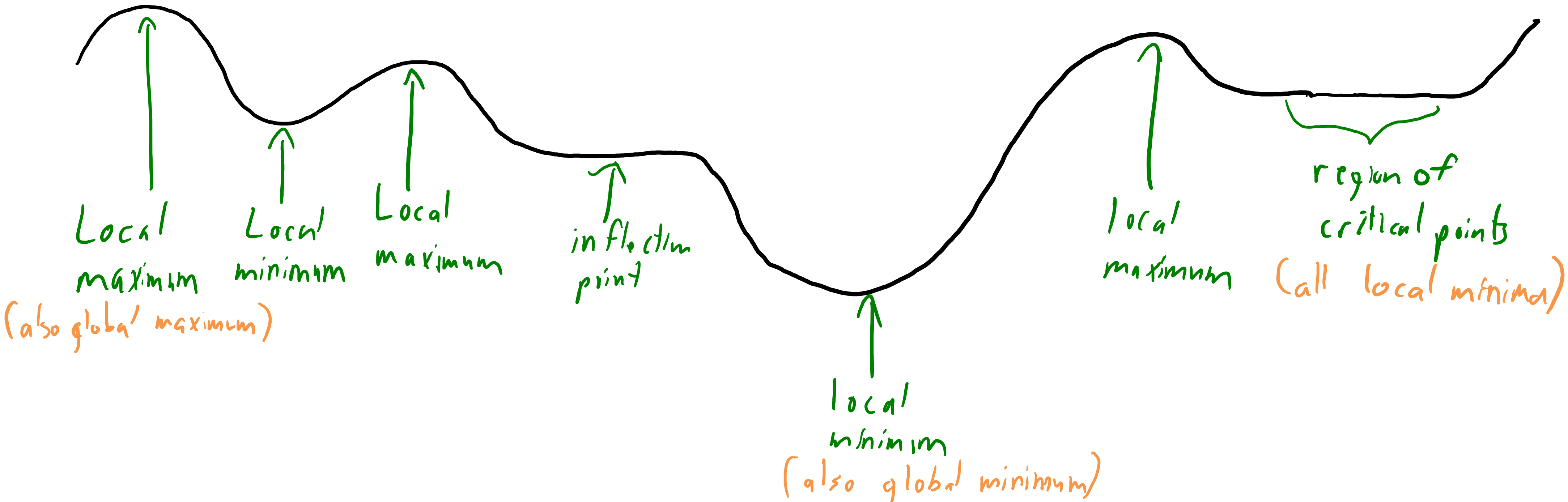


  - If we're minimizing, we would ideally like to find a global minimum.
    - But for some problems the best we can do is find a stationary point where ∇ f(w)=0.

Motivation: Large-Scale Least Squares

- Normal equations find 'w' with ∇ f(w) = 0 in O(nd^2 + d^3) time.

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

$\rightarrow$ 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

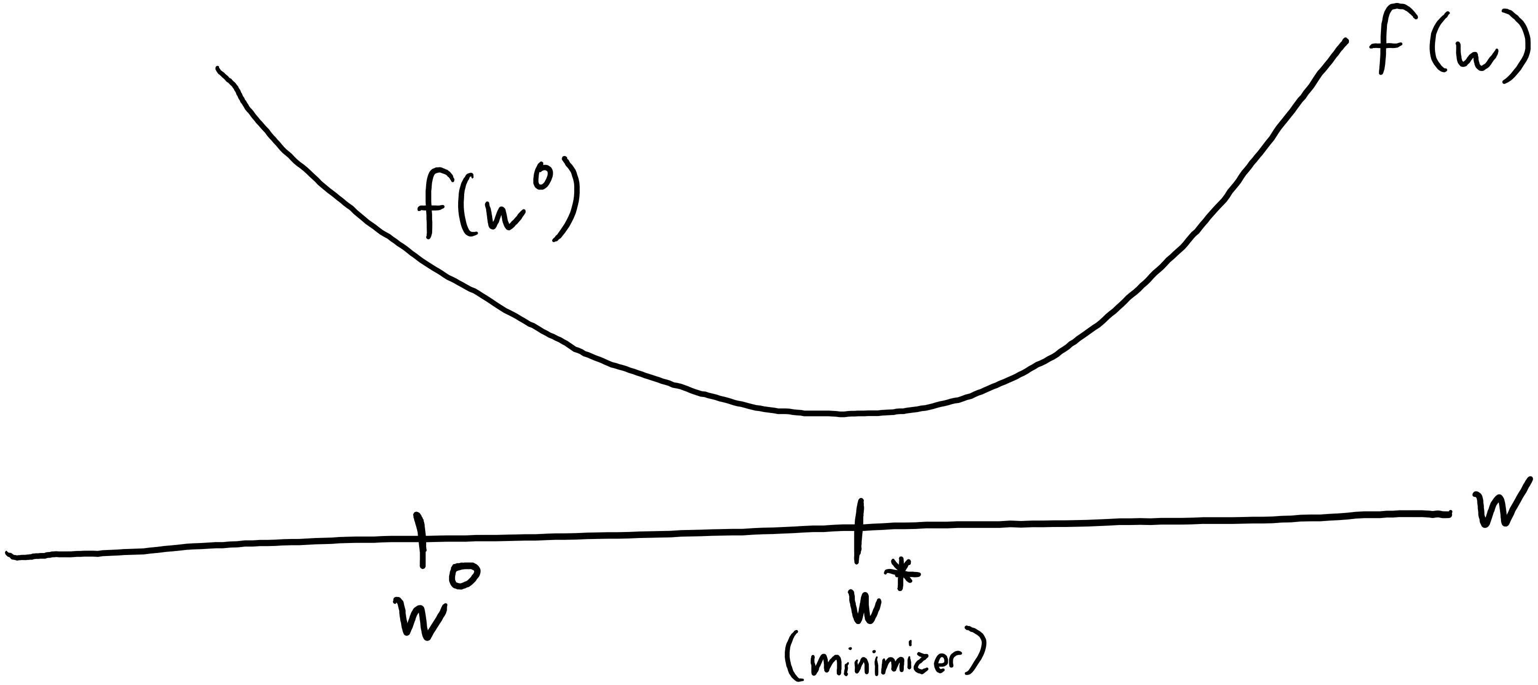
- Gradient descent is an iterative optimization algorithm:
  - It starts with a "guess" w^0.
  - It uses the gradient $\nabla f(w^0)$ to generate a better guess w^1.
  - It uses the gradient $\nabla f(w^1)$ to generate a better guess w^2.
  - It uses the gradient $\nabla f(w^2)$ to generate a better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



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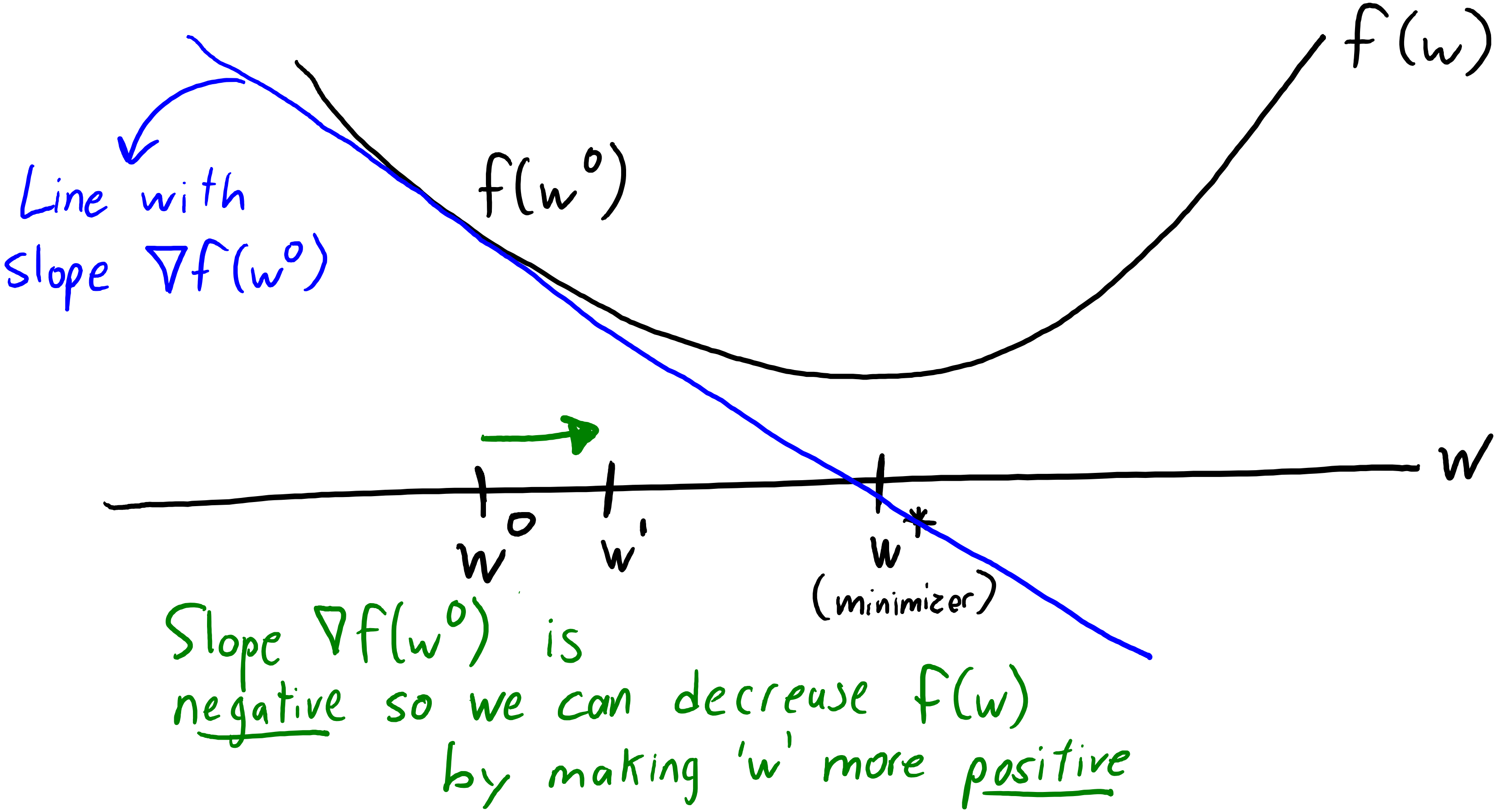

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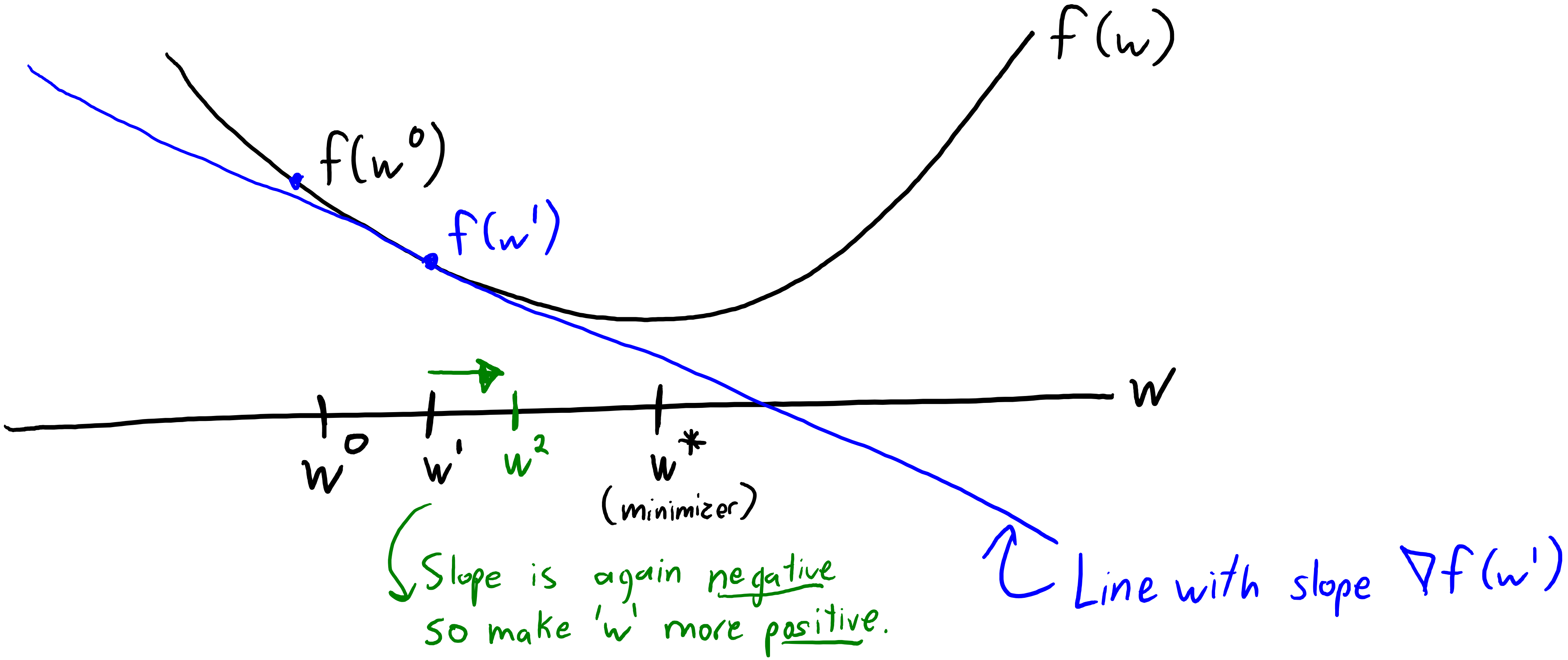

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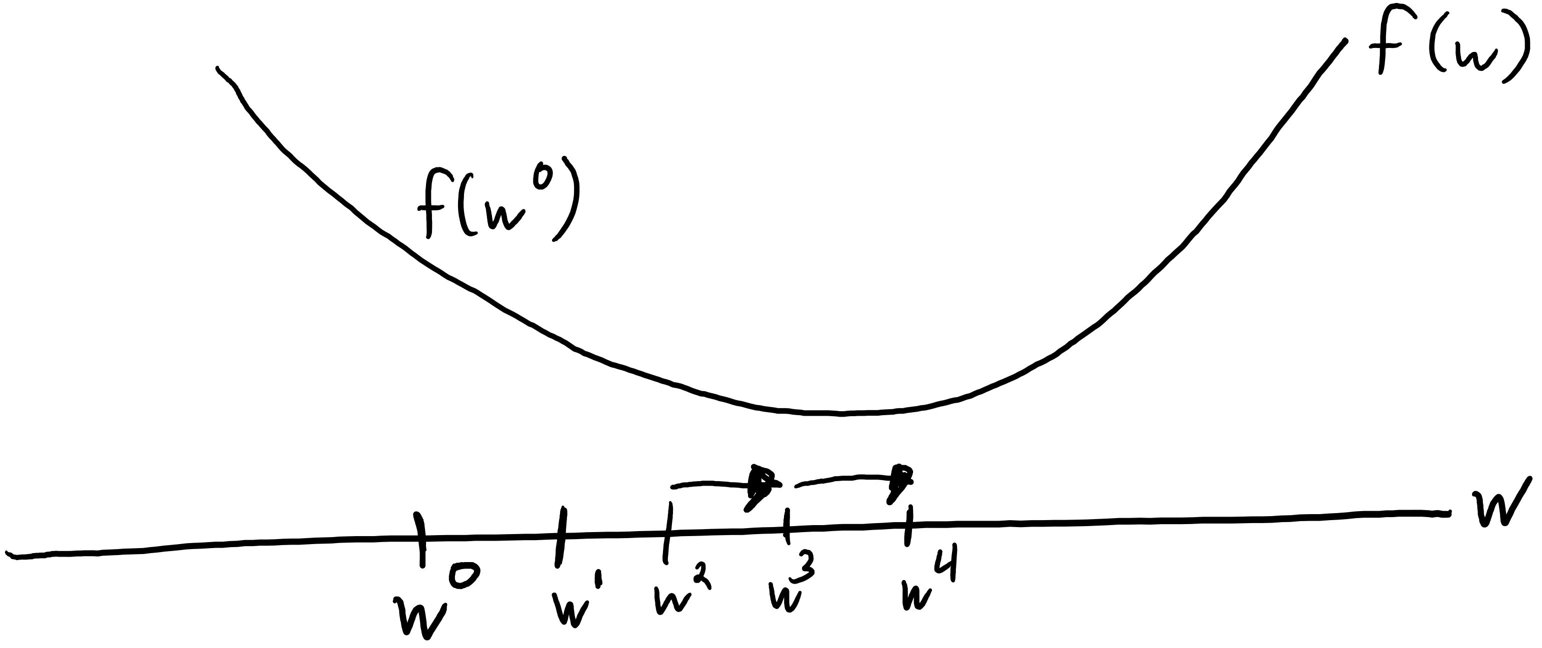

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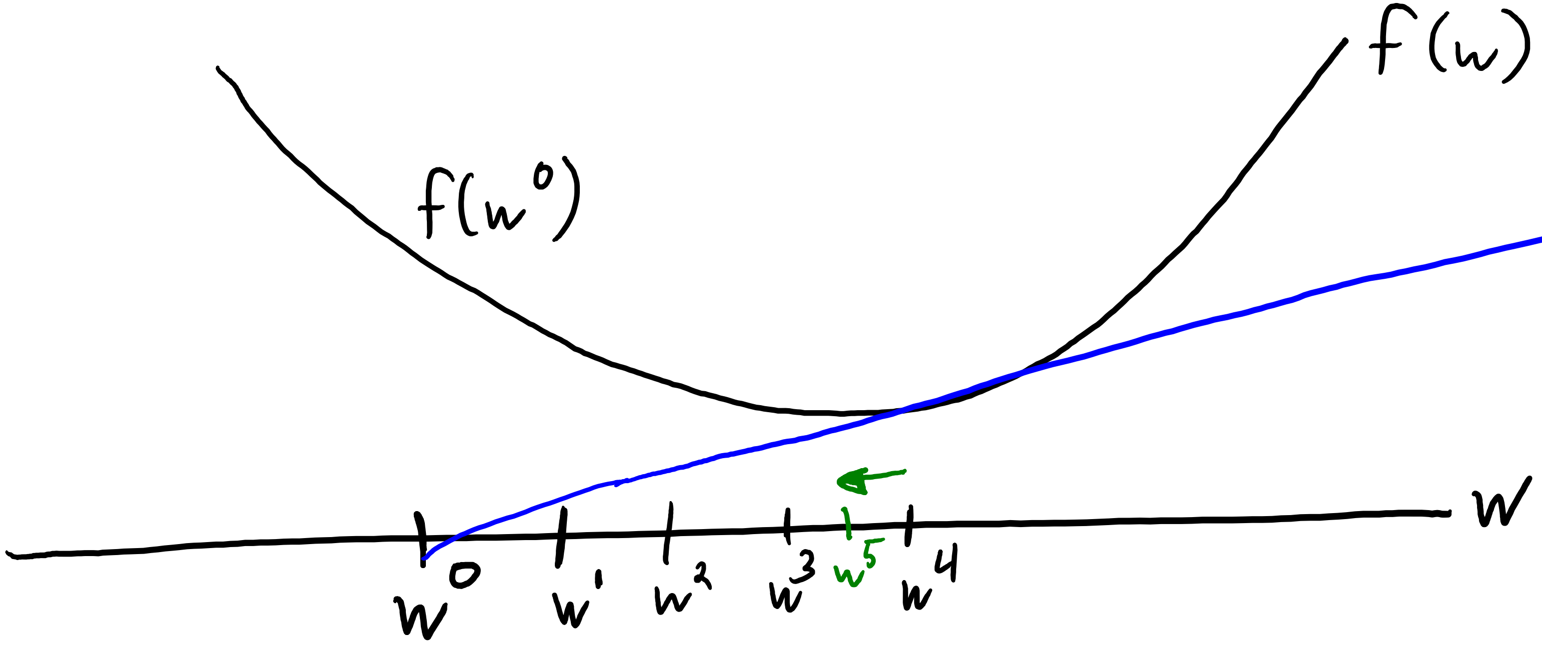


Now the slope $\nabla f(w^4)$ is positive so we move in the negative direction.

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").

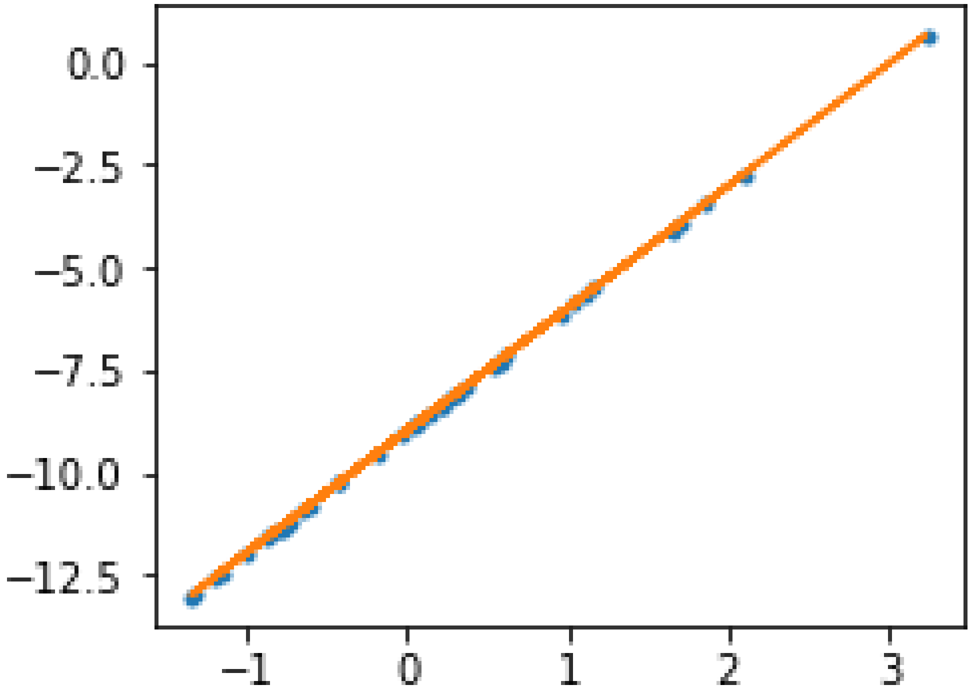
– Repeat to successively refine the guess:

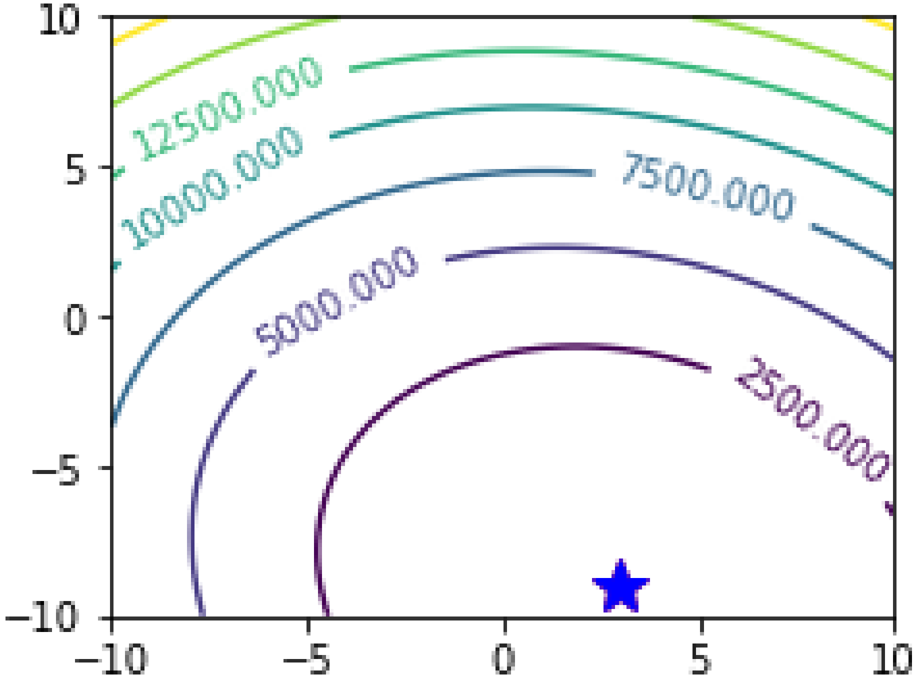
$$w^{t+1} = w^t - \alpha^t \nabla f(w^t) \quad \text{for } t = 1, 2, 3, \ldots$$

– Stop if not making progress or $\underbrace{\|\nabla f(w^t)\| \leq \varepsilon}_{\text{Approximate local minimum}}$ ↳ Some small scalar.

Data Space vs. Parameter Space

- Usual regression plot is in the “x vs. y” data space (left):

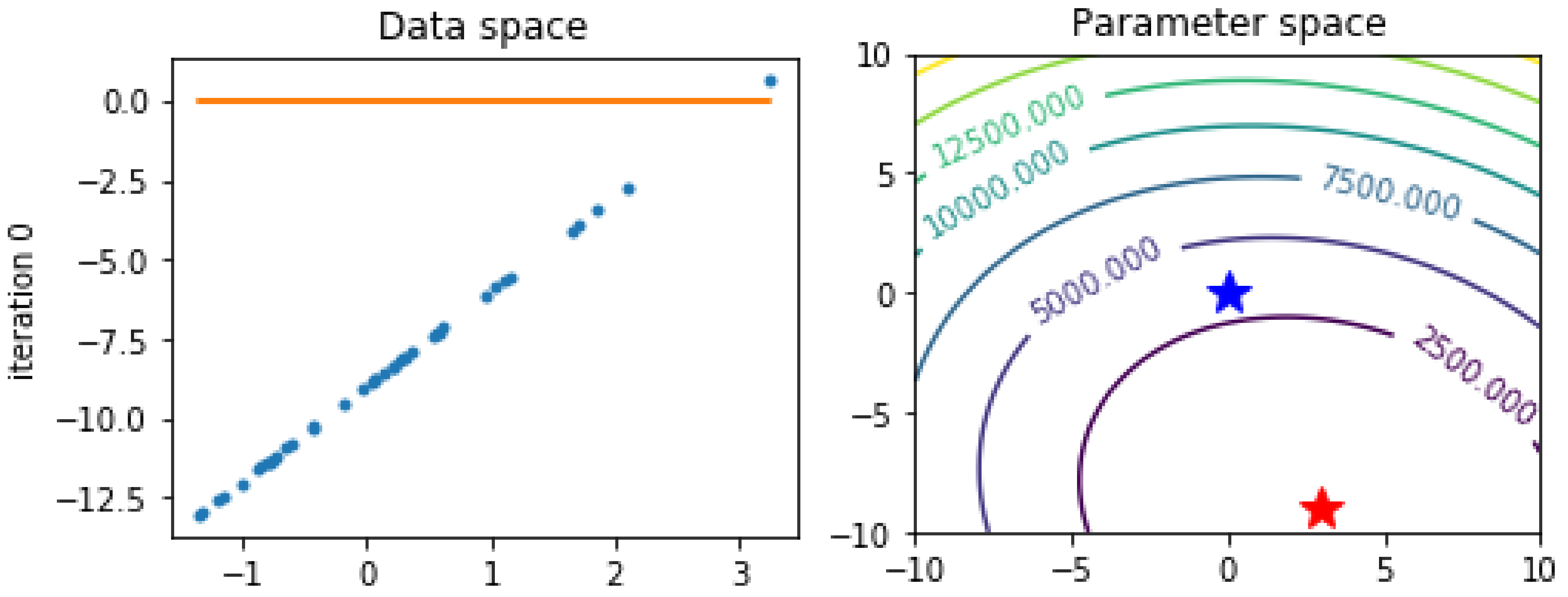




- On the right is plot of the “intecerpt vs. slope” parameter space.
  – Points in parameter space correspond to models (* is least squares parameters).

Gradient Descent in Data Space vs. Parameter Space

- Gradient descent starts with an initial guess in parameter space:



  – And each iteration tries to move guess closer to solution.

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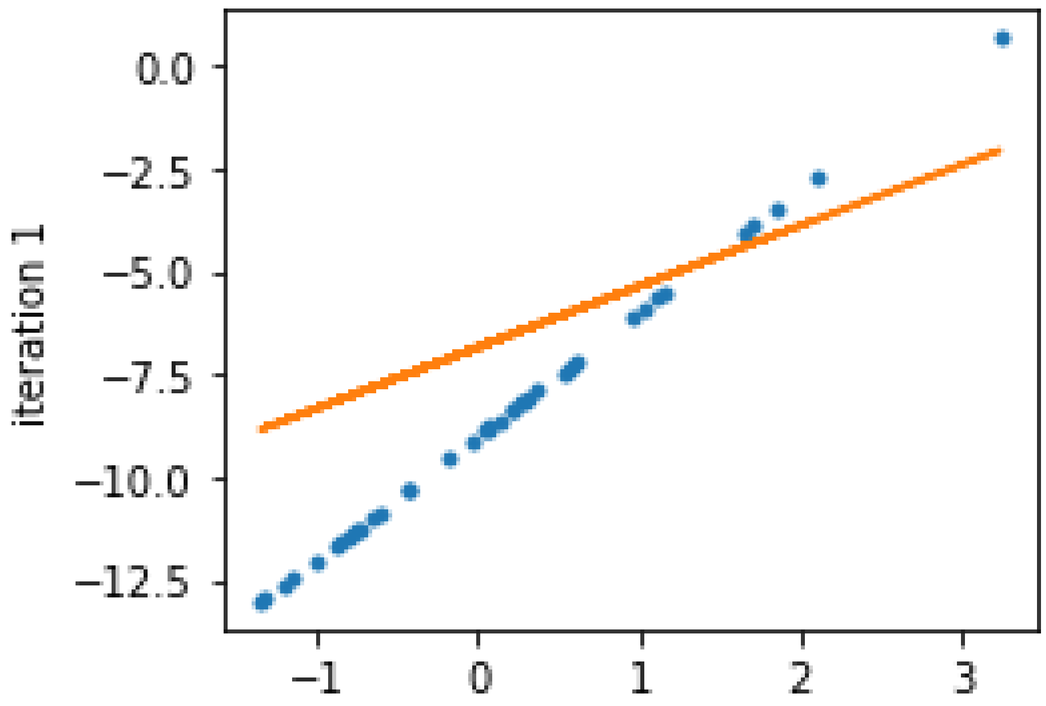

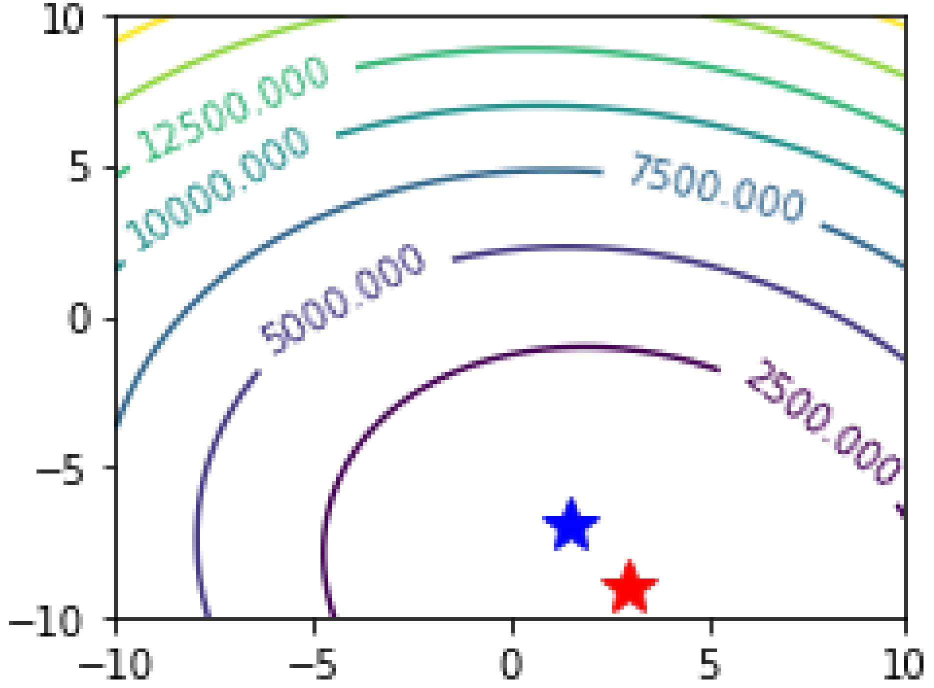

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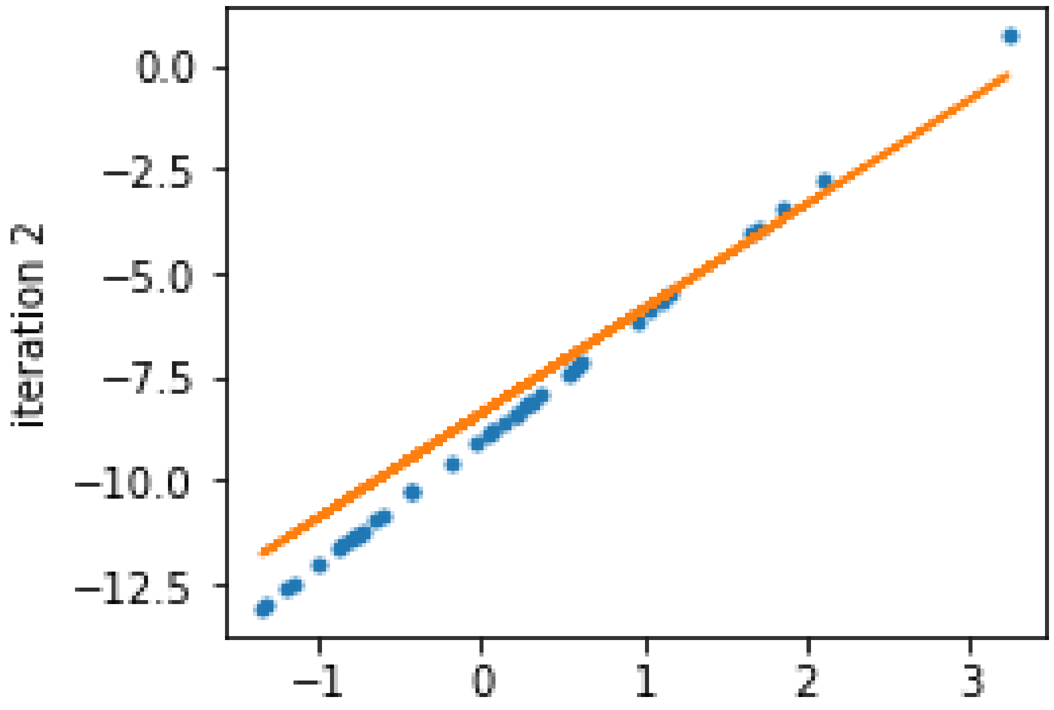

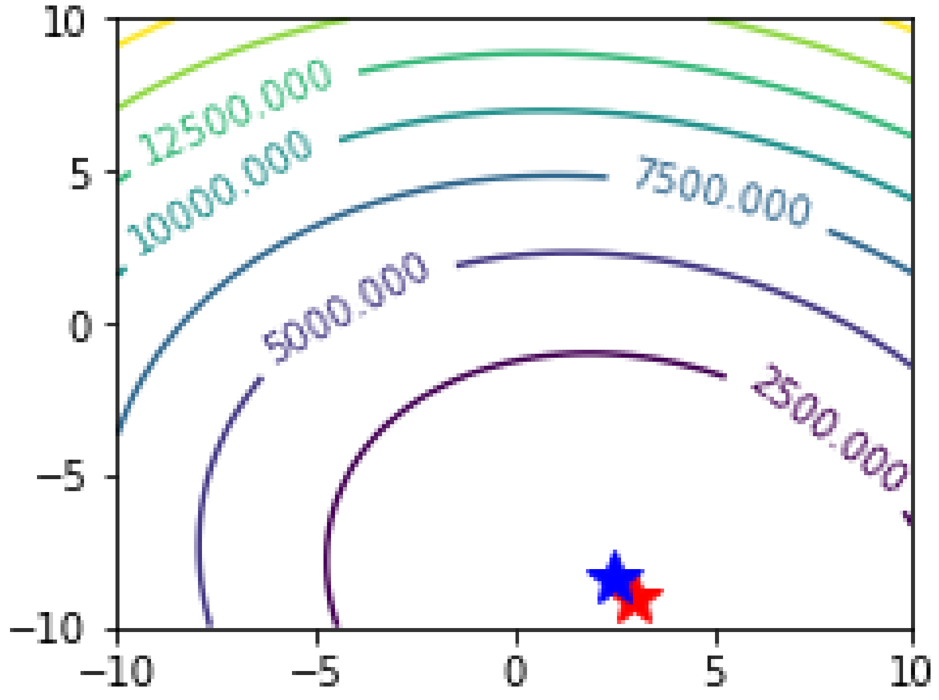

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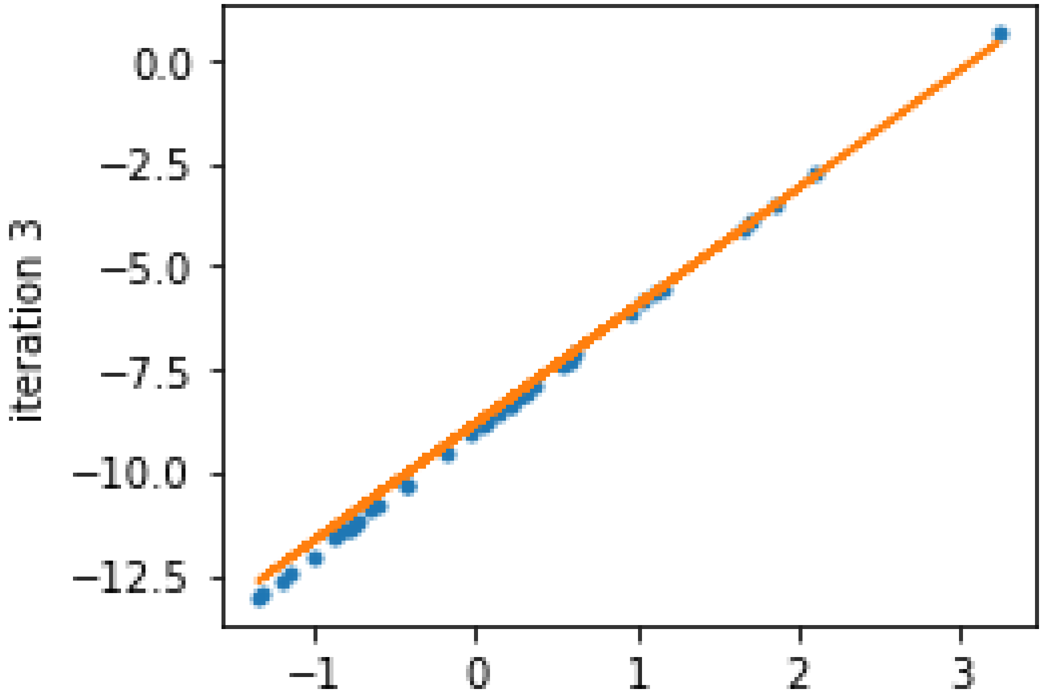
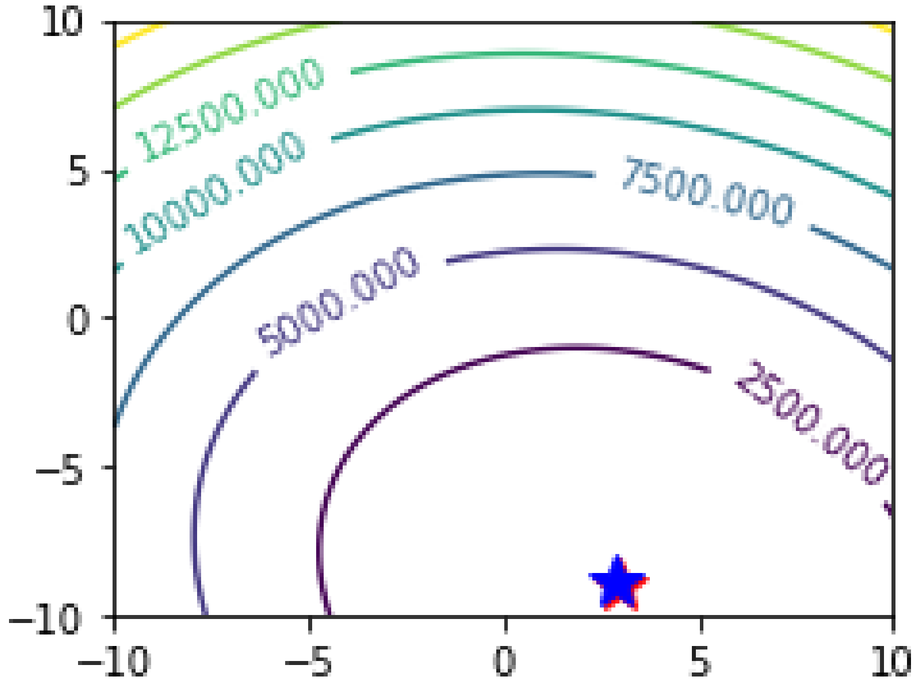
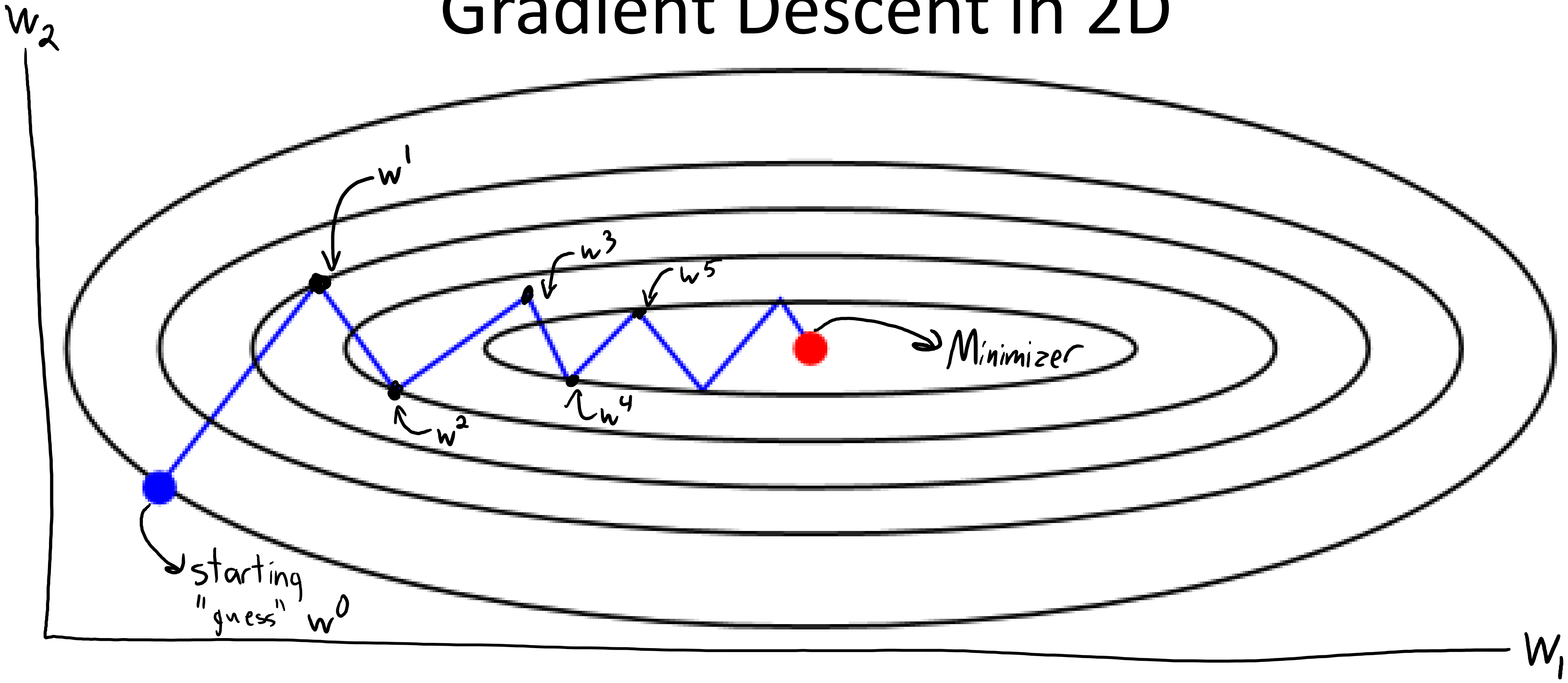




  - And each iteration tries to move guess closer to solution.

Gradient Descent in 2D



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

Gradient Descent for Least Squares

- The least squares objective and gradient:

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

- Gradient descent iterations for least squares:

$$w^{t+1} = w^t - \alpha^t \underbrace{X^T(Xw^t - y)}_{\nabla f(w^t)}$$

- Cost of gradient descent iteration is O(nd) (no need to form X^TX).

Bottleneck is computing $\nabla f(w^t) = \underbrace{X^T\underbrace{(\underbrace{Xw^t}_{O(nd)} - y)}_{O(n)}}_{O(nd)}$

Normal Equations vs. Gradient Descent

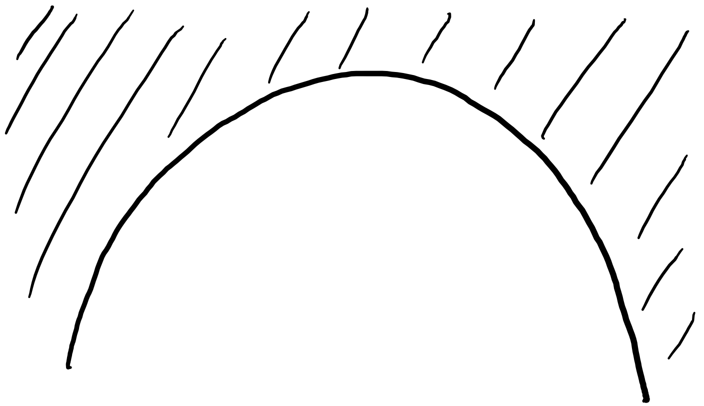
- Least squares via normal equations vs. gradient descent:
  - Normal equations cost $O(nd^2 + d^3)$.
  - Gradient descent costs $O(ndt)$ to run for 't' iterations.
    - Each of the 't' iterations costs $O(nd)$.
  - Gradient descent can be faster when 'd' is very large:
    - If solution is "good enough" 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

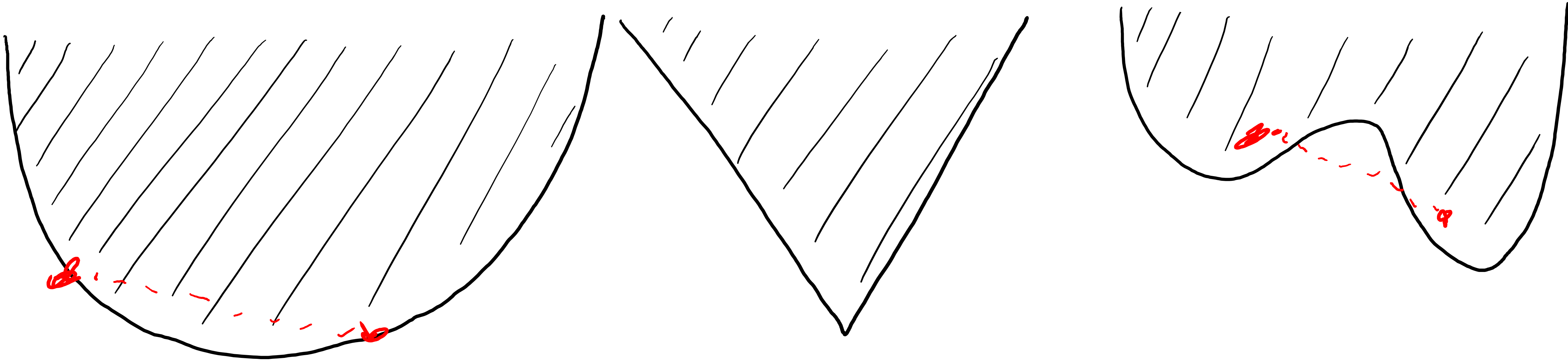
- There are many variations on gradient descent.
  - Methods employing a “line search” to choose the step-size.
  - “Conjugate” gradient and “accelerated” gradient methods.
  - Newton’s method (which uses second derivatives).
  - Quasi-Newton and Hessian-free Newton methods.
  - Stochastic gradient (later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

Convex Functions



- Is finding a ‘w’ with $\nabla f(w) = 0$ good enough?
  - Yes, for convex functions.



- A function is convex if the area above the function is a convex set.
  - All values between any two points above function stay above function.

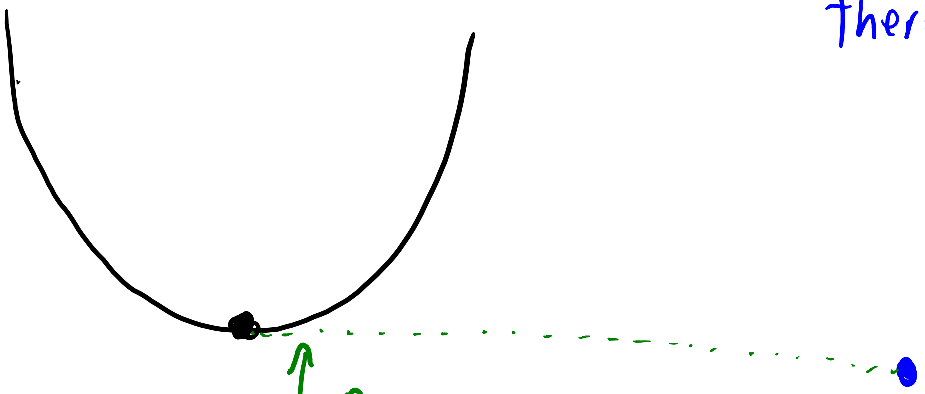
Convex Functions

- All ‘w’ with $\nabla f(w) = 0$ for convex functions are global minima.

Proof by contradiction:

Consider a local minimum

If this is not global minimum, there must a smaller value.



By convexity we can move along line to global minimum and decrease objective.

But this contradicts that we are at a local minimum.

  - Normal equations find a global minimum because of convexity.

How do we know if a function is convex?

- Some useful tricks for showing a function is convex:
  - 1-variable, twice-differentiable function is convex iff $f''(w) \geq 0$ for all 'w'.

Consider $f(w) = \frac{1}{2}aw^2$ for $a > 0$.

We have $f'(w) = aw$

and $f''(w) = a > 0$

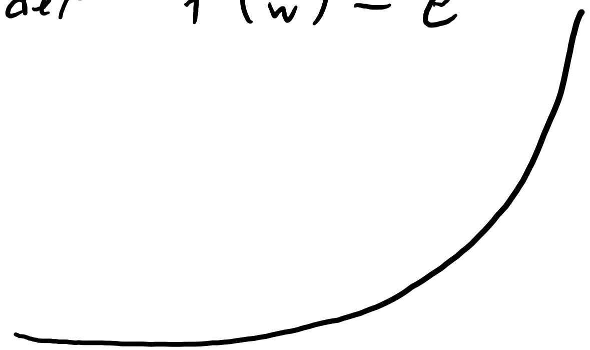
By assumption

Consider $f(w) = e^w$

We have $f'(w) = e^w$

and $f''(w) = e^w > 0$

By definition of exponential function.



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- Some useful tricks for showing a function is convex:
  - 1-variable, twice-differentiable function is convex iff $f''(w) \geq 0$ for all ‘w’.
  - A convex function multiplied by non-negative constant is convex.

We showed that $f(w) = e^w$ is convex, so $f(w) = 10e^w$ is convex.

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  - Norms and squared norms are convex.

$\|w\|$, $\|w\|^2$, $\|w\|_1$, $\|w\|_\infty$, $\|w\|_1^2$, and so on are all convex.

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  - The sum of convex functions is a convex function.

$$f(w) = \underbrace{10e^{w}}_{\text{From earlier}} + \underbrace{\frac{\lambda}{2}}_{\text{constant}}\underbrace{\|w\|^2}_{\text{norm squared}} \quad \text{is convex}$$

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$$f(w) = w^T x_i = \underbrace{w_1 x_{i1}}_{\text{convex}} + \underbrace{w_2 x_{i2}}_{\text{convex}} + \cdots + \underbrace{w_d x_{id}}_{\text{convex}}$$

Second derivative of each term is 0.

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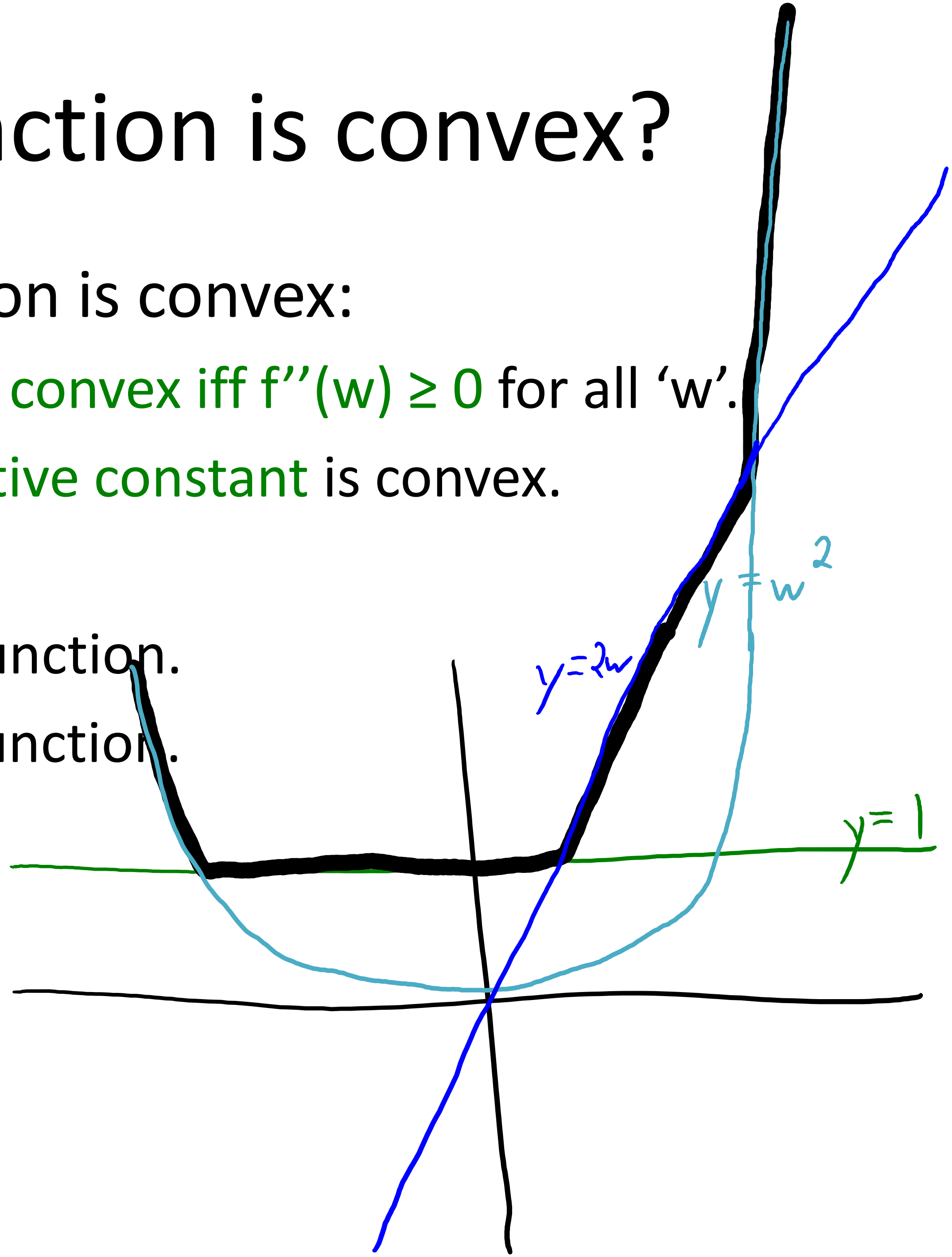
  - The max of convex functions is a convex function.

$f(w) = \max\{1, 2w, w^2\}$ is convex.

convex



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  - The sum of convex functions is a convex function.
  - The max of convex functions is a convex function.
  - Composition of a convex function and a linear function is convex.

If $f(w) = g(\underbrace{Xw - y}_{\text{linear function}})$ then 'f' is convex if 'g' is convex.

How do we know if a function is convex?

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  - The sum of convex functions is a convex function.
  - The max of convex functions is a convex function.
  - Composition of a convex function and a linear function is convex.
- But: not true that composition of convex with convex is convex:

Even if 'f' is convex and 'g' is convex, $f(g(w))$ might <u>not</u> be convex.

E.g. x^2 is convex and $-\log(x)$ is convex but $-\log(x^2)$ is <u>not</u> convex.

Example: Convexity of Linear Regression

- Consider linear regression objective with squared error:

$$f(w) = \|Xw - y\|^2$$

- We can use that this is a convex function composed with linear:

Let $g(r) = \|r\|^2$, which is convex because it's a squared norm.

Then $f(w) = g(Xw - y)$, which is convex because it's a convex function composed with a linear function

Convexity in Higher Dimensions

- Twice-differentiable ‘d’-variable function is convex iff:
  – Eigenvalues of Hessian $\nabla^2 f(w)$ are non-negative for all ‘w’.

- True for least squares where $\nabla^2 f(w) = X^TX$ for all ‘w’.
  – It may not be obvious that this matrix has non-negative eigenvalues.

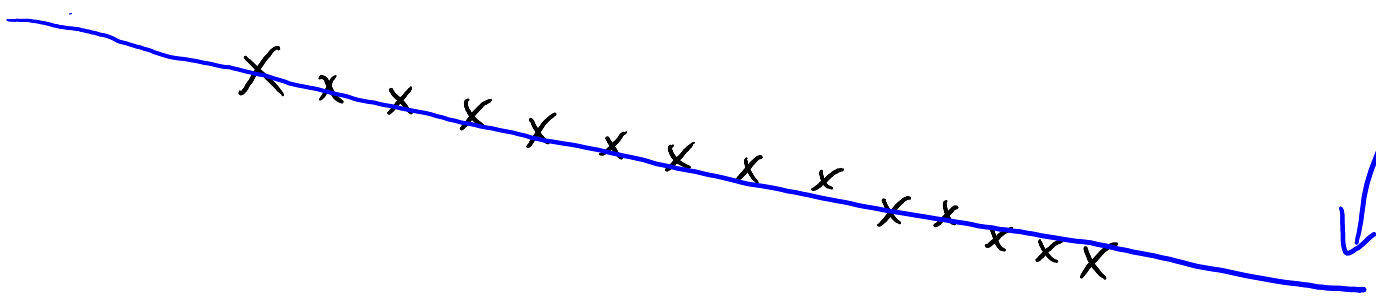
- Unfortunately, sometimes hard to show convexity this way.
  – Usually easier to just use some of the rules as we did on the last slide.

(pause)

Least Squares with Outliers

- Consider least squares problem with outliers in ‘y’:

x ← "outlier" that doesn't follow trend



This is what we want least squares to do.

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

Least Squares with Outliers

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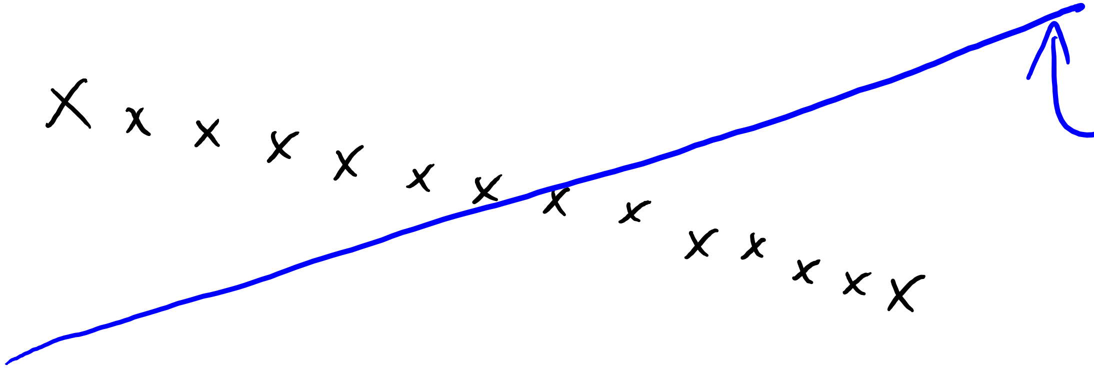
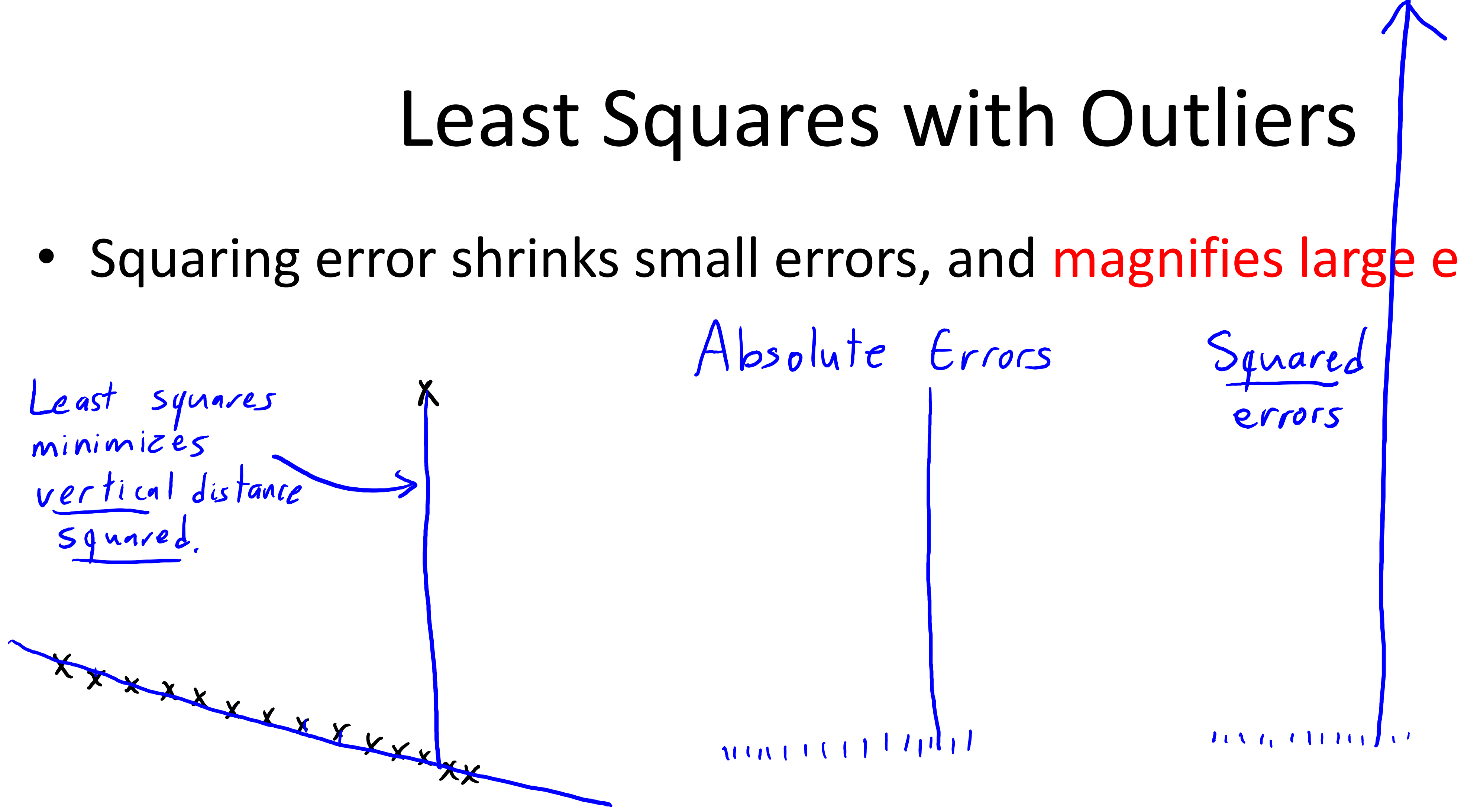


This is what least squares will actually do.

- 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

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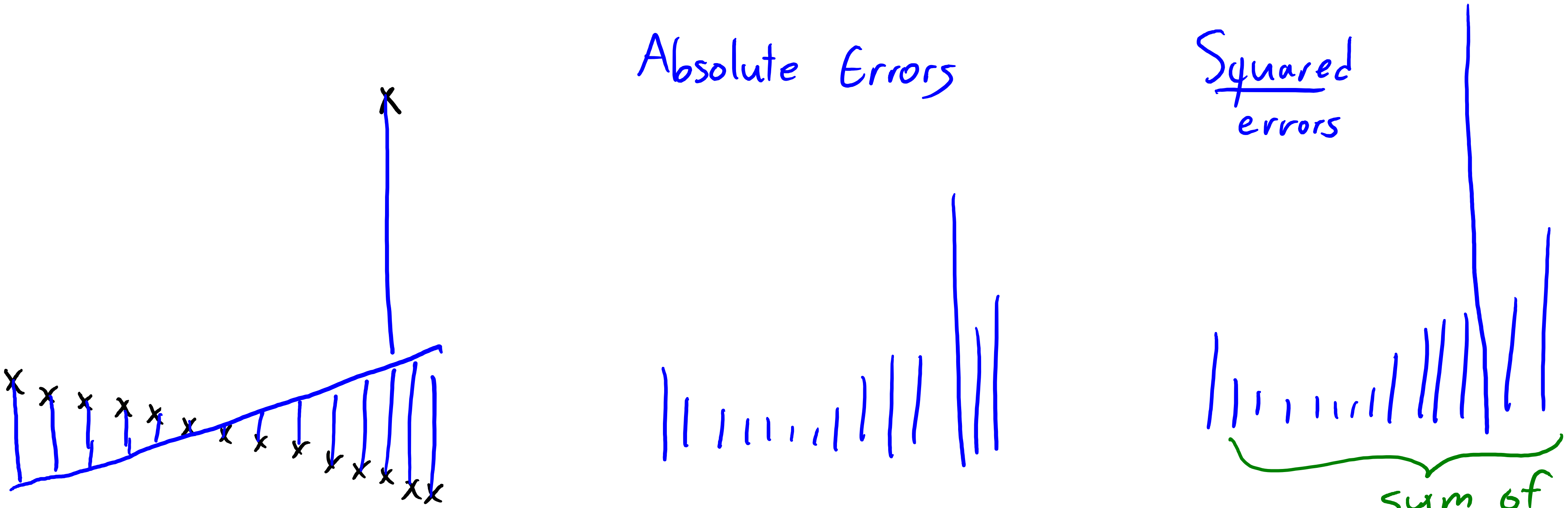


- Outliers (large error) influence 'w' much more than other points.
  - Good if outlier means 'plane crashes', bad if it means 'data entry error'.

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

Summary

- Gradient descent finds critical point of differentiable function.
  - Finds global optimum if function is convex.
- Convex functions:
  - Set of functions with property that $\nabla f(w) = 0$ implies 'w' is a global min.
  - Can (usually) be identified using a few simple rules.
- Outliers in 'y' can cause problem for least squares.

- Next time:
  - Linear regression without the outlier sensitivity…

Constraints, Continuity, Smoothness

- Sometimes we need to optimize with constraints:
  - Later we'll see "non-negative least squares".

$$\min_{w \geq 0} \frac{1}{2}\sum_{i=1}^{n}(w^Tx_i - y_i)^2$$

  - A vector 'w' satisfying w ≥ 0 (element-wise) is said to be "feasible".
- Two factors affecting difficulty are continuity and smoothness.
  - Continuous functions tend to be easier than discontinuous functions.
  - Smooth/differentiable functions tend to be easier than non-smooth.
  - See the calculus review here if you haven't heard these words in a while.

Convexity, min, and argmin

- If a function is convex, then all critical points are global optima.

- However, convex functions don't necessarily have critical points:
  - For example, f(x) = a*x, f(x) = exp(x), etc.

- Also, more than one 'x' can achieve the global optimum:
  - For example, f(x) = c is minimized by any 'x'.

Why use the negative gradient direction?

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

$$f(w^{t+1}) = f(w^t) + \nabla f(w^t)^T (w^{t+1} - w^t) + \frac{1}{2}(w^{t+1} - w^t) \underbrace{\nabla^2 f(v)}_{\text{for some 'v' between } w^{t+1} \text{ and } w^t} (w^{t+1} - w^t)$$

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

$$f(w^{t+1}) = f(w^t) + \nabla f(w^t)^T (w^{t+1} - w^t) + \underbrace{O(\|w^{t+1} - w^t\|^2)}_{\text{becomes negigible as } w^{t+1} \text{ gets close to } w^t}$$

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

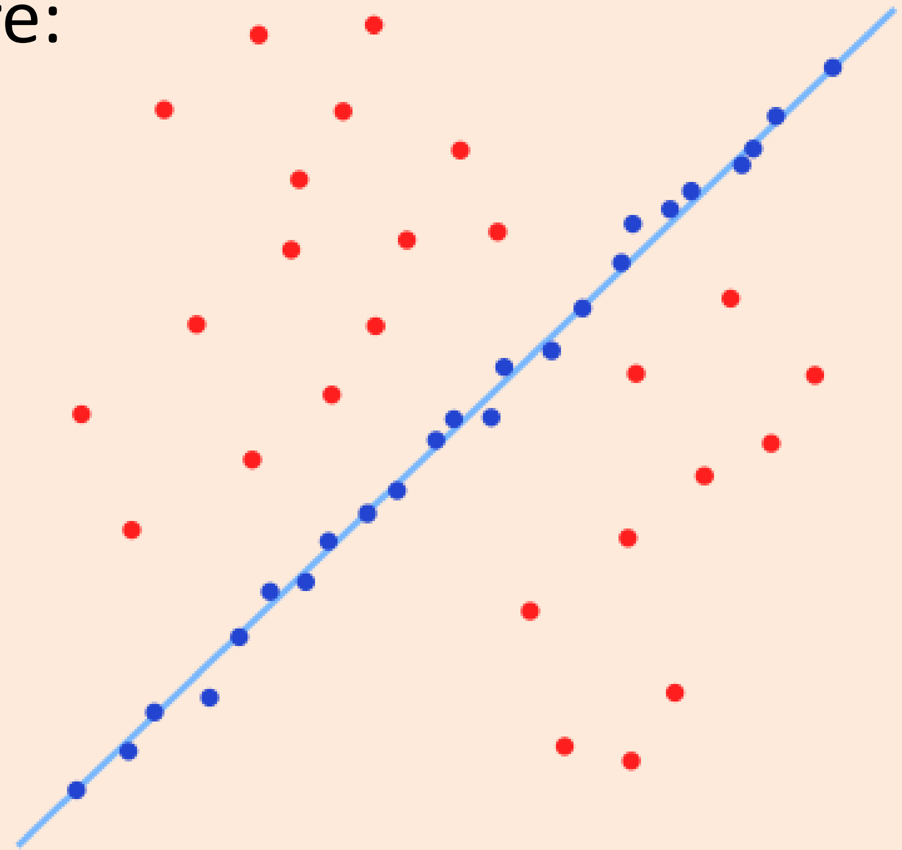
This will work for a while, but notice that

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

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

Random Sample Consensus (RANSAC)

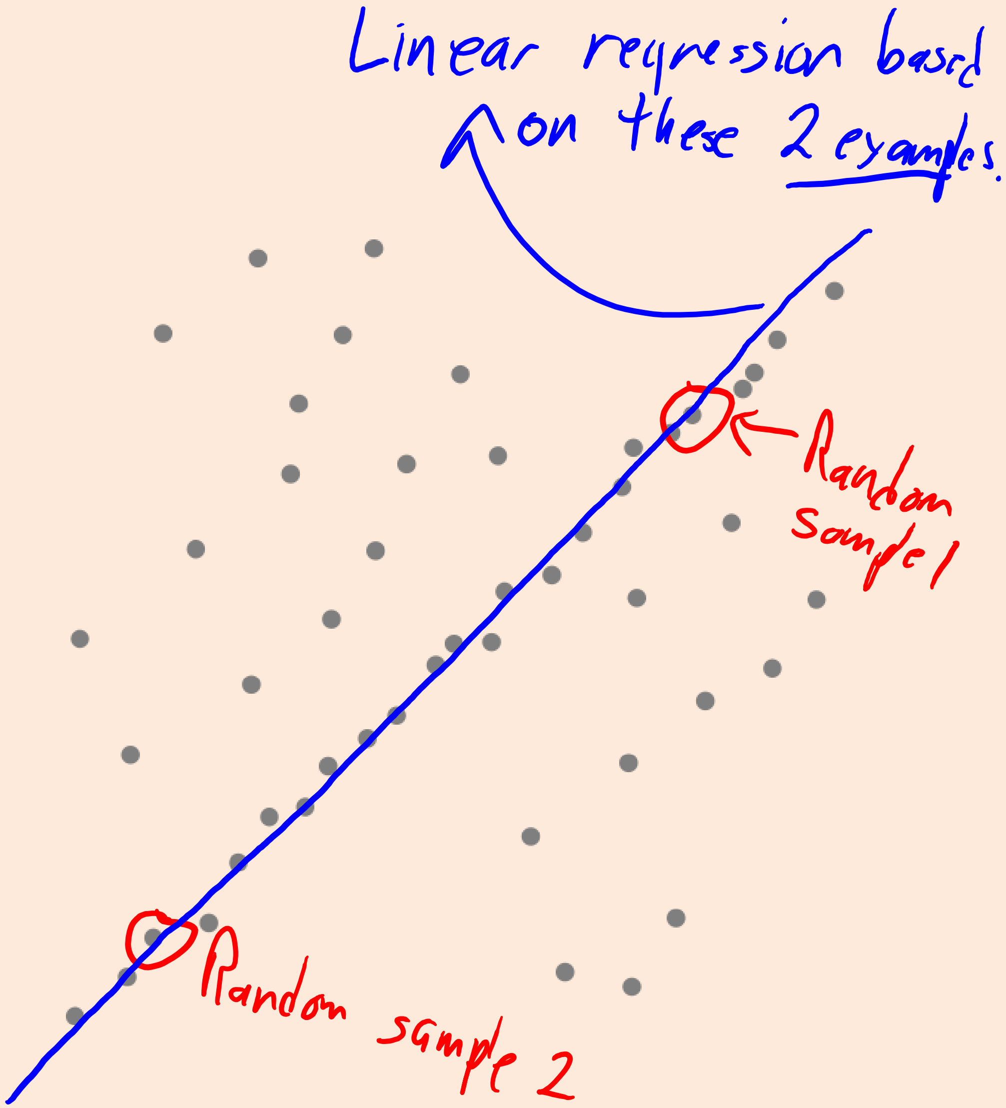
- In computer vision, a widely-used generic framework for robust fitting is random sample consensus (RANSAC).
- This is designed for the scenario where:
  - You have a large number of outliers.
  - Majority of points are “inliers”: it’s really easy to get low error on them.



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".



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