CS 6375
Linear Regression

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Slides adapted from Nick Rouzzi and Sriraam Natarajan

Recap: Course Topics

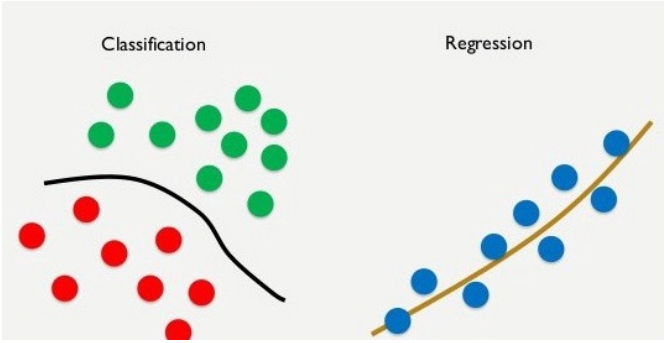
- **Supervised Learning**
  - SVMs & kernel methods
  - Decision trees, Random Forests, Gradient Boosted Trees
  - Nearest Neighbor: KNN Classifiers
  - Logistic Regression
  - Neural networks
  - Probabilistic models: Bayesian networks, Naïve Bayes
- **Unsupervised Learning**
  - Clustering: k-means & 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:** $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(M)}, y^{(M)}\right)$ ← Training Dataset
  - $x^{(m)}$ is the m^{th} data item and $y^{(m)}$ is the m^{th} **label**

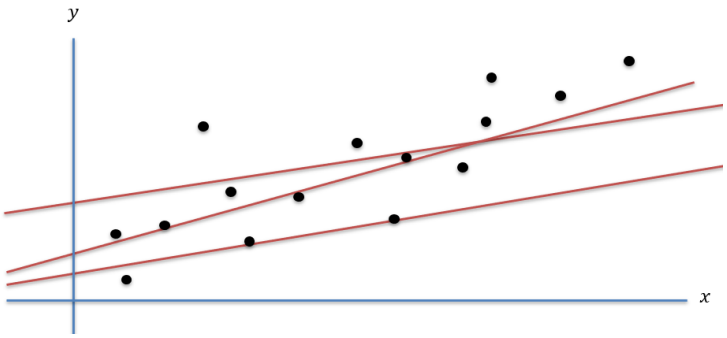
- **Goal:** find a function f such that $f\left(x^{(m)}\right)$ is a "good approximation" to $y^{(m)}$
  - Can use it to predict y values for previously unseen x values

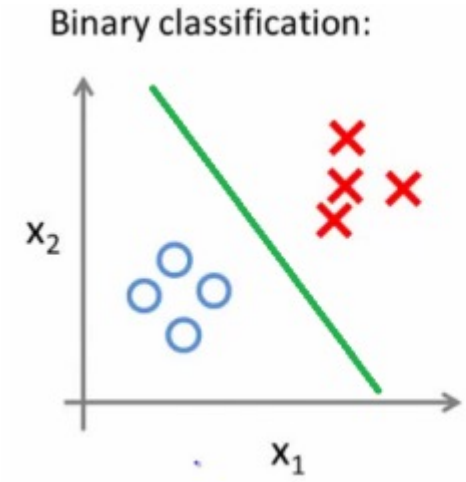


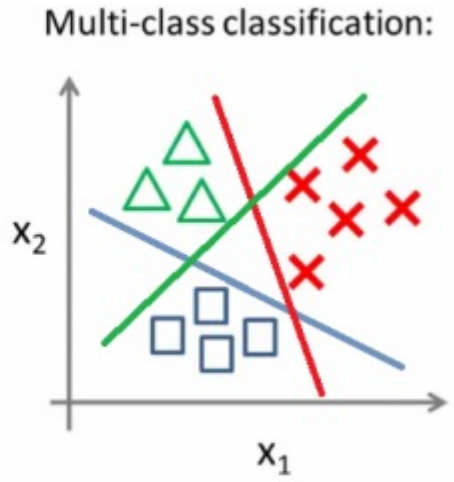
Recap: Classification vs Regression

Classification vs Regression

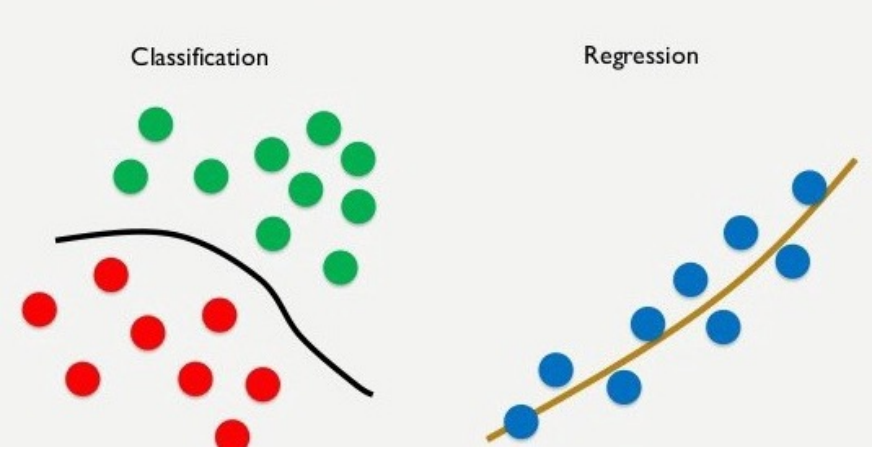
- Input: pairs of points $(x^{(1)}, y^{(1)}), \ldots, (x^{(M)}, y^{(M)})$ with $x^{(m)} \in \mathbb{R}^d$ d = # Features
- Regression case: $y^{(m)} \in \mathbb{R}$ $y^{(m)}$ is continuous
- Classification case: $y^{(m)} \in [0, k-1]$ [k-class classification]
- If k = 2, we get Binary classification







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

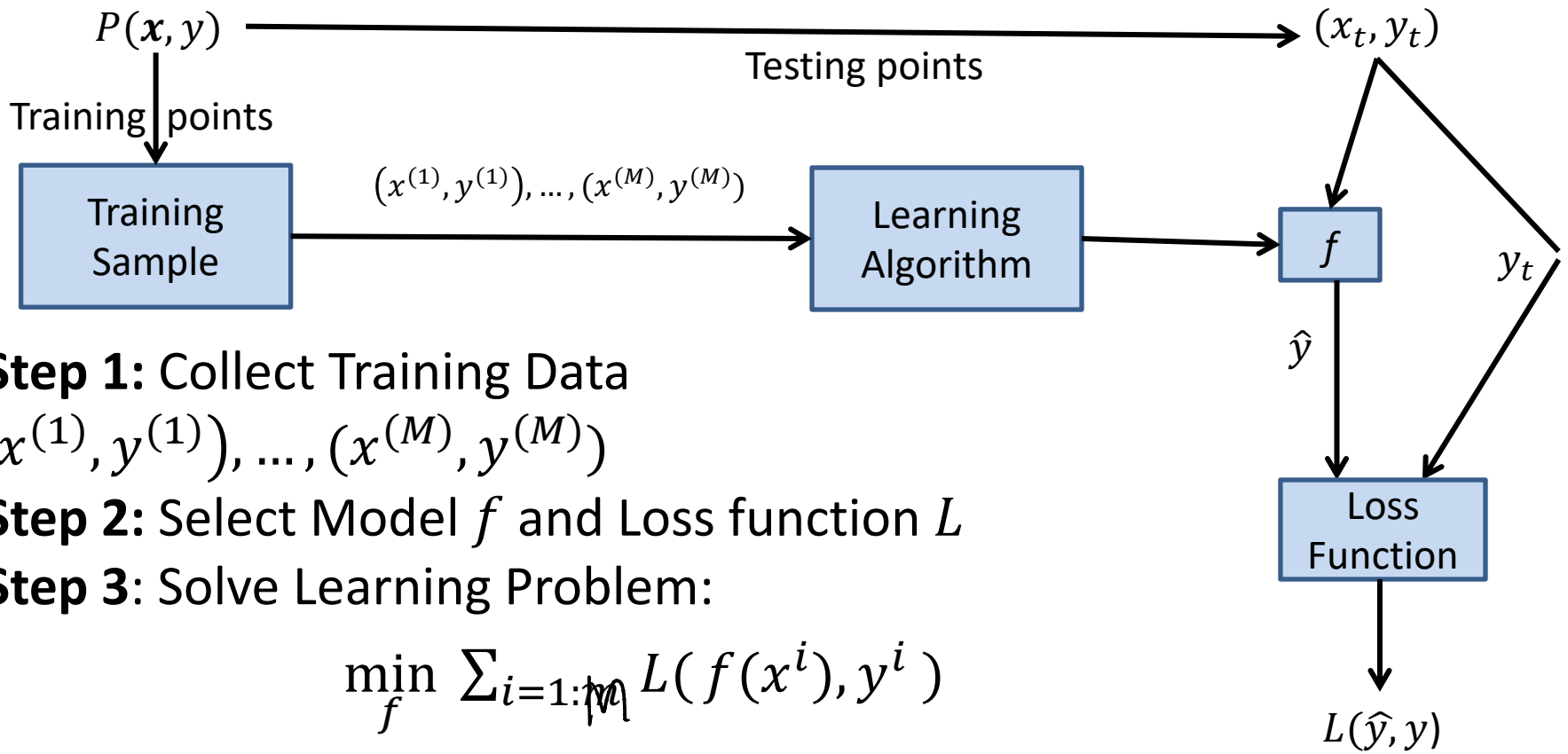
- Hypothesis space (Aka Model): set of allowable functions $f: X \rightarrow Y$

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

  - How do we measure the quality of f?

"Linear" → Hypothesis Space.

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 $Err(\hat{y}_t, y_t)$

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

$$L(\hat{y}, y) = Err(\hat{y}, y) = (\hat{y} - y)^2 \;/\; |\hat{y} - y|$$

Square Error

Absolute Error.

For a single instance (x, y) $\quad (\hat{y}, y)$, where $\hat{y} = f(x)$

$$L(\hat{y}, y) = [y - \hat{y}]^2 = Err(\hat{y}, y)$$

$$(x^1, y^1) \ \ldots \ (x^M, y^M) \rightarrow D$$

$$Err_D = L_D = \frac{1}{M} \sum_{i=1}^{M} L(y^i, \hat{y}^i)$$

$$L(y, \hat{y}) = [y - \hat{y}]^2$$

$$Err_D = L_D = \frac{1}{M} \sum_{i=1}^{M} [y^i - \hat{y}^i]^2$$

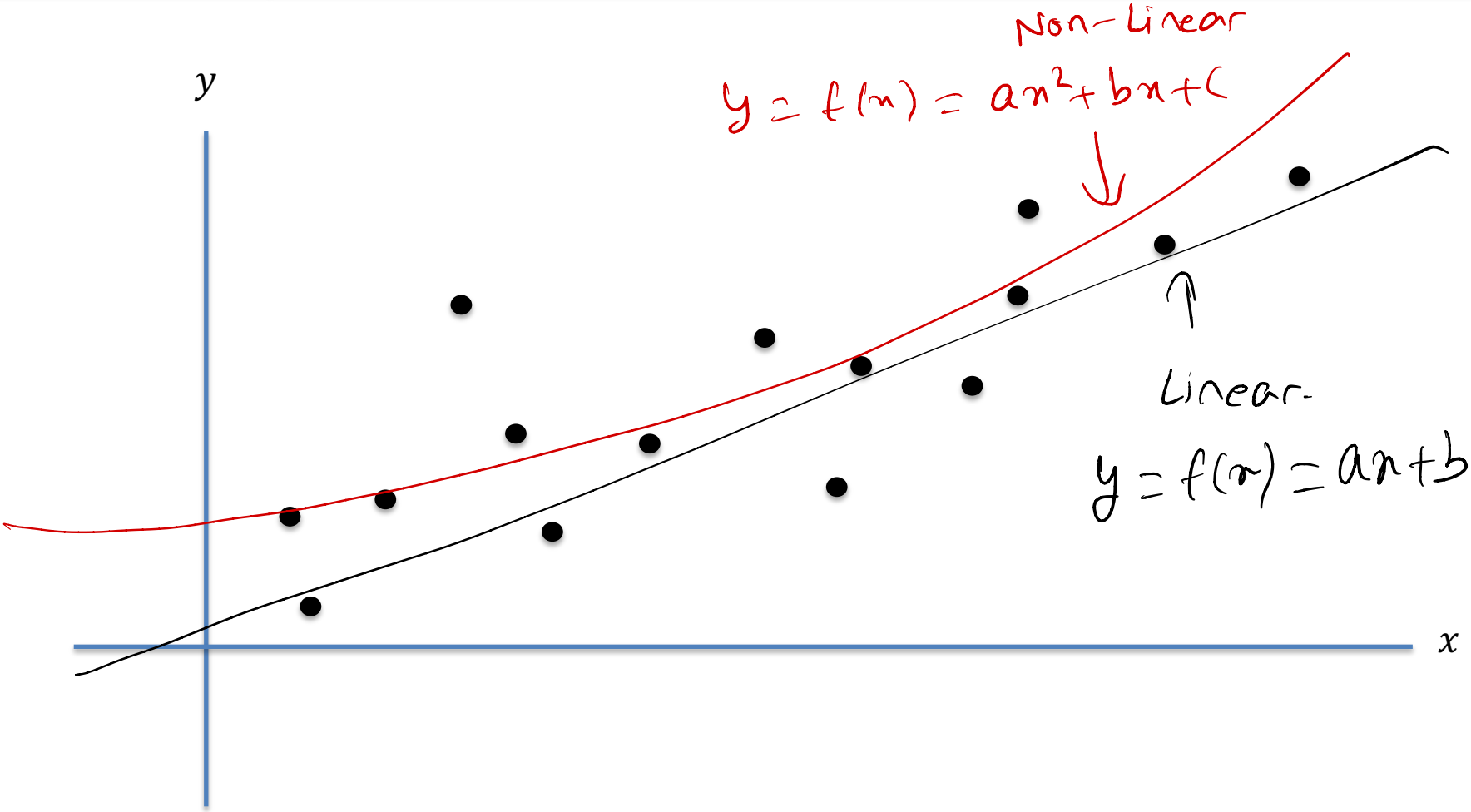
Mean Square Error (MSE)

$$L(y, \hat{y}) = |y - \hat{y}|$$

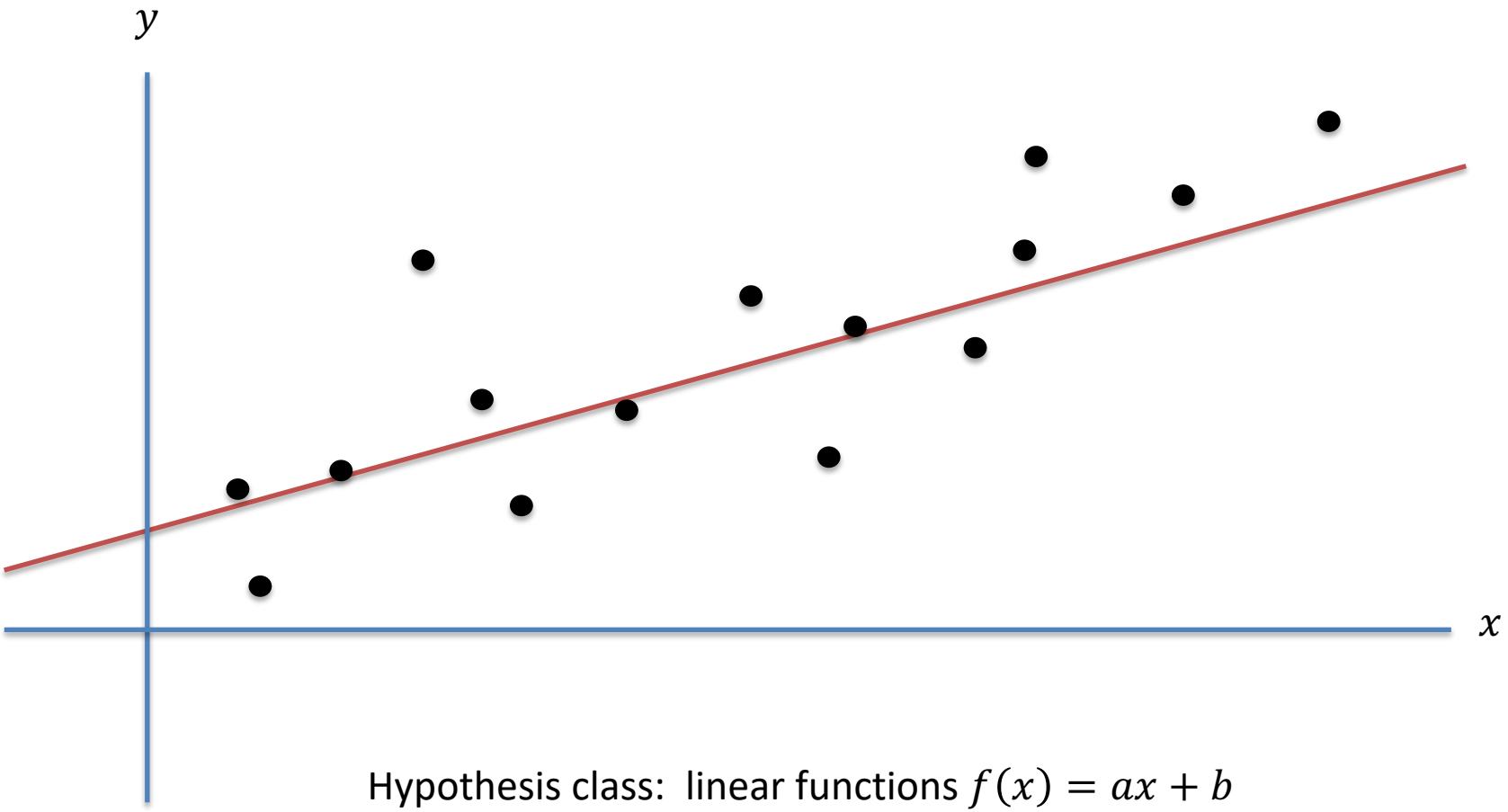
$$Err_D = L_D = \frac{1}{M} \sum_{i=1}^{M} |y^i - \hat{y}^i|$$

Mean Absolute Error (MAE)

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

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

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

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

Linear Regression

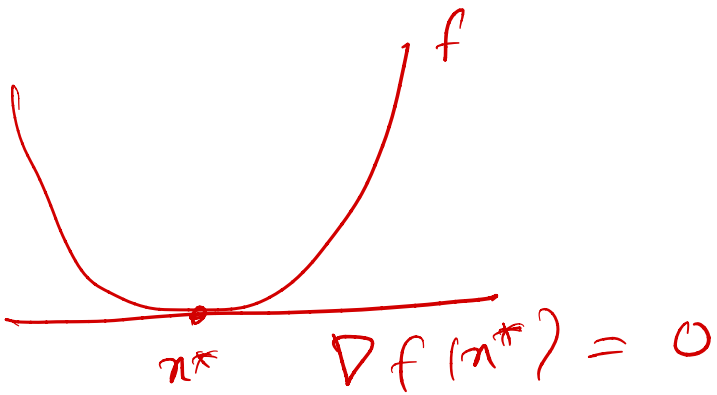
$$\min_{a,b} \frac{1}{M} \sum_{m} \left(ax^{(m)} + b - y^{(m)} \right)^2$$

- How do we find the optimal a and b?

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!) ← $O(d^3)$
  - Solution 2: use gradient descent

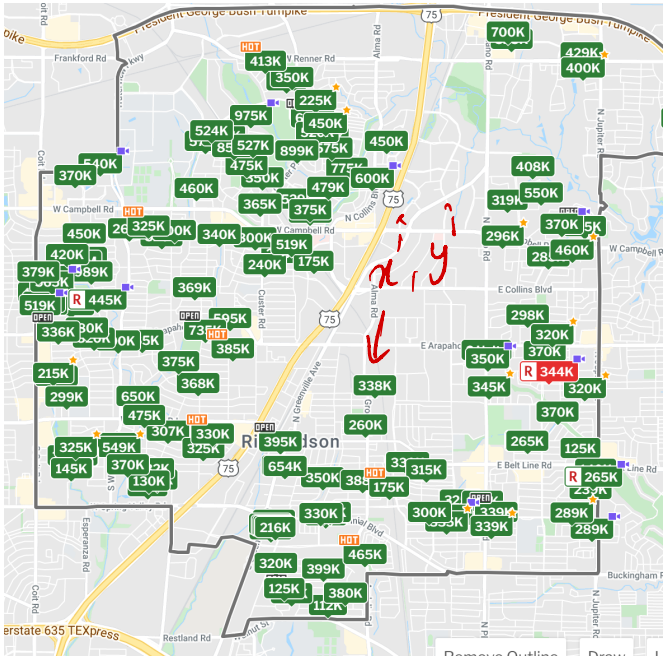


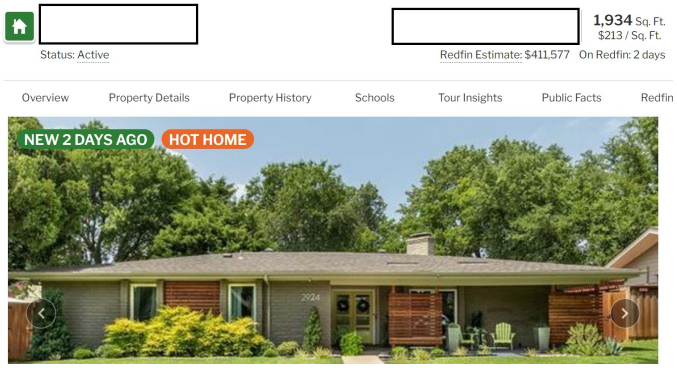
Linear Regression

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

- 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

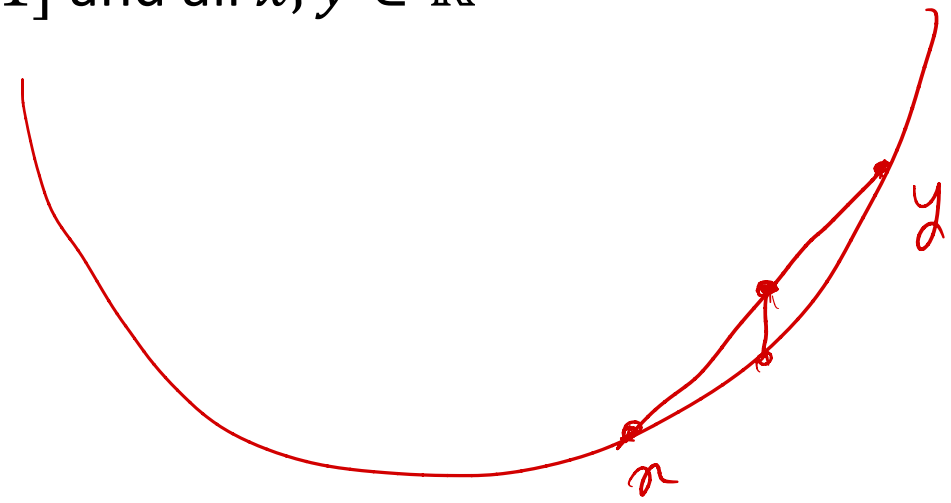
Gradient Descent

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 $x, y \in \mathbb{R}^n$



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)

Convergence

1. $\|x^{t+1} - x^t\|_2 \leq \varepsilon \rightarrow$ (e.g. $\varepsilon = 10^{-2}$)
2. $\|\nabla f(x^t)\|_2 \leq \varepsilon$
3. $|f(x^{t+1}) - f(x^t)| \leq \varepsilon$

$$\|x\|_2^2 = \sum_{i=1}^{d} x_i^2 \quad , \quad \|x\|_2 = \sqrt{\sum_{i=1}^{d} x_i^2}$$

Basics of Convexity and Gradient Desc

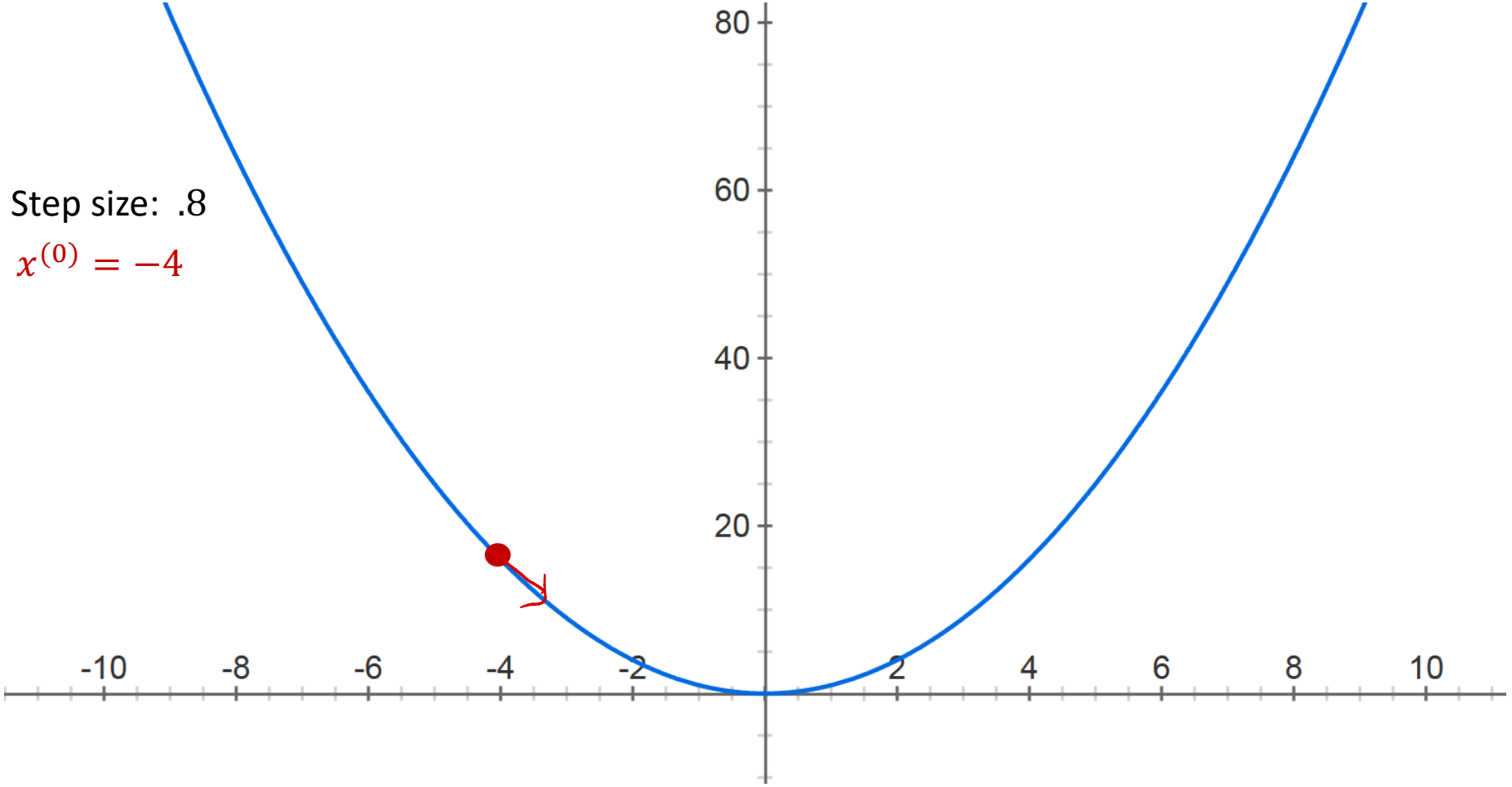
- For additional reading, please see some of my slides from my Spring 2020 Class “Optimization in Machine Learning”
- Github Location for Lecture Notes and Slides: https://github.com/rishabhk108/OptimizationML
- Please skim through:
  - Lectures 1 and 2 for basics
  - Lectures 3-5 for convex functions
  - 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

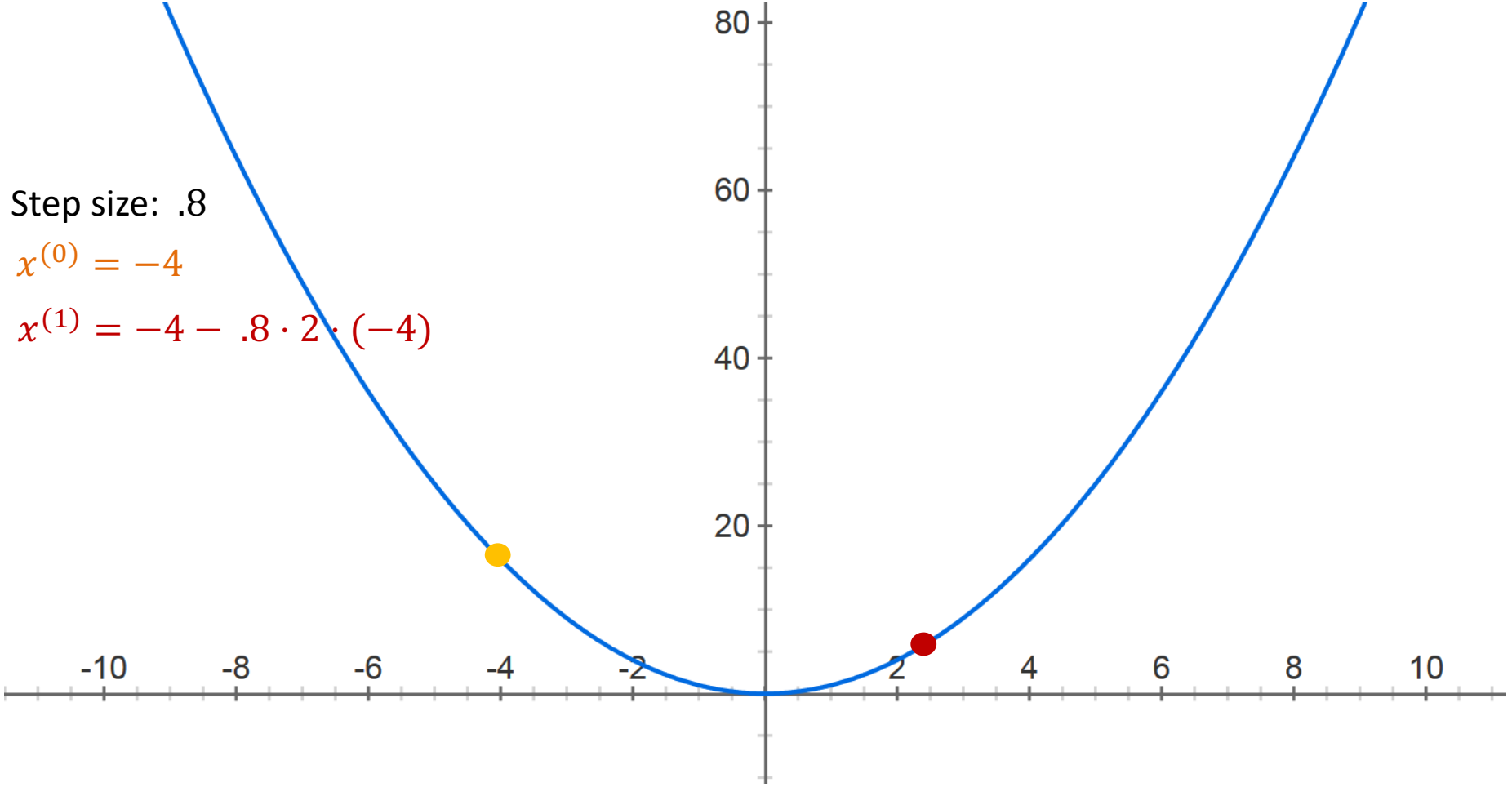
$f(x) = x^2$

$\nabla f(x) = 2x$

Step size: .8

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

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



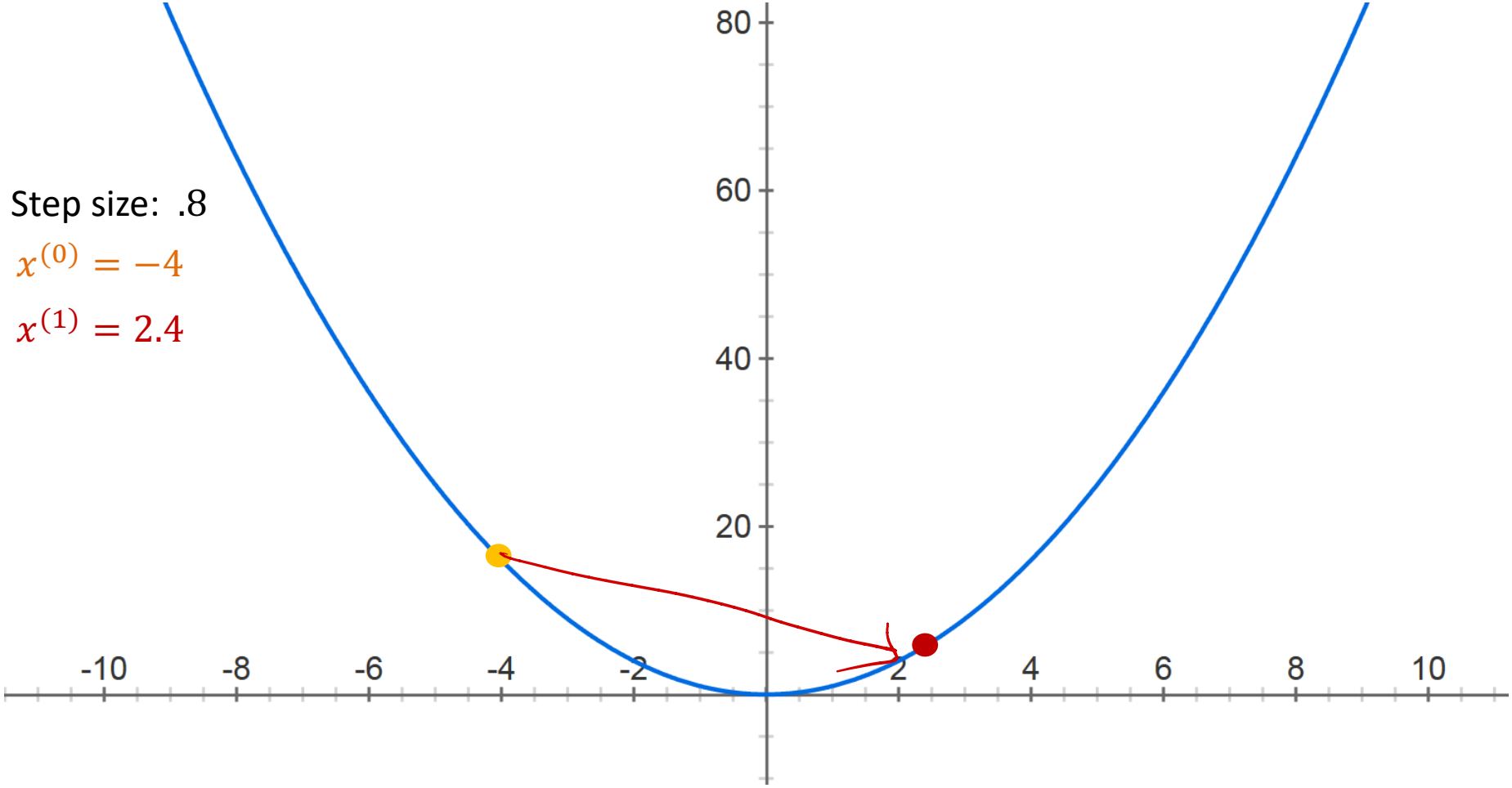
Gradient Descent

$f(x) = x^2$

Step size: .8

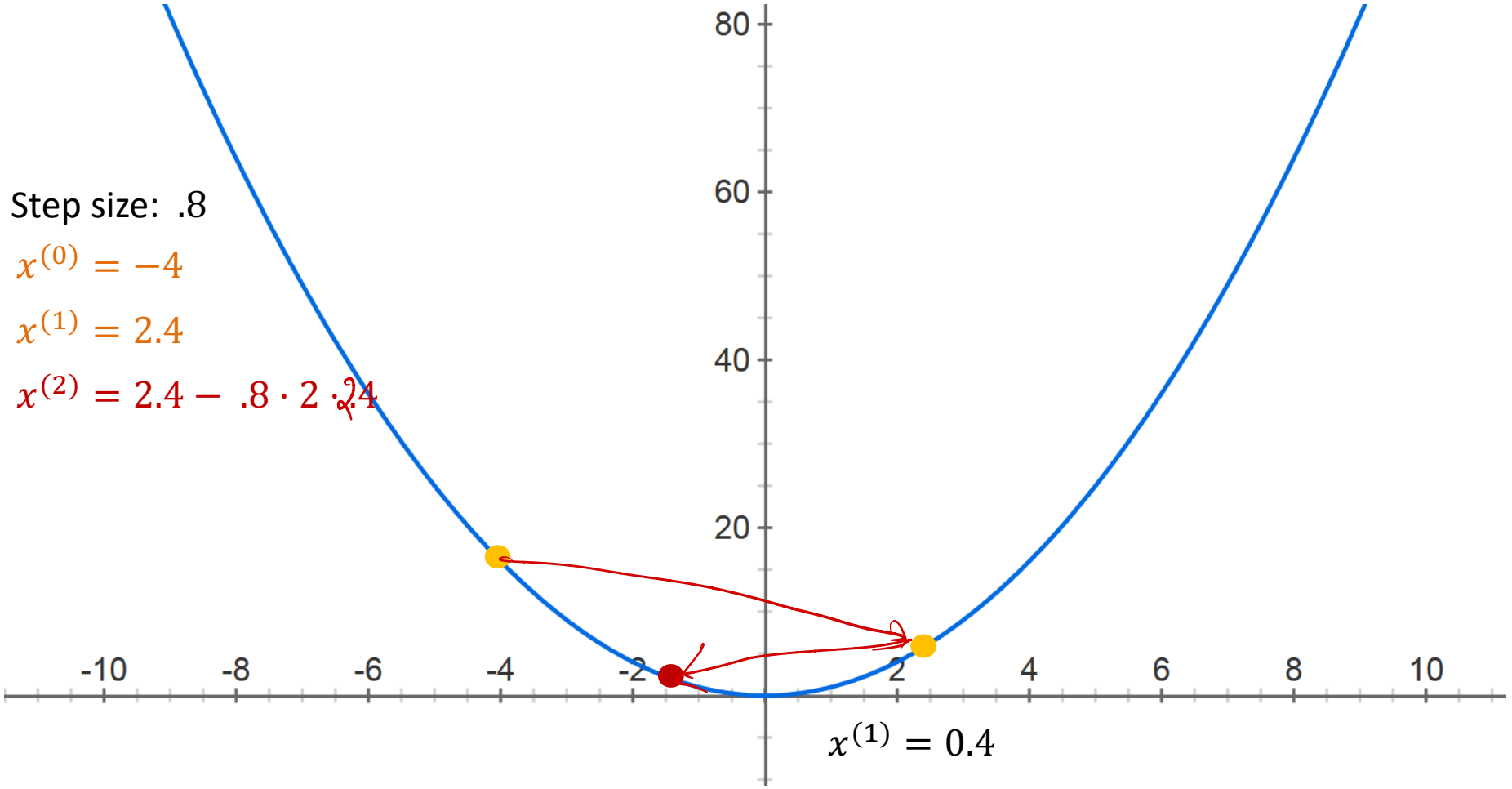
$x^{(0)} = -4$

$x^{(1)} = 2.4$



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

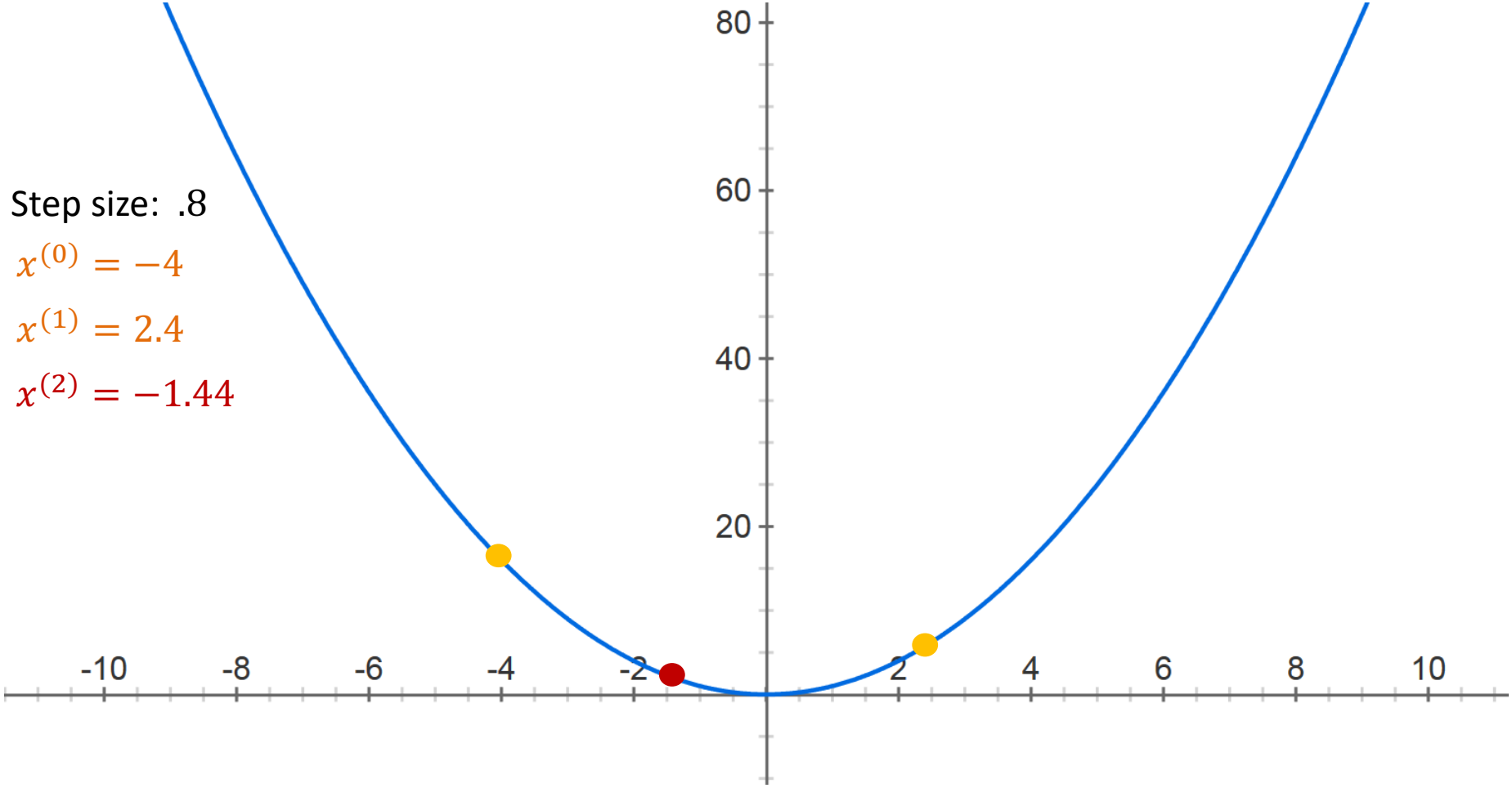
$f(x) = x^2$

Step size: .8

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

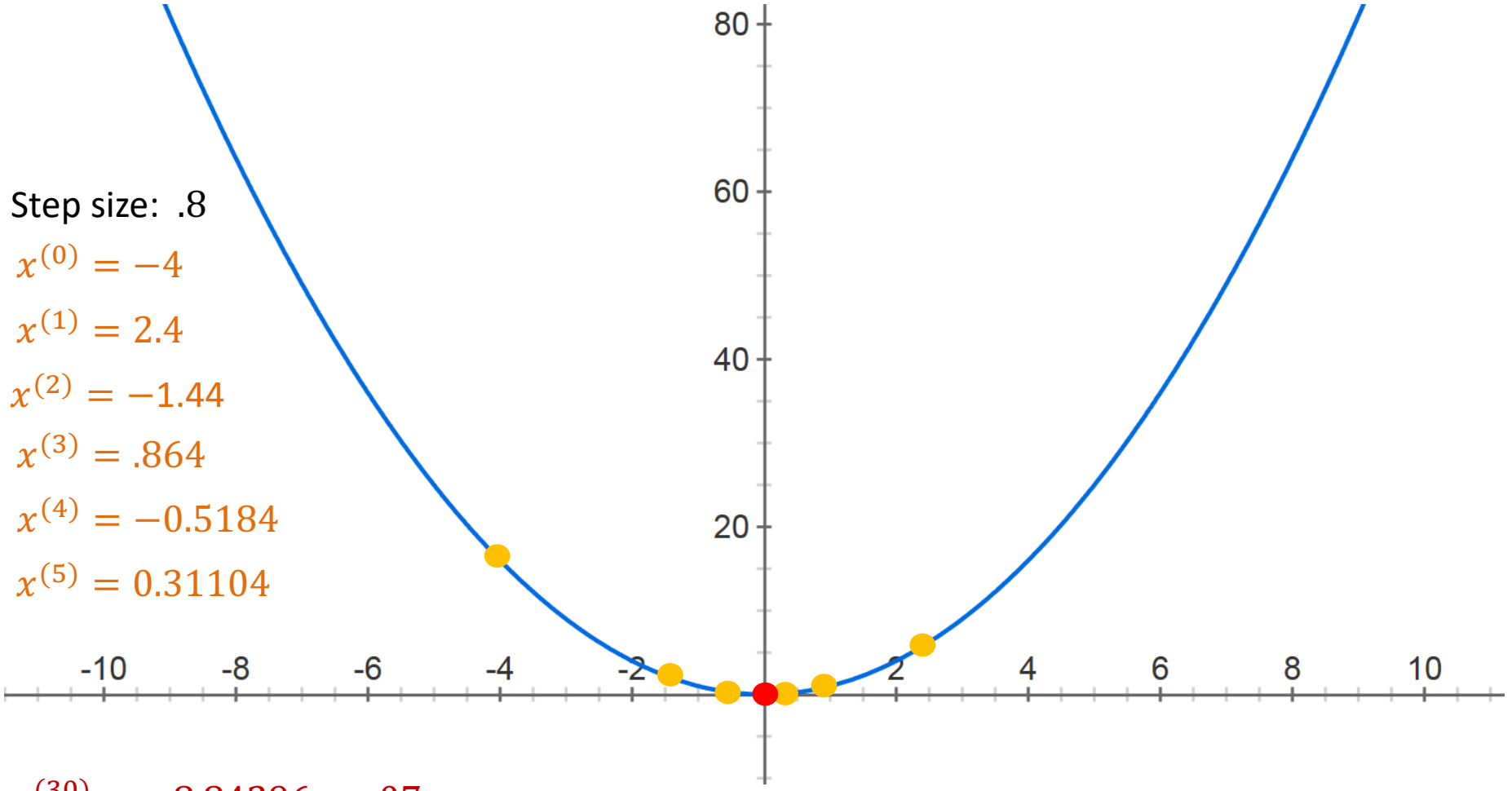
$x^{(1)} = 2.4$

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



Gradient Descent

$f(x) = x^2$



Step size: .8

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

$x^{(1)} = 2.4$

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

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

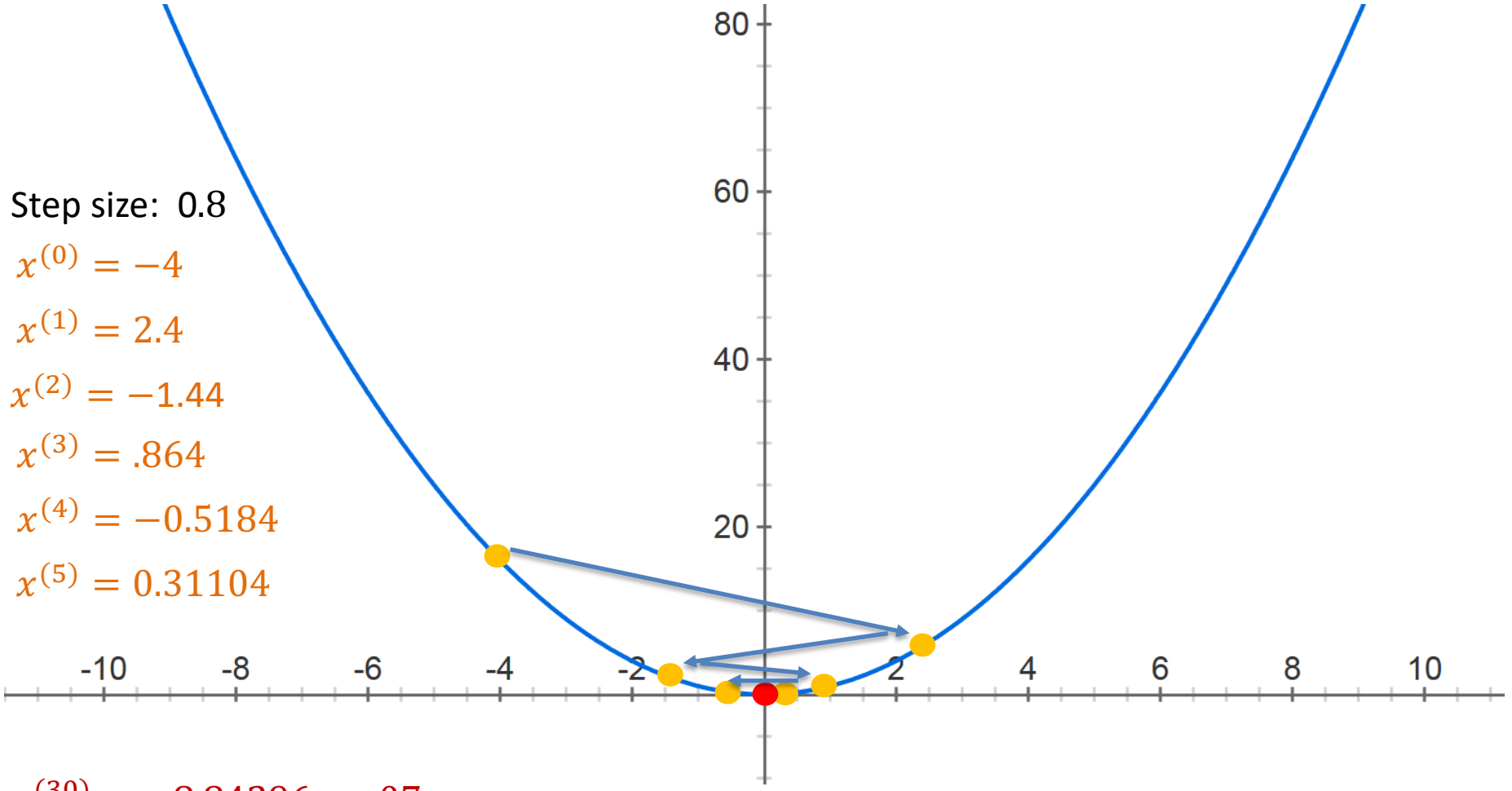
$x^{(4)} = -0.5184$

$x^{(5)} = 0.31104$

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

Gradient Descent: Good Convergence

$f(x) = x^2$



Step size: 0.8

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

$x^{(1)} = 2.4$

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

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

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

$x^{(5)} = 0.31104$

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

Gradient Descent: Slow Convergence

$f(x) = x^2$

Step size: 0.08

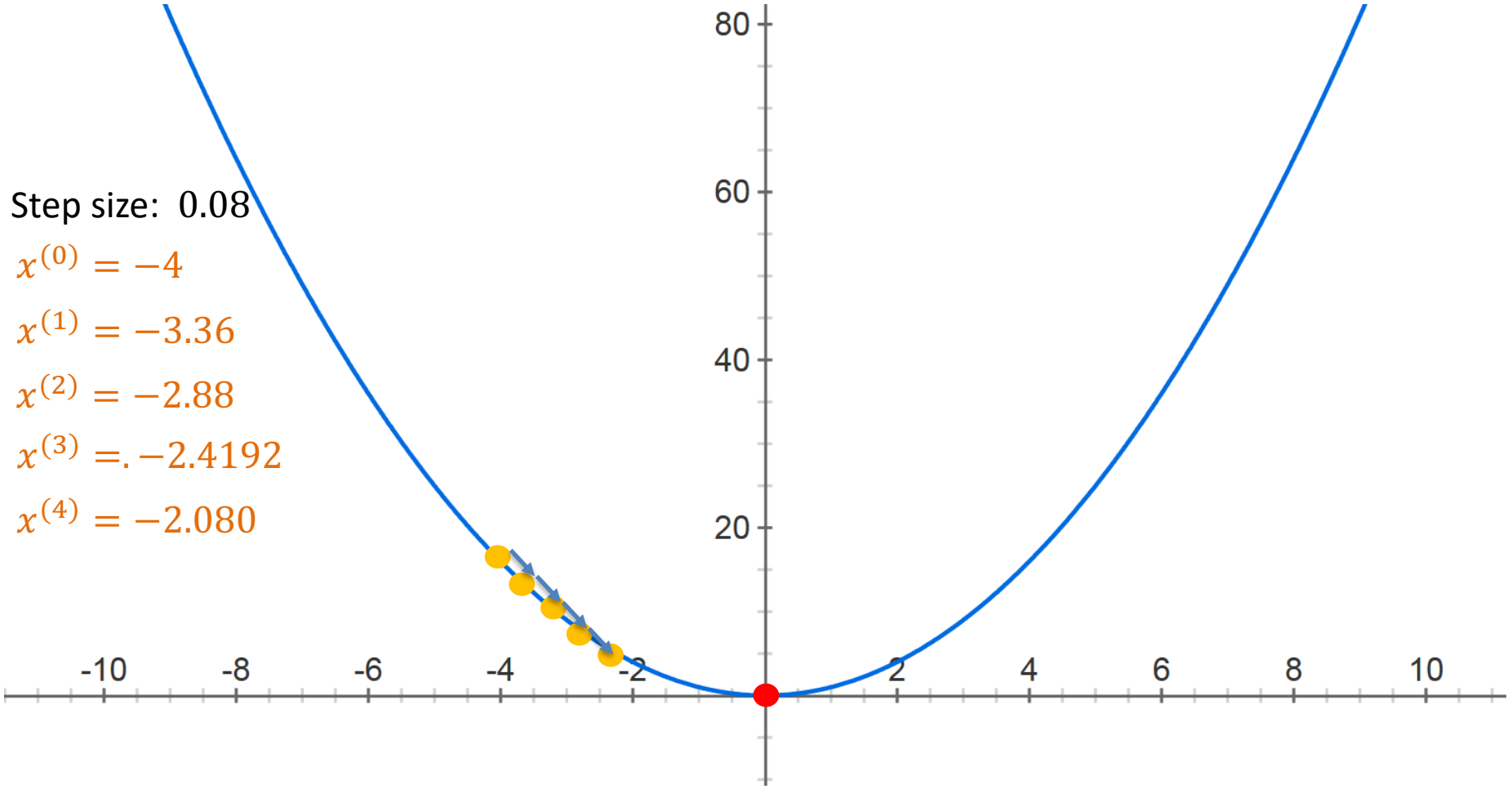
$x^{(0)} = -4$

$x^{(1)} = -3.36$

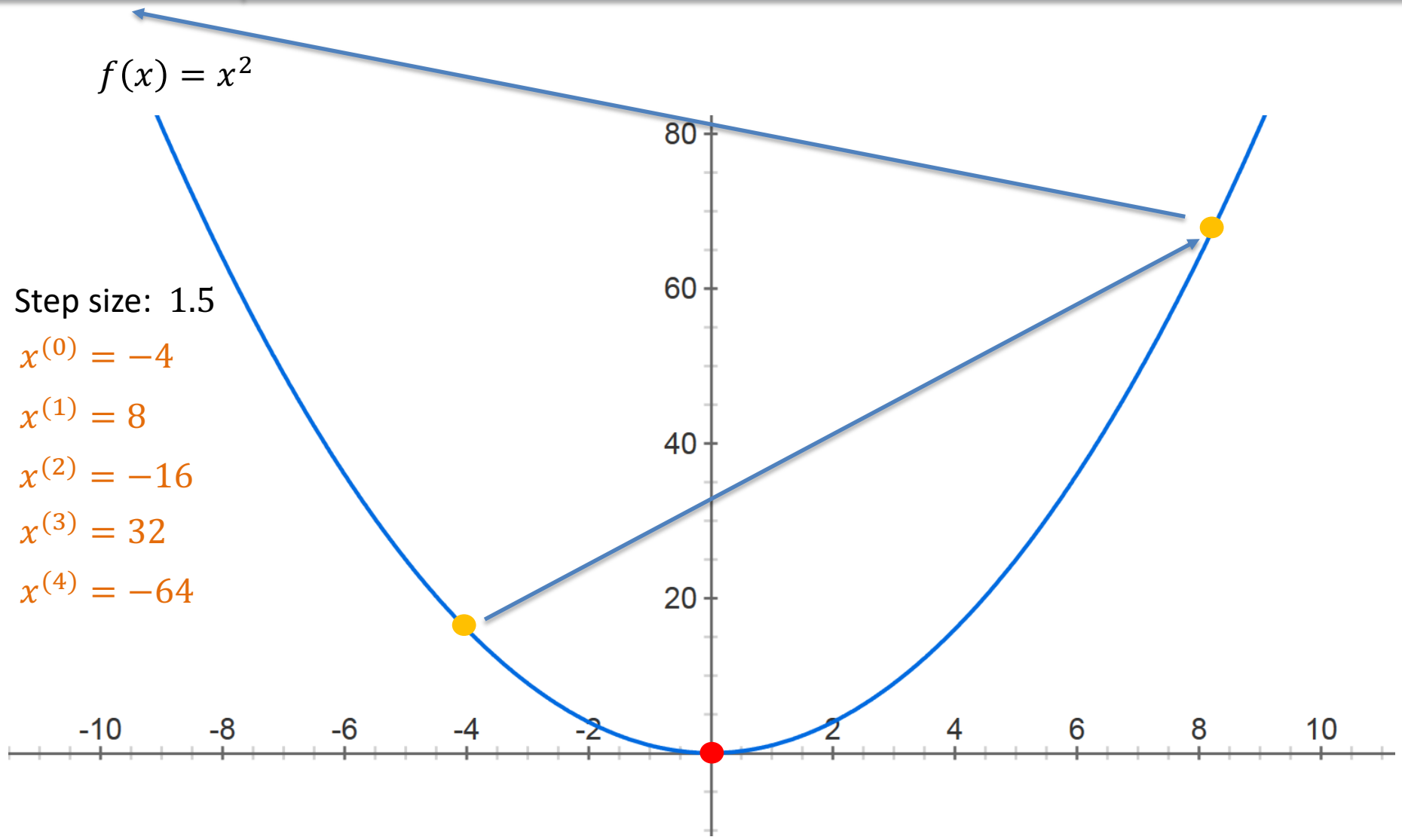
$x^{(2)} = -2.88$

$x^{(3)} = .-2.4192$

$x^{(4)} = -2.080$



Gradient Descent: Divergence



Step size: 1.5

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

$x^{(1)} = 8$

$x^{(2)} = -16$

$x^{(3)} = 32$

$x^{(4)} = -64$

Gradient Descent

$$\begin{bmatrix} a \\ b \end{bmatrix}$$

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

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

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

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

$$\nabla_b L = \frac{1}{M}\sum_{m=1}^{M} 2\left(ax^{(m)} + b - y^{(m)}\right]$$

Chain rule

$$L(a) = F(G(a))$$

$$L'(a) = \frac{dF(G)}{dG}\,\frac{dG(a)}{da}$$

Gradients for Linear Regression

- The Loss Function for Linear Regression is:

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

- The gradients with respect to a and b are:

$$\nabla L_a(a,b) = \frac{1}{M}\sum_m 2(ax^{(m)} + b\ - y^m)\ x^{(m)}$$

$$\nabla L_b(a,b) = \frac{1}{M}\sum_m 2(ax^{(m)} + b\ - y^m)$$

- The gradients can be obtained by using the chain rule

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

$$L(a) = \|a\|^2 = \sum_{i=1}^{d} a_i^2 \quad , \quad a \in \mathbb{R}^d$$

$$\nabla_a L = \begin{bmatrix} \frac{\partial L}{\partial a_1} \\ \frac{\partial L}{\partial a_2} \\ \vdots \\ \frac{\partial L}{\partial a_d} \end{bmatrix} = \begin{bmatrix} 2a_1 \\ 2a_2 \\ \\ \\ 2a_d \end{bmatrix} = 2a.$$

Gradient Descent

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

$f(x) = ax + b$ ← Linear

$f(x) = ax^2 + bx + c$ (Quad)

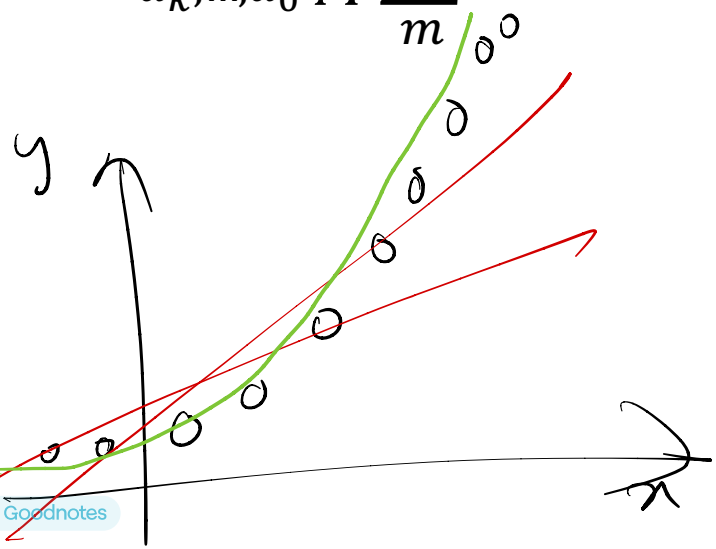
$f(x) = ax^3 + bx^2 + cx + d$ (Cubic)

} Poly functions

Polynomial Regression

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

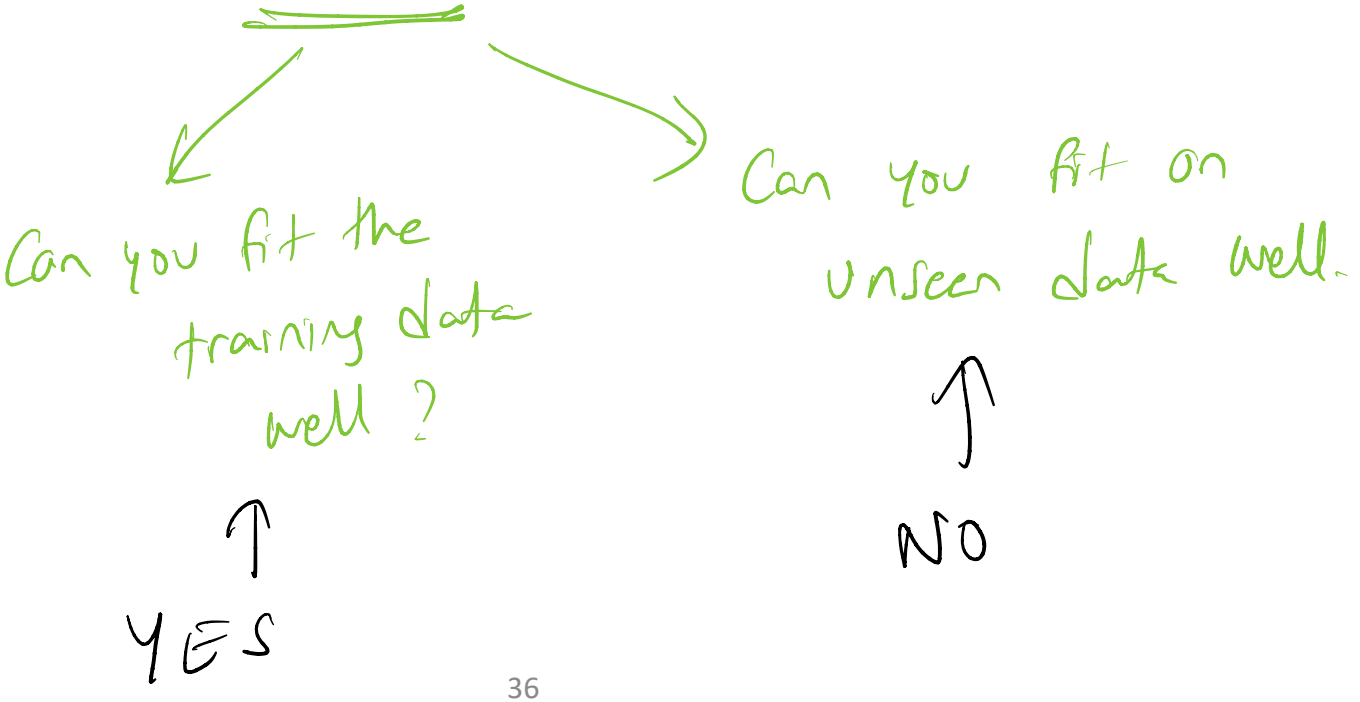
$$\min_{a_k,\ldots,a_0} \frac{1}{M} \sum_m \left(a_k \left(x^{(m)}\right)^k + \cdots + a_1 x^{(m)} + a_0 - y^{(m)} \right)^2$$



$(x^{(m)}, y^{(m)})$

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

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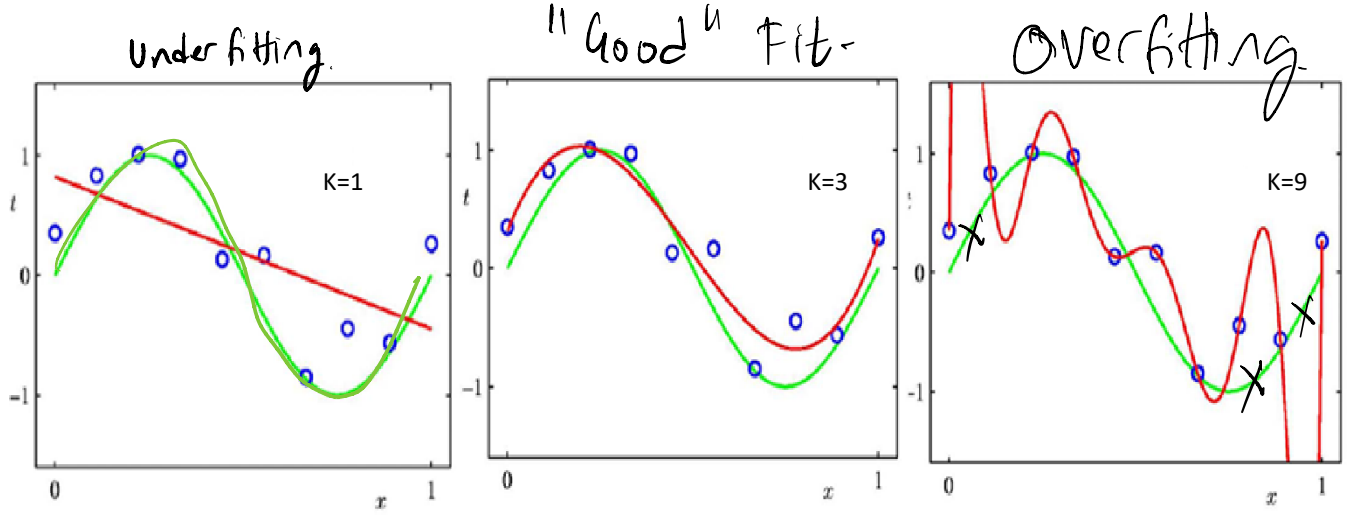


Polynomial Regression

$$x \in \mathbb{R}^d = (x_1, x_2, \ldots, x_d)$$

$$a_{11} x_1 + a_{12} x_2 + \ldots + a_{1d} x_d \quad \leftarrow \quad d$$

$$+ a_{21} x_1^2 + a_{22} x_2^2 + \ldots + a_{2d} x_d^2 \quad \leftarrow \quad d$$

$$+ \sum_{\substack{i,j \\ i<j}} b_{ij} x_i x_j \quad \longleftrightarrow \quad \binom{d}{2}$$

$$+ c$$

Polynomial Regression $\equiv$ Linear Regression with Polynomial Features

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

$$= [a_0, a_1, a_2 \cdots, a_k] \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^k \end{bmatrix}$$

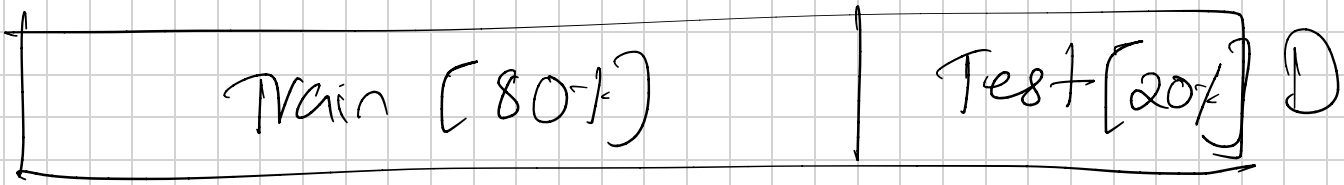
a

$$a^T \phi(x)$$

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)

Train VS Test Data.



How to split into train/test

→ Random Split

→ Uniform split [Maintains distribution]

→ Temporal Split

How much to assign?

(1) |Train| >> |Test|

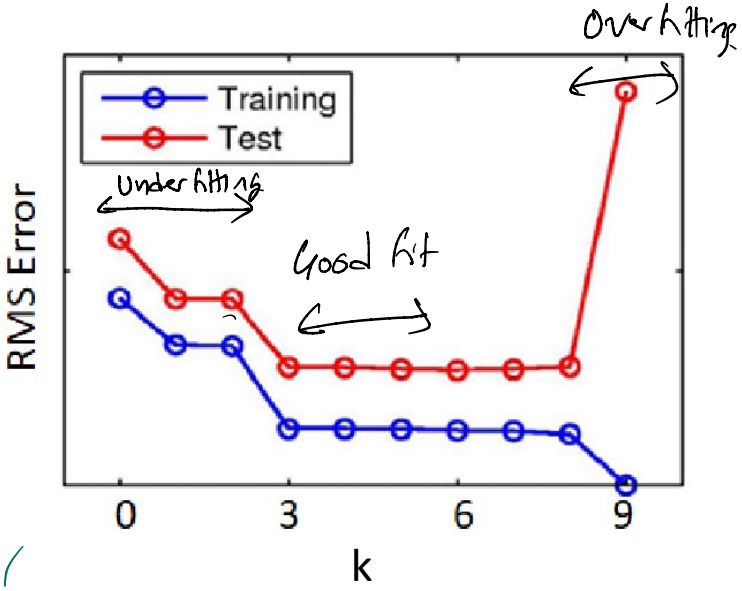
(2) Test set should be non trivial.

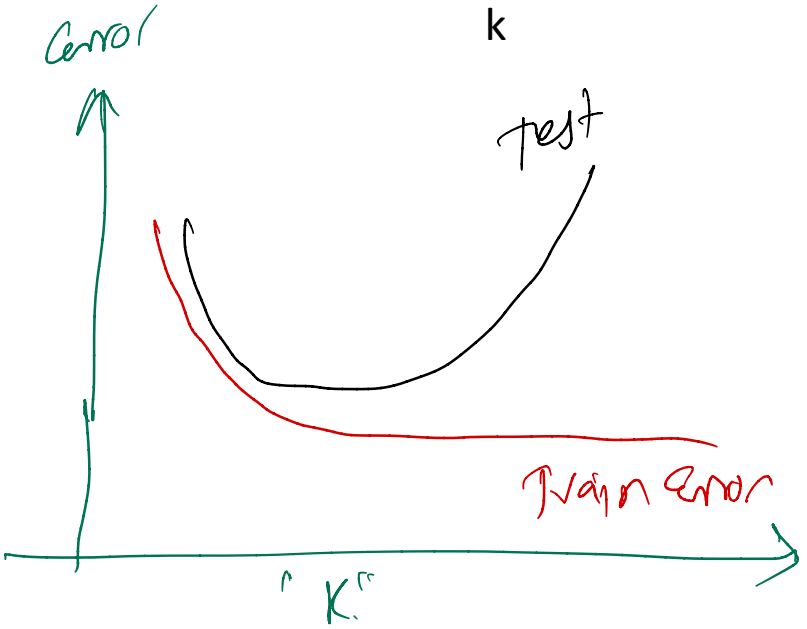
Train → Learn the model.

Test → measure generalization.

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)





L1 vs L2 Loss

Mean Absolute Error

L1 Loss

$$L(\theta) = |a^T x + b - y|$$

Penalizes Errors Linearly

Large Error does not dominate.

Median Fit

Non Differentiable, Convex

Mean Square Error

L2 Loss

$$L(\theta) = [a^T x + b - y]^2$$

Penalizes Errors Quadratically

Large Error can dominate.

Mean Fit

Differentiable, Smooth & Convex

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

Target [y]

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