CS 4375
Linear Regression

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Slides adapted from Nick Rouzzi and Sriraam Natarajan

Recap: Course Topics

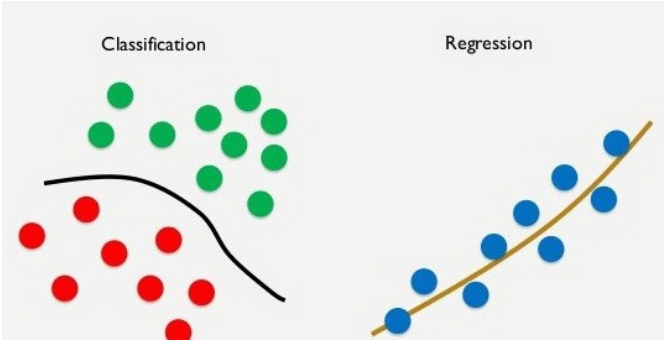
- **Supervised Learning**
  - SVMs & kernel methods
  - Decision trees, Random Forests, Gradient Boosted Trees
  - Nearest Neighbor: KNN Classifiers
  - Logistic Regression
  - Neural networks
  - Probabilistic models: Bayesian networks, Naïve Bayes
- **Unsupervised Learning**
  - Clustering: k-means & spectral clustering
  - Dimensionality reduction
  - PCA
  - Matrix Factorizations
- **Parameter estimation**
  - Bayesian methods, MAP estimation, maximum likelihood estimation, expectation maximization, …
- **Evaluation**
  - AOC, cross-validation, precision/recall
- **Statistical Methods**
  - Boosting, bagging, bootstrapping
  - Sampling
- **Reinforcement Learning, Semi-supervised Learning, Active Learning, ….**

Part I: Recap of Supervised Learning and Linear Regression Setup

Recap: Supervised Learning

- **Input:** $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(M)}, y^{(M)}\right)$
  - $x^{(m)}$ is the m^{th} data item and $y^{(m)}$ is the m^{th} **label**

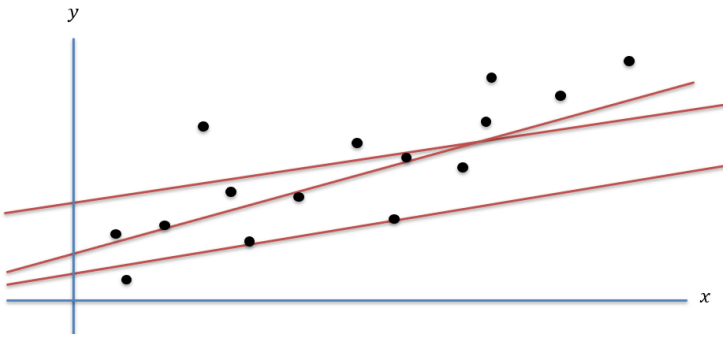
- **Goal:** find a function f such that $f\left(x^{(m)}\right)$ is a "good approximation" to $y^{(m)}$
  - Can use it to predict y values for previously unseen x values

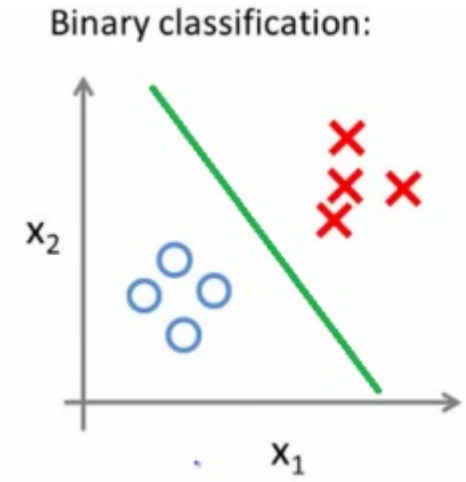


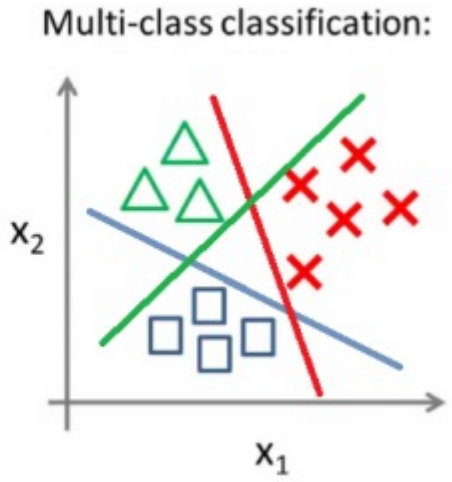
Recap: Classification vs Regression

Classification vs Regression

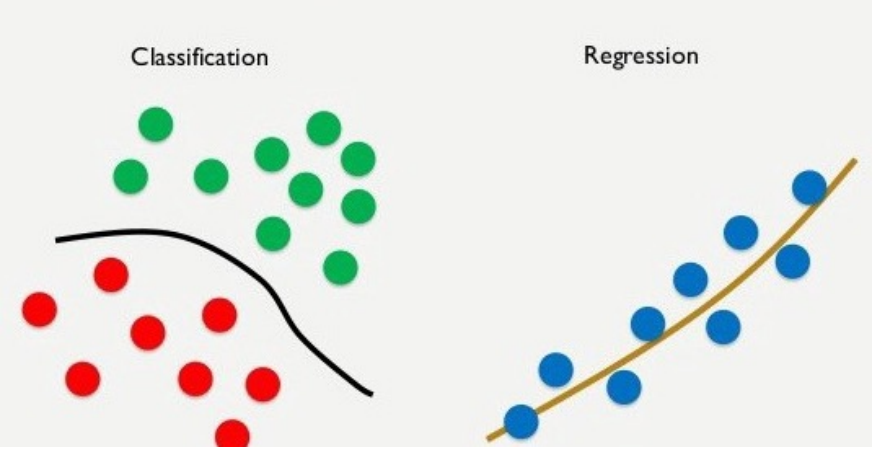
- Input: pairs of points $\left(x^{(1)}, y^{(1)}\right), \ldots, (x^{(M)}, y^{(M)})$ with $x^{(m)} \in \mathbb{R}^n$
- Regression case: $y^{(m)} \in \mathbb{R}$
- Classification case: $y^{(m)} \in [0, k-1]$ [k-class classification]
- If k = 2, we get Binary classification







Recap: Examples of Supervised Learning



Classification

- Spam email detection
- Handwritten digit recognition
- Medical Diagnosis
- Fraud Detection
- Face Recognition

Regression

- Housing Price Prediction
- Stock Market Prediction
- Weather Prediction
- Market Analysis and Business Trends

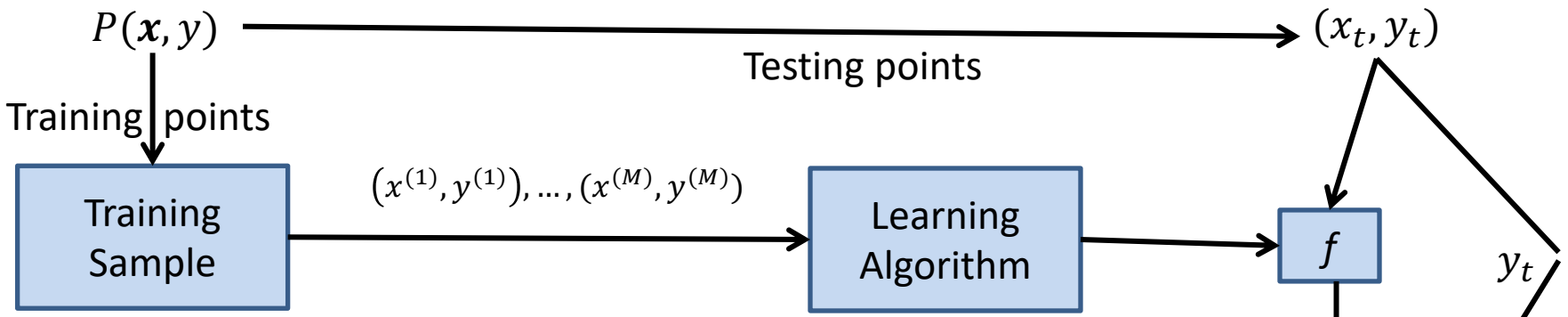
Recap: Hypothesis Space

- Hypothesis space (Aka Model): set of allowable functions $f: X \rightarrow Y$

- Goal: find the "best" element of the hypothesis space

  - How do we measure the quality of f?

Recap: Supervised Learning Workflow



- **Step 1:** Collect Training Data
  $(x^{(1)}, y^{(1)}), \ldots, (x^{(M)}, y^{(M)})$
- **Step 2:** Select Model f and Loss function L
- **Step 3**: Solve Learning Problem:

$$\min_f \sum_{i=1:m} L(f(x^i), y^i)$$

- **Step 4:** Obtain Predictions $\hat{y}_t = f(x_t)$ on all **Test Data**
- **Step 5:** Evaluation -- Measure the error $Err(\hat{y}_t, y_t)$

Train set

Generalization

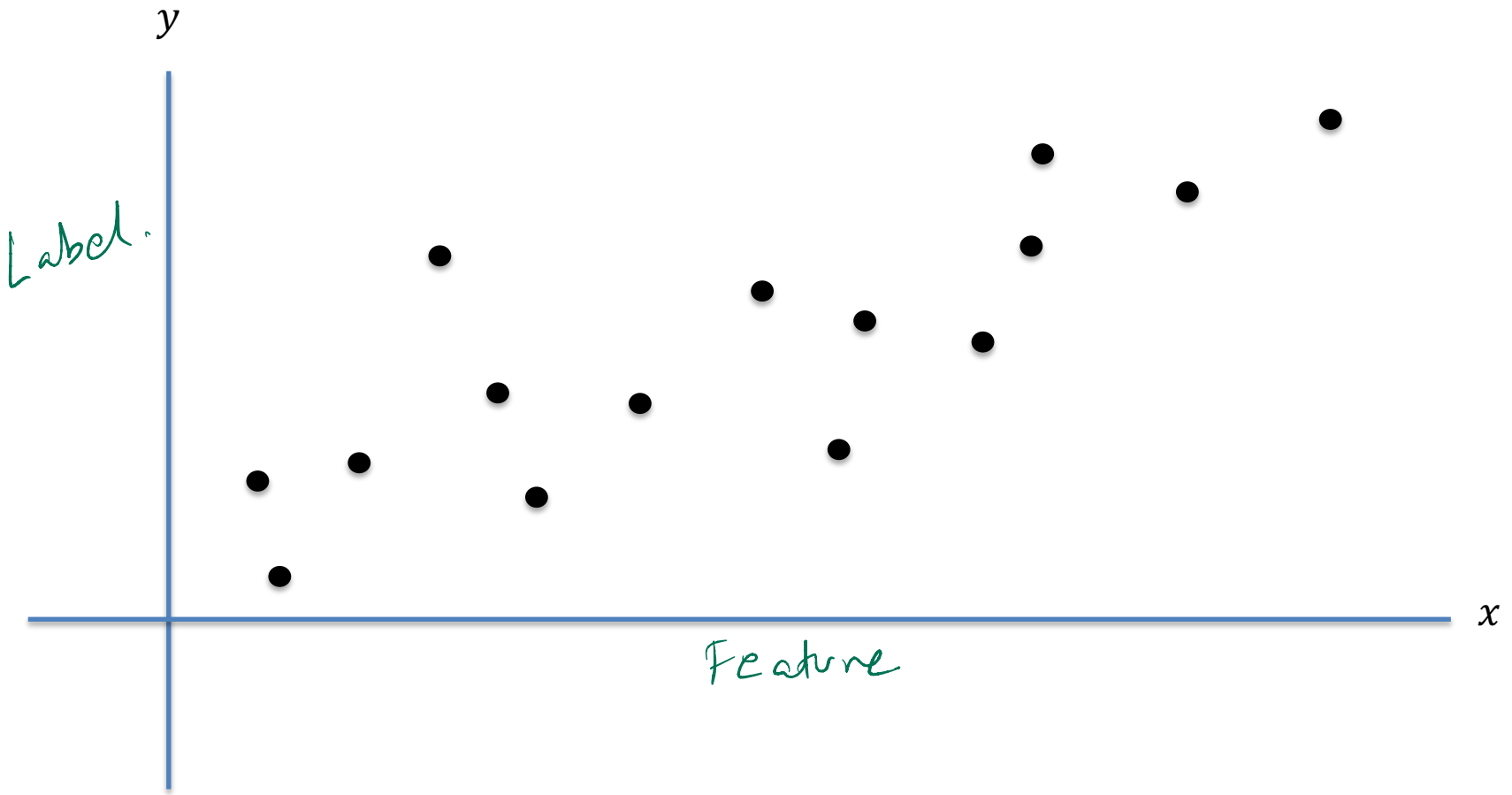
Test set

Linear Regression

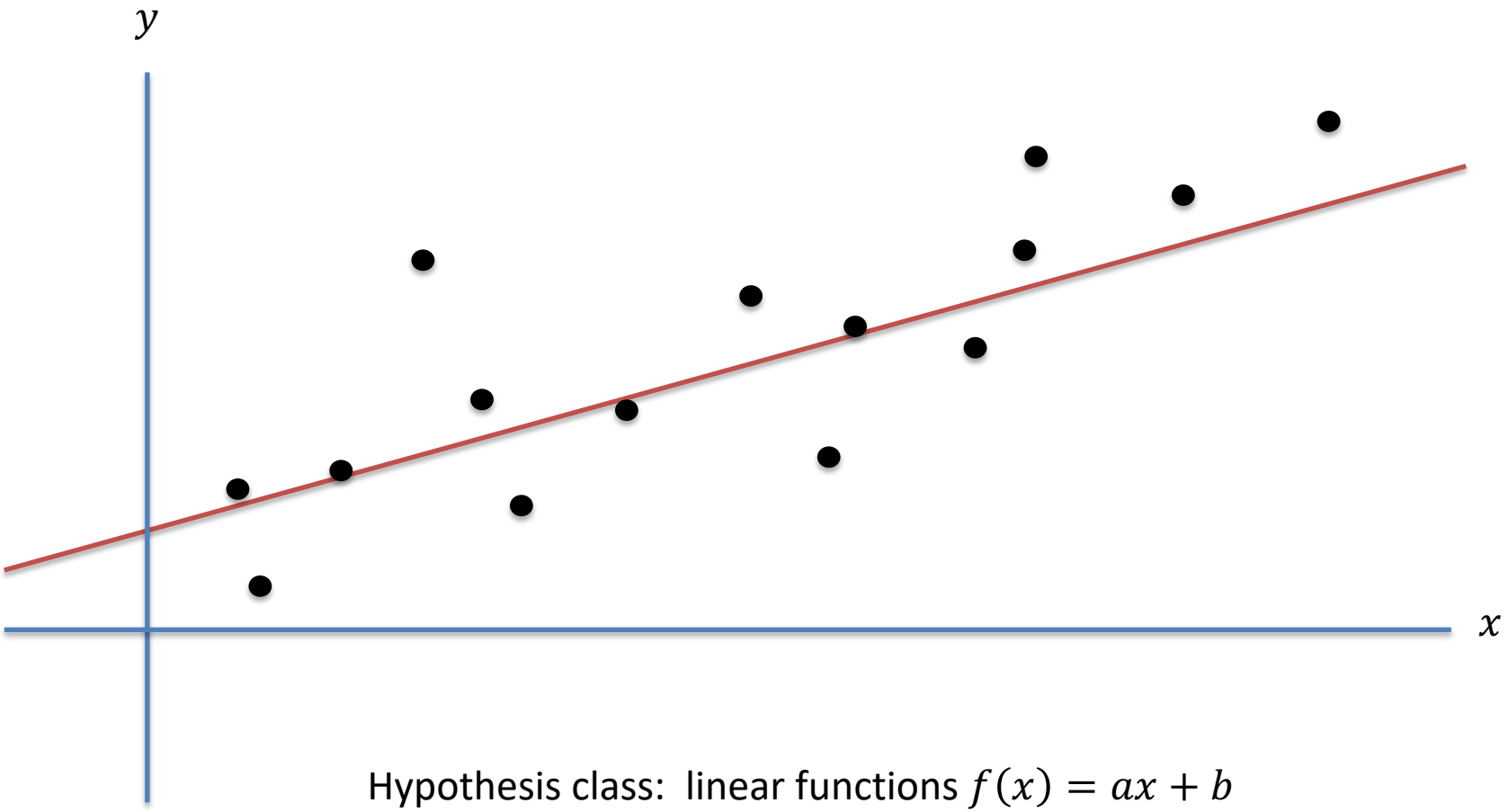
- Simple linear regression
  - Input: pairs of points $(x^{(1)}, y^{(1)}), \ldots, (x^{(M)}, y^{(M)})$ with $x^{(m)} \in \mathbb{R}^d$ and $y^{(m)} \in \mathbb{R}$ (Regression)
  - Hypothesis space: set of linear functions $f(x) = a^T x + b$ with $a \in \mathbb{R}^d, b \in \mathbb{R}$
  - In one dimension, $a, b \in \mathbb{R}$ and $f(x) = ax + b$
  - Error metric and Loss Function: squared difference between the predicted value and the actual value

$[y - f(x)]^2$, $|y - f(x)|$

Regression



Regression



Hypothesis class: linear functions $f(x) = ax + b$

How do we compute the error of a specific hypothesis?

Linear Regression

- For any data point, x, the learning algorithm predicts $f(x)$
- In typical regression applications, measure the fit using a squared loss function

normalization

$$L(f) = \frac{1}{M}\sum_{m=1}^{M}\left(f\left(x^{(m)}\right) - y^{(m)}\right)^2$$

(a, b)

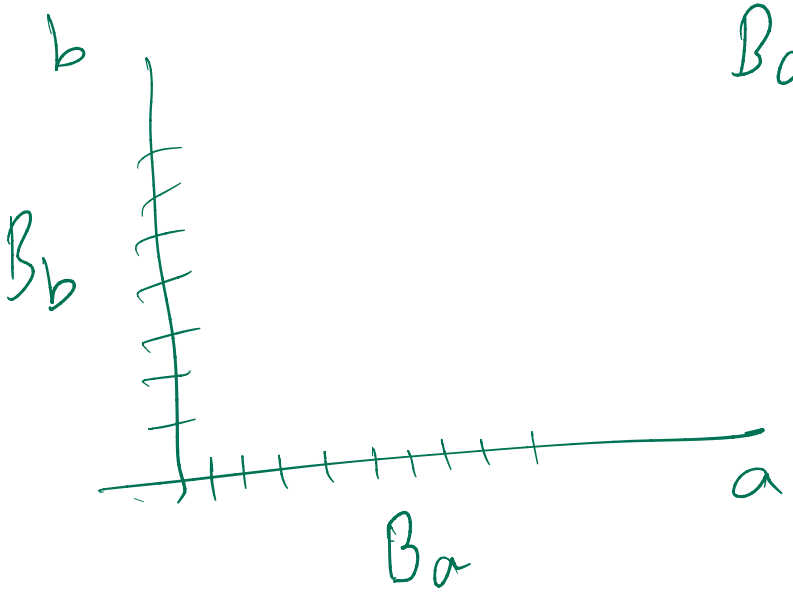
- Want to minimize the average loss on the training data
- The optimal linear hypothesis is then given by

$$\min_{a,b} \frac{1}{M}\sum_{m=1}^{M}\left(ax^{(m)} + b - y^{(m)}\right)^2$$

Linear Regression

$$\min_{a,b} \frac{1}{M} \sum_{m} \left(ax^{(m)} + b - y^{(m)} \right)^2$$

- How do we find the optimal a and b?



$B_{a_1} \times B_{a_2} \cdots \times B_{a_d} \times B_b$

Linear Regression

$$\min_{a,b} \frac{1}{M} \sum_{m} \left(ax^{(m)} + b - y^{(m)} \right)^2$$

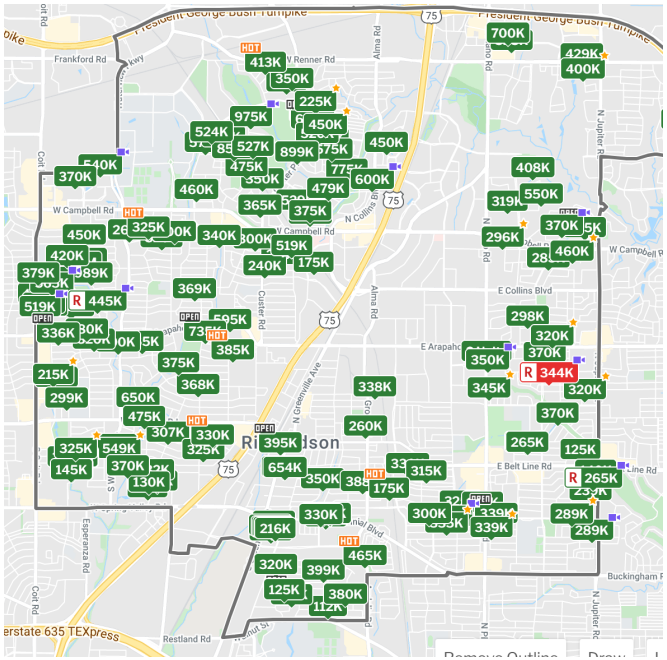
- How do we find the optimal a and b?
  - Solution 1: take derivatives and solve
    (there is a closed form solution!)
  - Solution 2: use gradient descent

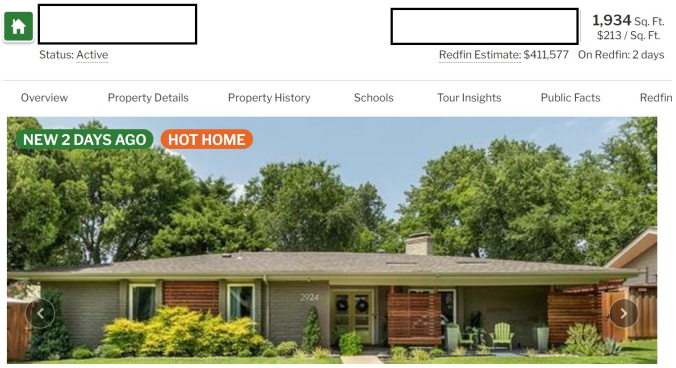
Linear Regression

$$\min_{a,b} \frac{1}{M} \sum_{m} \left(a x^{(m)} + b - y^{(m)} \right)^2$$

- How do we find the optimal a and b?
  - Solution 1: take derivatives and solve
    (there is a closed form solution!)
  - Solution 2: use gradient descent
    - This approach is much more likely to be useful for general loss functions

Recap – Housing Price Prediction Application





Home Facts

Status	Active	Time on Redfin	2 days
Property Type	Residential, Single Family	HOA Dues	$4/month
Year Built	1969	Style	Single Detached, Mid-Century Modern, Ranch, Traditional
Community	Canyon Creek Country Club 9	Lot Size	10,019 Sq. Ft.
MLS#	14375892		

Part II: Gradient Descent and Optimization

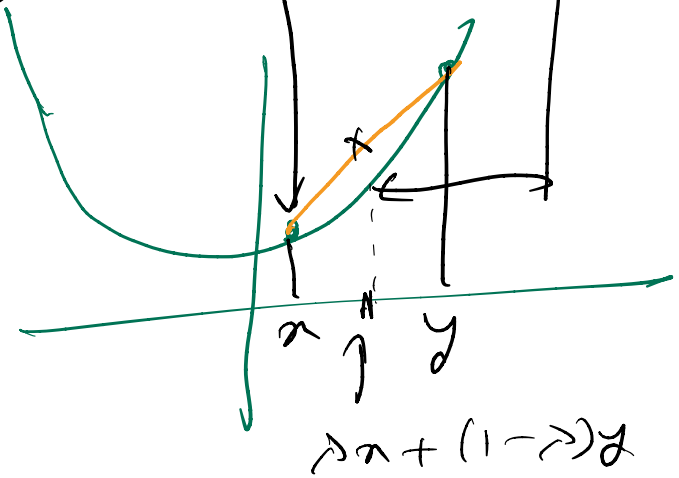
Gradient Descent

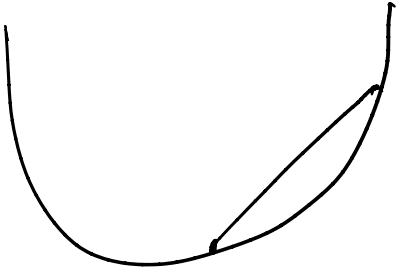
Iterative method to minimize a (convex) differentiable function f

A function $f: \mathbb{R}^n \to \mathbb{R}$ is convex if

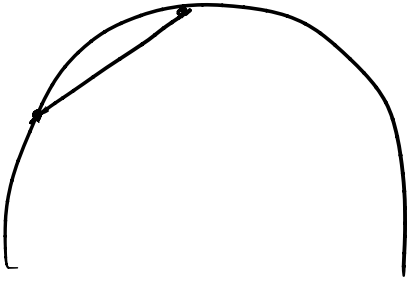
$$\lambda f(x) + (1-\lambda) f(y) \geq f(\lambda x + (1-\lambda) y)$$

for all $\lambda \in [0,1]$ and all $x, y \in \mathbb{R}^n$

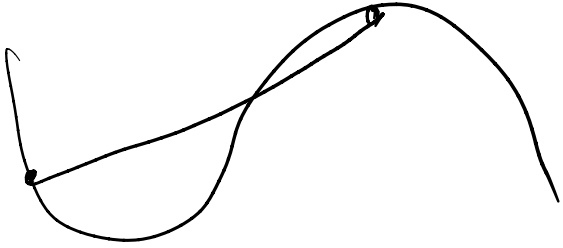




Convex



Concave



Not convex nor concave.

Gradient Descent

Iterative method to minimize a (convex) differentiable function f

- Pick an initial point x_0
- Iterate until convergence

$$x_{t+1} = x_t - \gamma_t \nabla f(x_t)$$

where γ_t is the t^{th} step size (sometimes called learning rate)

$$x_{t+1} = x_t - \gamma_t \frac{df}{dx_t}$$

Basics of Convexity and Gradient Desc

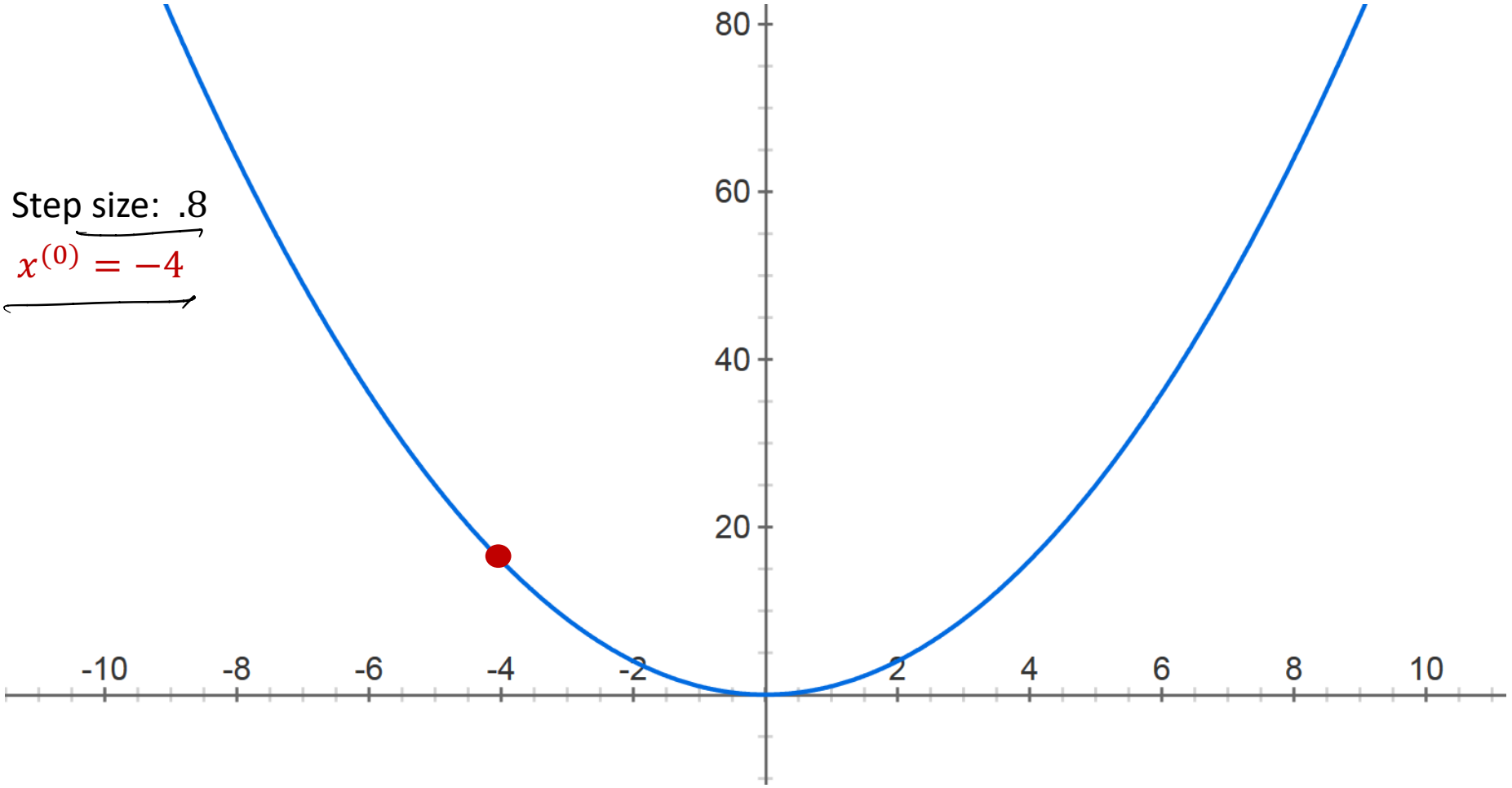
- For additional reading, please see some of my slides from my Spring 2020 Class “Optimization in Machine Learning”
- Github Location for Lecture Notes and Slides: https://github.com/rishabhk108/OptimizationML
- Please skim through:
  - Lectures 1 and 2 for basics
  - Lectures 3-5 for convex functions
  - Lectures 6-8 on Gradient Descent
  - This includes slightly more mathematical details like convergence analysis and proofs for convergence etc.

Gradient Descent

$f(x) = x^2$

Step size: .8

$x^{(0)} = -4$



Gradient Descent

$f(x) = x^2$

$\frac{df}{dx} = 2x$

$\gamma = 0.8$

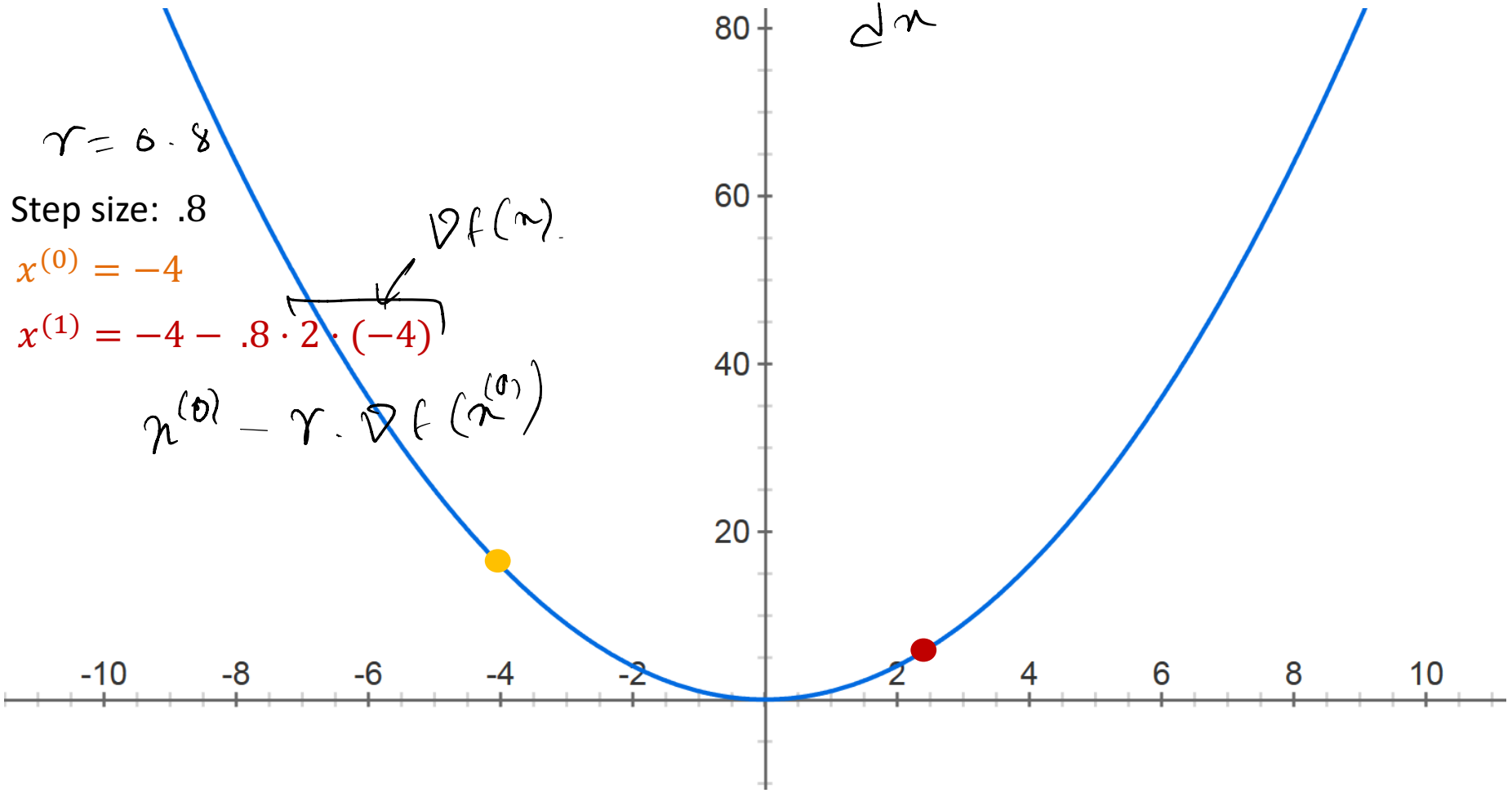
Step size: .8

$x^{(0)} = -4$

$\nabla f(x)$

$x^{(1)} = -4 - .8 \cdot 2 \cdot (-4)$

$x^{(0)} - \gamma \cdot \nabla f(x^{(0)})$



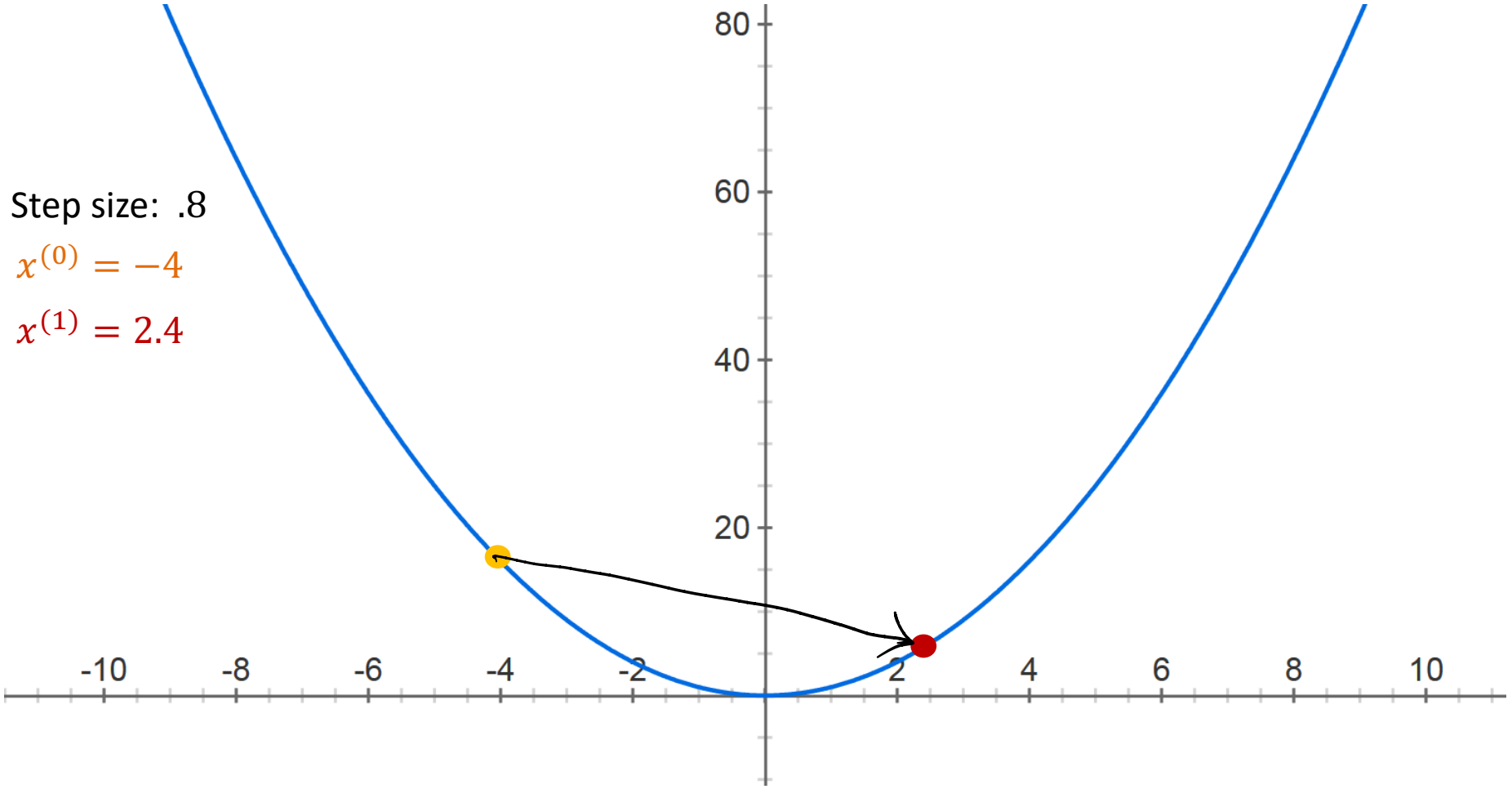
Gradient Descent

$f(x) = x^2$

Step size: .8

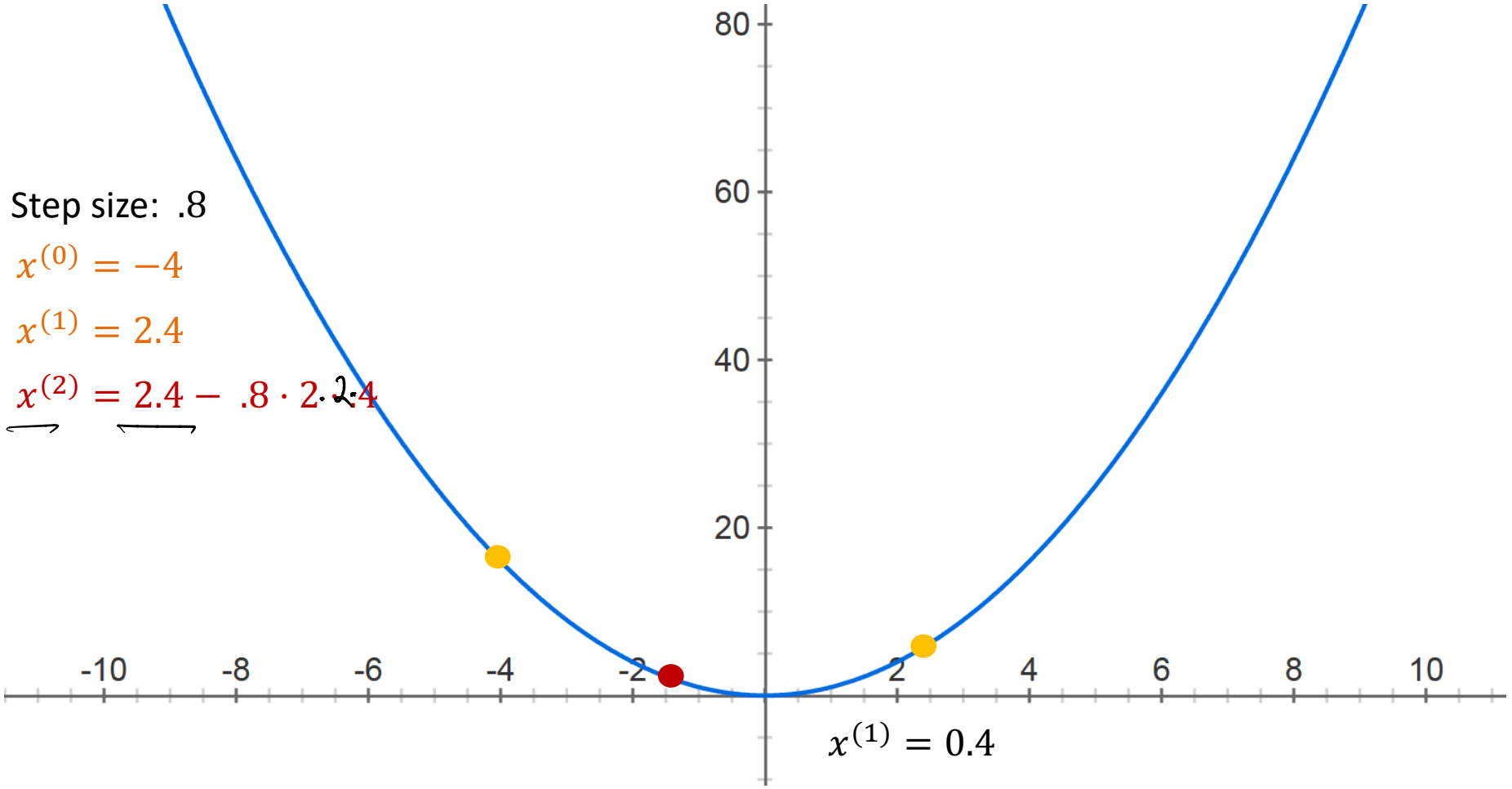
$x^{(0)} = -4$

$x^{(1)} = 2.4$



Gradient Descent

$f(x) = x^2$



Step size: .8

$x^{(0)} = -4$

$x^{(1)} = 2.4$

$x^{(2)} = 2.4 - .8 \cdot 2.4$

Gradient Descent

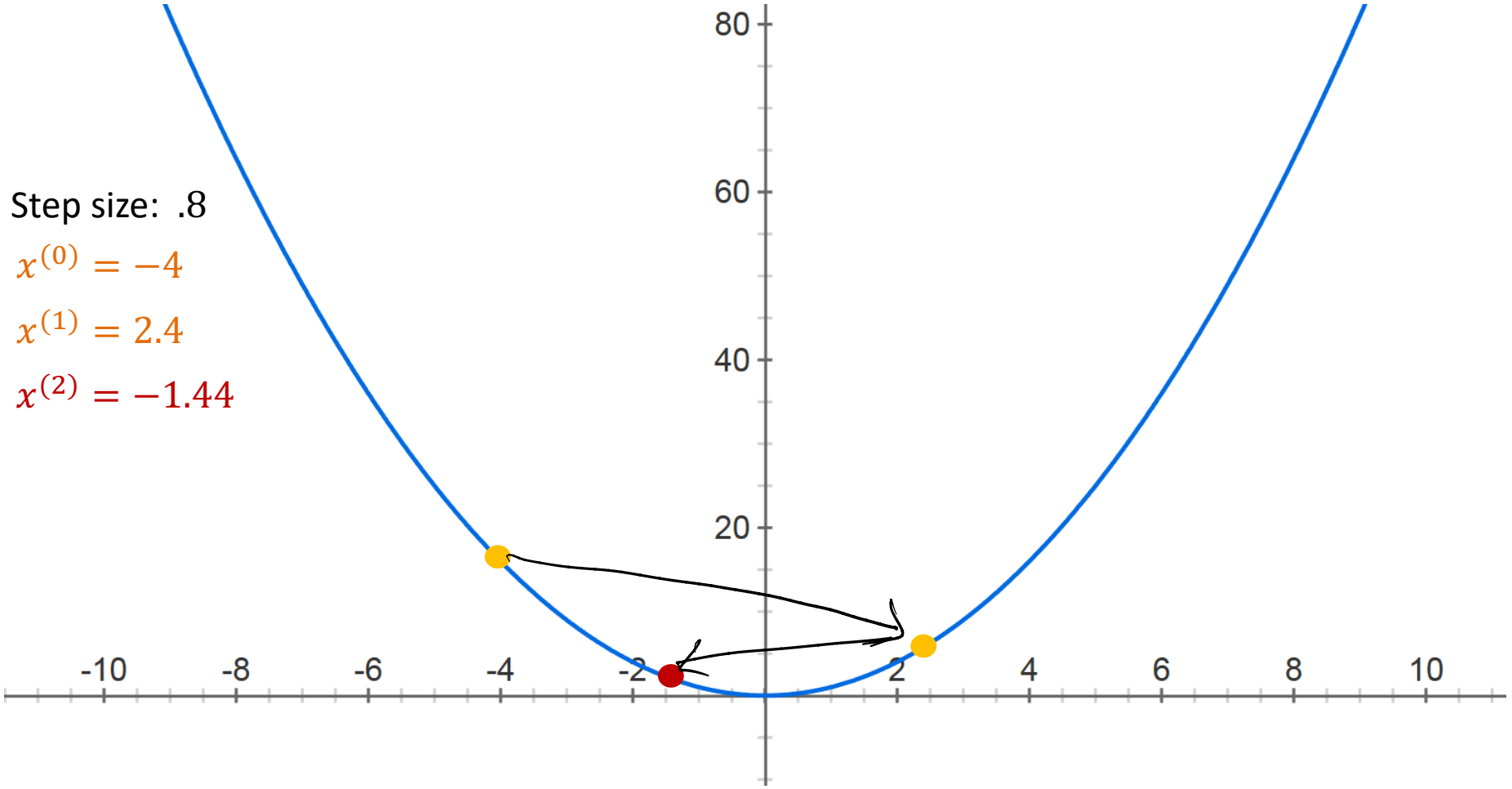
$f(x) = x^2$

Step size: .8

$x^{(0)} = -4$

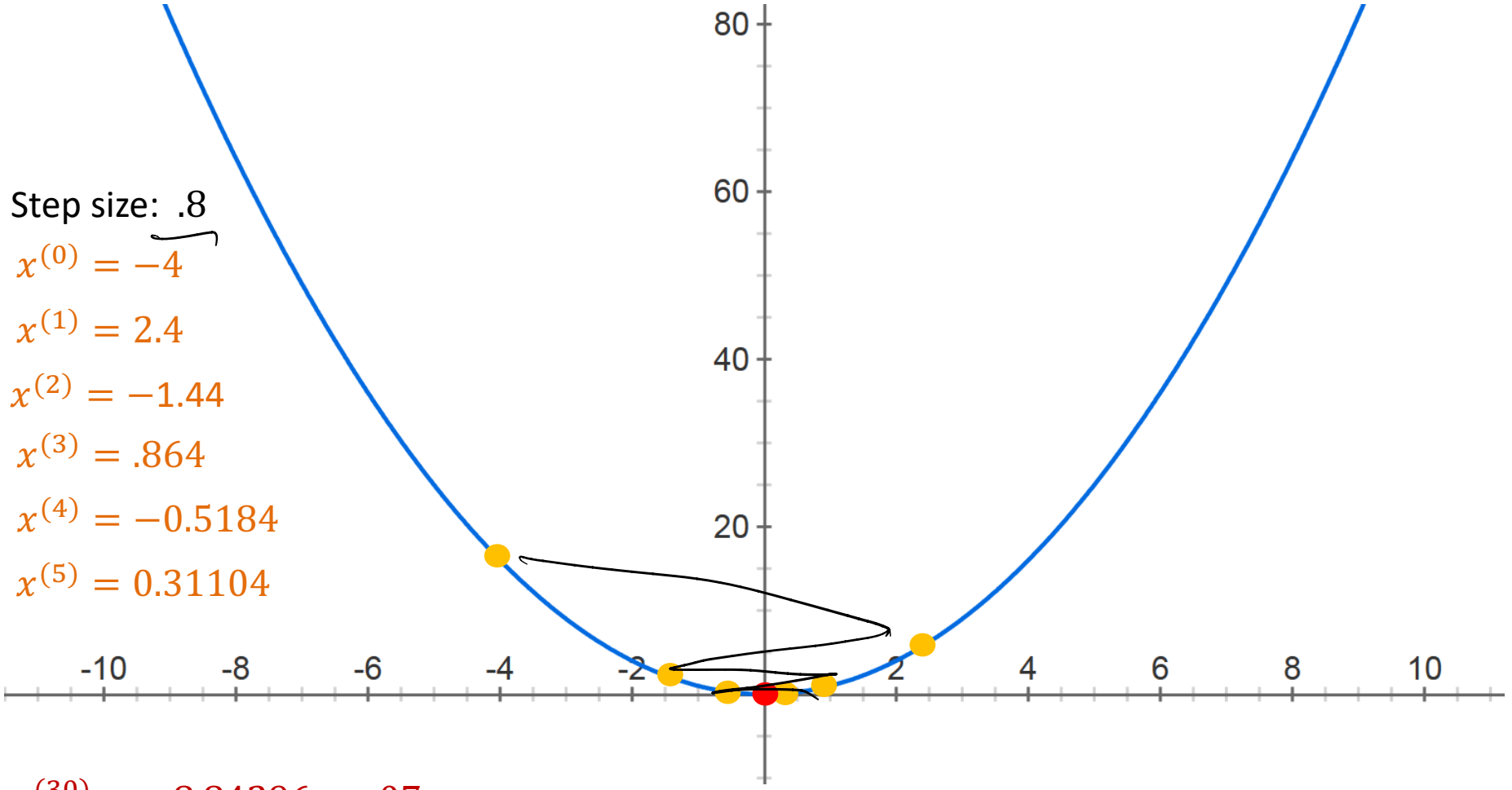
$x^{(1)} = 2.4$

$x^{(2)} = -1.44$



Gradient Descent

$f(x) = x^2$



Step size: .8

$x^{(0)} = -4$

$x^{(1)} = 2.4$

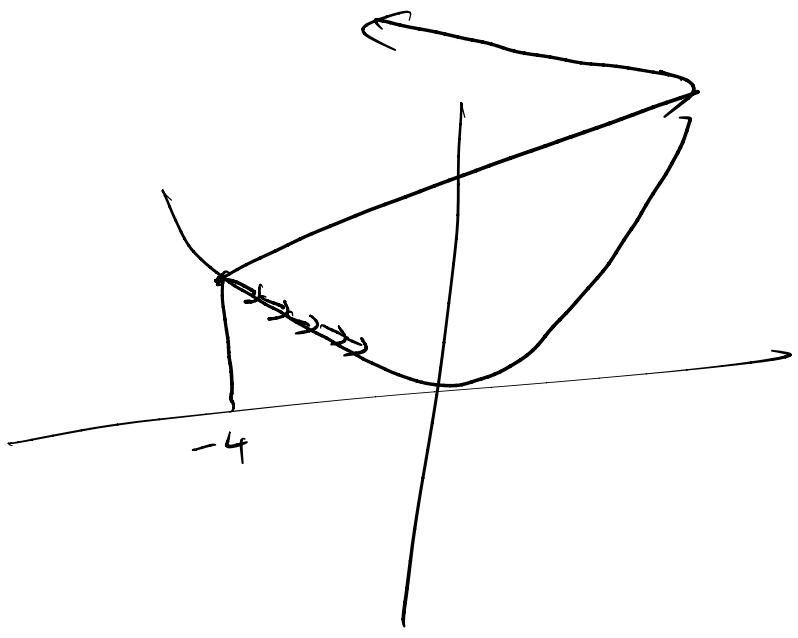
$x^{(2)} = -1.44$

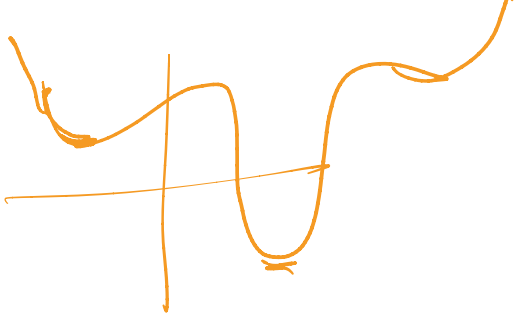
$x^{(3)} = .864$

$x^{(4)} = -0.5184$

$x^{(5)} = 0.31104$

$x^{(30)} = -8.84296e - 07$





$x^{(0)} = -4$

$r = 0.08$

$x^{(1)} = -4 - 2(-4)(0.08)$

$= -4 + 8 \cdot (0.08)$

$= -3.46$

$x^{(0)} = -4$

$r = 8$

$x^{(1)} = -4 - 2(-4)(8)$

$= 60$

Gradient Descent

$$\min_{a,b} \frac{1}{M} \sum_{m} \left(ax^{(m)} + b - y^{(m)} \right)^2$$

- What is the gradient of this function?
- What does a gradient descent iteration look like for this simple regression problem?

Derivation of the Gradient (one dim)

$$L(a,b) = \frac{1}{M} \sum_m \left(a x^{(m)} + b - y^{(m)}\right)^2$$

$$\nabla_a L = \frac{\partial L}{\partial a} = \frac{1}{M} \sum_m \frac{\partial}{\partial a} \left(a x^{(m)} + b - y^{(m)}\right)^2$$

$$\nabla_a L = \frac{1}{M} \sum_m 2 \left(a x^{(m)} + b - y^{(m)}\right) x^{(m)}$$

$$\nabla_b L = \frac{\partial L}{\partial b} = \frac{1}{M} \sum_m \frac{\partial}{\partial b} \left(a x^{(m)} + b - y^{(m)}\right)^2$$

$$= \frac{1}{M} \sum_m 2 \left(a x^{(m)} + b - y^{(m)}\right) \cdot 1$$

Linear Regression

- In higher dimensions, the linear regression problem is essentially the same with $x^{(m)} \in \mathbb{R}^n$

$$\min_{a \in \mathbb{R}^n, b} \frac{1}{M} \sum_{m} \left(a^T x^{(m)} + b - y^{(m)} \right)^2$$

- Can still use gradient descent to minimize this
  - Not much more difficult than the $n = 1$ case

Derivation of the Gradient (> 1 dim)

$$L(a,b) = \frac{1}{M}\sum_m \left(a^T x^{(m)} + b - y^{(m)}\right)^2$$

$$\nabla_a L = \frac{1}{M}\sum_m 2\left(a^T x^{(m)} + b - y^{(m)}\right) \nabla_a \left(a^T x^{(m)}\right)$$

$x^{(m)}$ is constant

$$a = (a_1, a_2, \ldots a_n), \quad a^T x^{(m)} = \sum_{i=1}^{n} a_i \cdot x_i^{(m)}$$

$$\nabla_a L = \begin{bmatrix} \partial L/\partial a_1 \\ \partial L/\partial a_2 \\ \vdots \\ \partial L/\partial a_n \end{bmatrix} = \begin{bmatrix} x_1^{(m)} \\ x_2^{(m)} \\ \vdots \\ x_n^{(m)} \end{bmatrix} = x^{(m)}$$

$$\nabla_a L = \frac{1}{M}\sum_m 2\left(a^T x^{(m)} + b - y^{(m)}\right) x^{(m)}$$

Gradient Descent

- Gradient descent converges under certain technical conditions on the function f and the step size γ_t

  $\nabla f = 0$

  - If f is convex, then any fixed point of gradient descent must correspond to a global minimum of f

  - In general, for a nonconvex function, may only converge to a local optimum

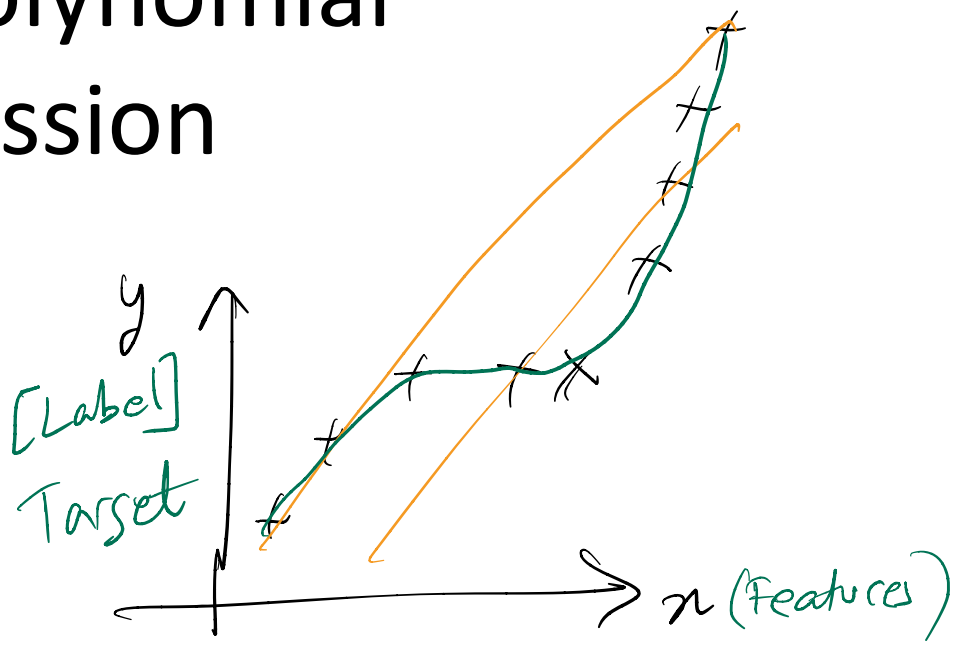
- Very fast convergence because the Linear Regression is *smooth* (loosely, think *differentiable*) and strongly convex (*loosely, bounded below by a quadratic function*)*

* See Lectures 6-8 for better understanding of smooth and strongly convex

Part III: Polynomial Regression

Linear Regression

$$y = a^T x + b$$



Polynomial Regression

- What if we enlarge the hypothesis class?
  - Quadratic functions: $ax^2 + bx + c$
  - k-degree polynomials: $a_k x^k + a_{k-1} x^{k-1} + \cdots + a_1 x + a_0$

$$y^{(m)} = a_k \left(x^{(m)}\right)^k + a_{k-1} \left(x^{(m)}\right)^{k-1} + \cdots + a_1 x^{(m)} + a_0$$

$$\min_{a_k,\ldots,a_0} \frac{1}{M} \sum_m \left(a_k \left(x^{(m)}\right)^k + \cdots + a_1 x^{(m)} + a_0 - y^{(m)} \right)^2$$

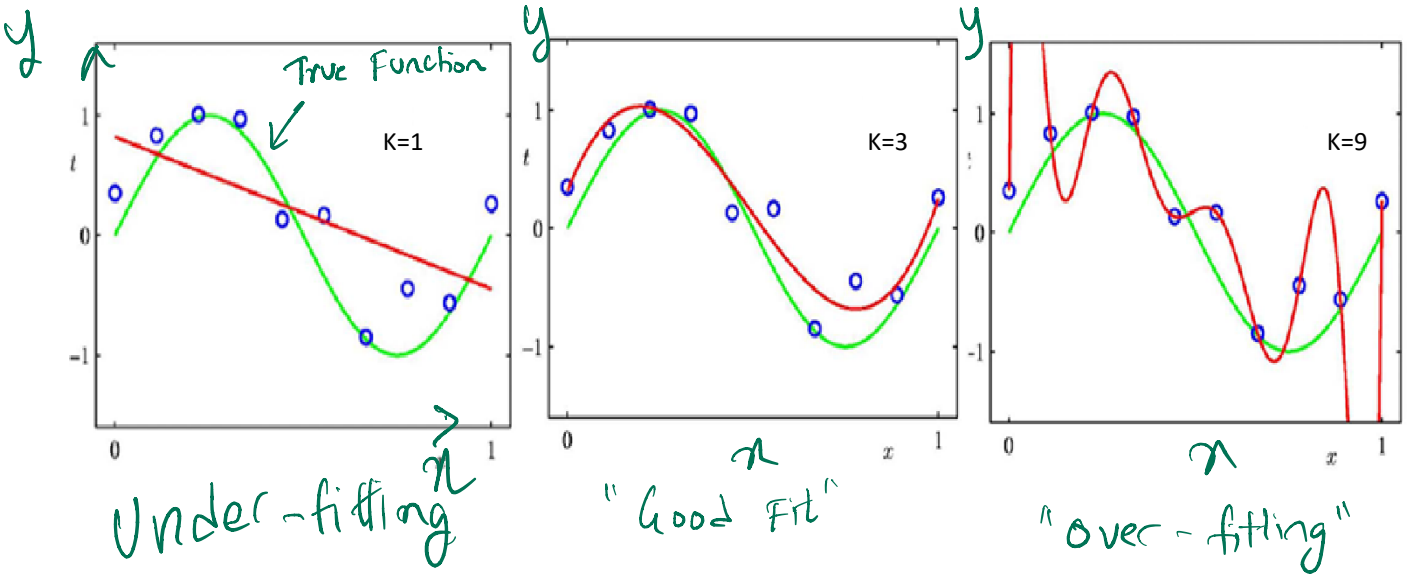
Polynomial Regression

- What if we enlarge the hypothesis class?
  - Quadratic functions: $ax^2 + bx + c$
  - k-degree polynomials: $a_k x^k + a_{k-1} x^{k-1} + \cdots + a_1 x + a_0$
- Can we always learn "better" with a larger hypothesis class?

Polynomial Regression

- What if we enlarge the hypothesis class?
  - Quadratic functions: $ax^2 + bx + c$
  - k-degree polynomials: $a_k x^k + a_{k-1} x^{k-1} + \cdots + a_1 x + a_0$
- Can we always learn "better" with a larger hypothesis class?

Not always true.

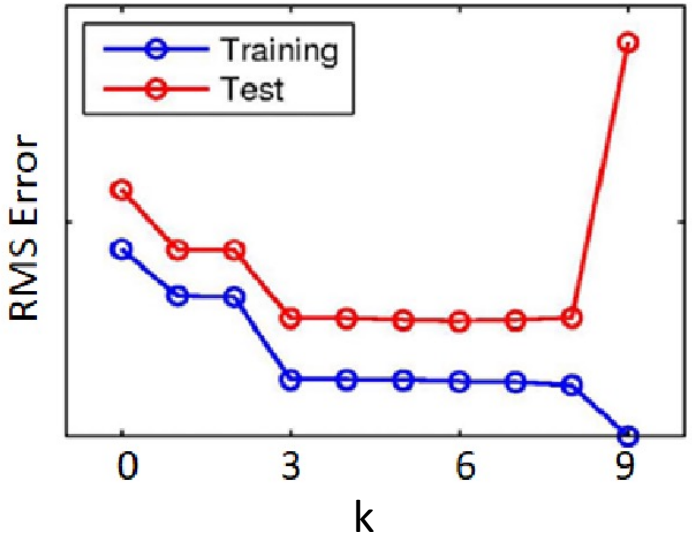


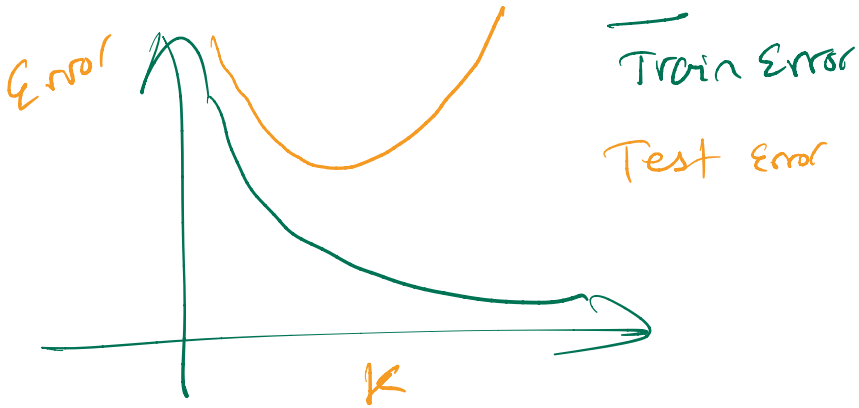
Caveats with Polynomial Regression

- Larger hypothesis space always decreases the cost function, but this does NOT necessarily mean better predictive performance
  - This phenomenon is known as overfitting
  - Ideally, we would select the simplest hypothesis consistent with the observed data
- In practice, we cannot simply evaluate our learned hypothesis on the training data, we want it to perform well on unseen data (otherwise, we can just memorize the training data!)
  - Report the loss on some held-out test data (i.e., data not used as part of the training process)

Overfitting

- As *the degree of the polynomial (k)* increases, training error decreases monotonically
- As *k* increases test error can increase
- Test error can decrease at first, but increases
- Overfitting can occur
  - When the model is too complex and trivially fits the data (i.e., too many parameters)
  - When the data is not enough to estimate the parameters
  - Model captures the noise (or the chance)





Quadratic Models

$$y = ax^2 + bx + c \quad , x \in \mathbb{R}.$$

$$x = [x_1, x_2, \ldots, x_d] \qquad x \in \mathbb{R}^d$$

$$y = a_1 x_1^2 + a_2 x_2^2 + \ldots + a_d x_d^2 + \sum_{i,j : i>j} a_{ij} x_i x_j + b_1 x_1 + b_2 x_2 + \ldots + b_d x_d + c$$

Polynomial Functions ≡ Polynomial Features with Linear Functions

$$y = a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k$$

$$= \underbrace{[a_1, a_2, \cdots, a_k]}_{A} \underbrace{\begin{bmatrix} x \\ x^2 \\ \vdots \\ x^k \end{bmatrix}}_{X^k} + a_0$$

$$= A^T X^k + a_0$$

$X^k \equiv$ Polynomial Features

Part IV: Hands On

House Price Prediction

- Boston House Price Dataset

CRIM: Per capita crime rate by town
ZN: Proportion of residential land zoned for lots over 25,000 sq. ft
INDUS: Proportion of non-retail business acres per town
CHAS: Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)
NOX: Nitric oxide concentration (parts per 10 million)
RM: Average number of rooms per dwelling
AGE: Proportion of owner-occupied units built prior to 1940
DIS: Weighted distances to five Boston employment centers
RAD: Index of accessibility to radial highways
TAX: Full-value property tax rate per $10,000
PTRATIO: Pupil-teacher ratio by town
B: $1000(Bk - 0.63)^2$, where Bk is the proportion of [people of African American descent] by town
LSTAT: Percentage of lower status of the population
MEDV: Median value of owner-occupied homes in $1000s

Feature

Label

Summary of the Hands On Portion

- Load the Dataset
- Exploratory Data Analysis
- Training a Linear Regression Model
- Training a Polynomial Regression Model
- Training a Linear/Poly Regression from scratch using gradient descent

Evaluation Criteria

$$MSE = \sum_{i=1}^{n} \left[y^{(i)} - \hat{y}^{(i)} \right]^2$$

$$RMSE = \sqrt{MSE}$$

$$R2 = 1 - \frac{RMSE}{RMSE_{Avg}}$$

$$RMSE_{Avg} = \sqrt{\sum_{i=1}^{n} \left[y^{(i)} - \frac{\sum_{i=1}^{n} y^{(i)}}{n} \right]^2}$$