CS 6375
Linear Regression

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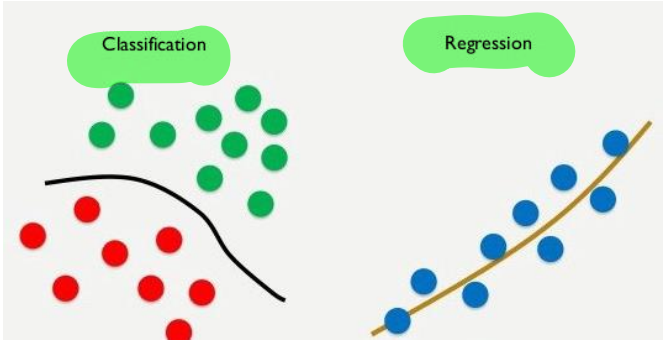
Slides adapted from Nick Rouzzi and Sriraam Natarajan

Part I: Recap of Supervised Learning and Linear Regression Setup

Recap: Supervised Learning

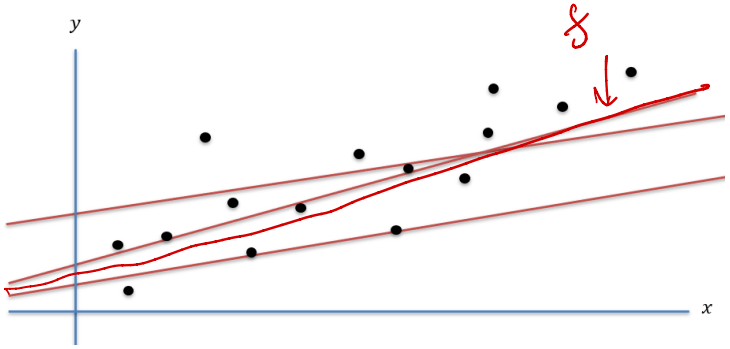
- **Input:** $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(M)}, y^{(M)}\right)$ ← Training Data
  - $x^{(m)}$ is the m^{th} data item and $y^{(m)}$ is the m^{th} **label**
    - $x^{(m)}$: Feature vector
    - $y^{(m)}$: Label
    - $y^m \in [0, K-1]$
    - $y^m \in \mathbb{R}$
- **Goal:** find a function f such that $f\left(x^{(m)}\right)$ is a "good approximation" to $y^{(m)}$ ⇒ $\min \sum L(f(x^m), y^m)$
  - Depends on loss fn
  - Can use it to predict y values for previously unseen x values

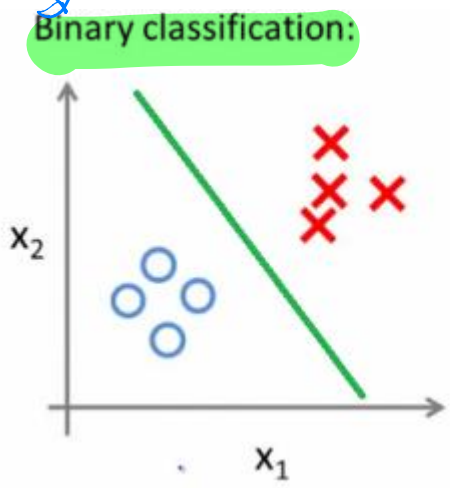


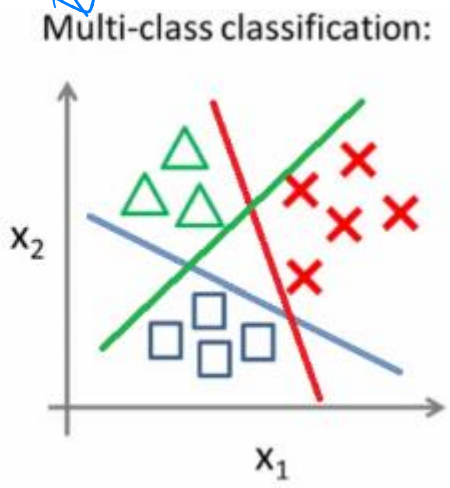
Recap: Classification vs Regression

Classification vs Regression

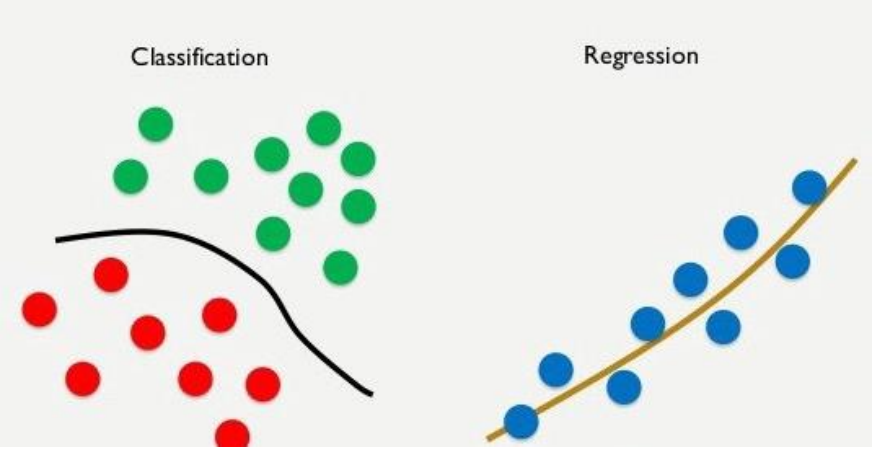
- Input: pairs of points $(x^{(1)}, y^{(1)}), \ldots, (x^{(M)}, y^{(M)})$ with $x^{(m)} \in \mathbb{R}^n$ [Feature vector]
- Regression case: $y^{(m)} \in \mathbb{R}$
- Classification case: $y^{(m)} \in [0, k-1]$ [k-class classification]
- If k = 2, we get Binary classification







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?

$f(x) = a^T x + b = a \cdot x + b$

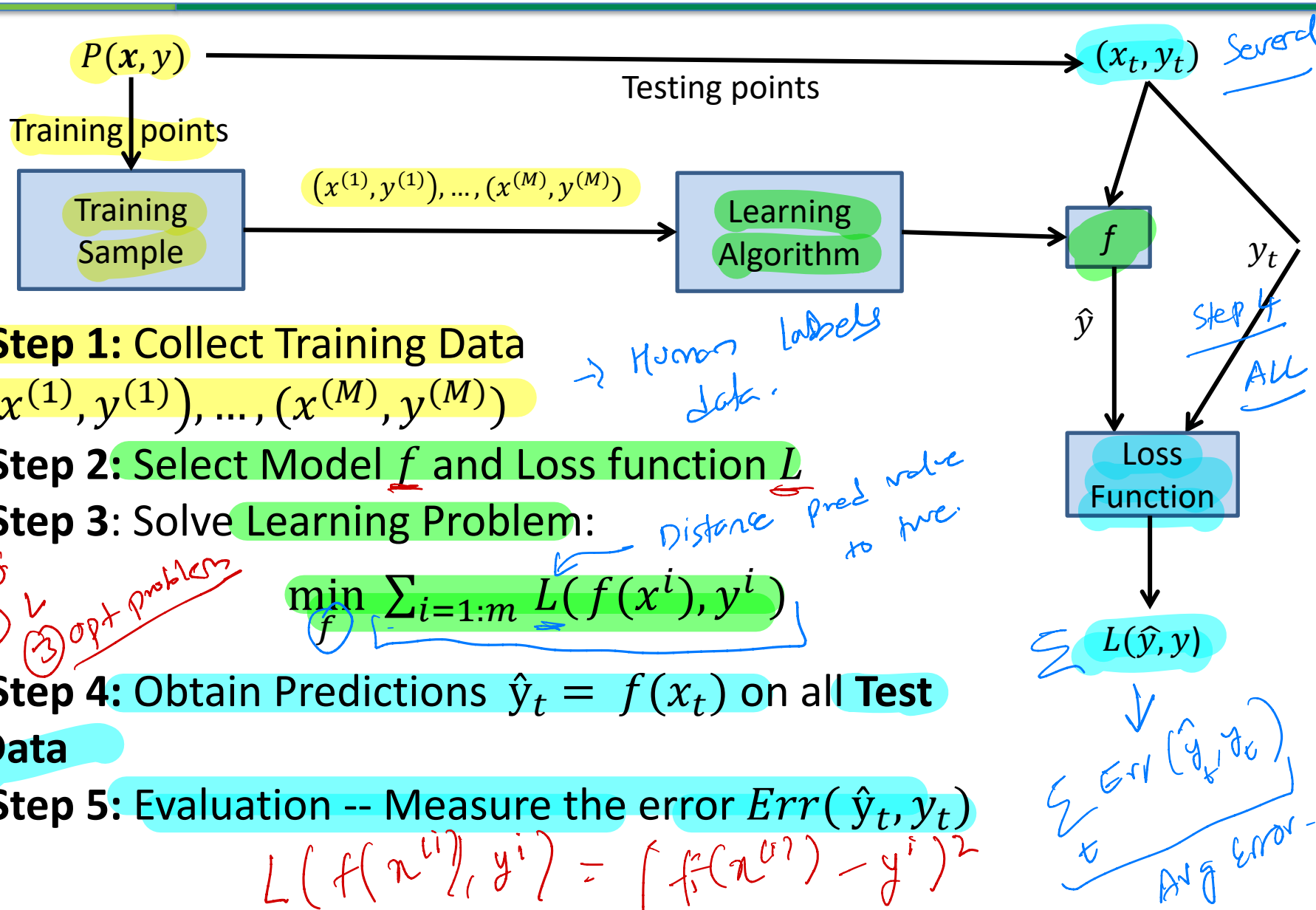
Linear

$f(\phi(x)) = a^T \phi(x) + b$

Poly

↑ richer feats

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

$$L(f(x^{(i)}), y^i) = (f(x^{(i)}) - y^i)^2$$

Linear Regression

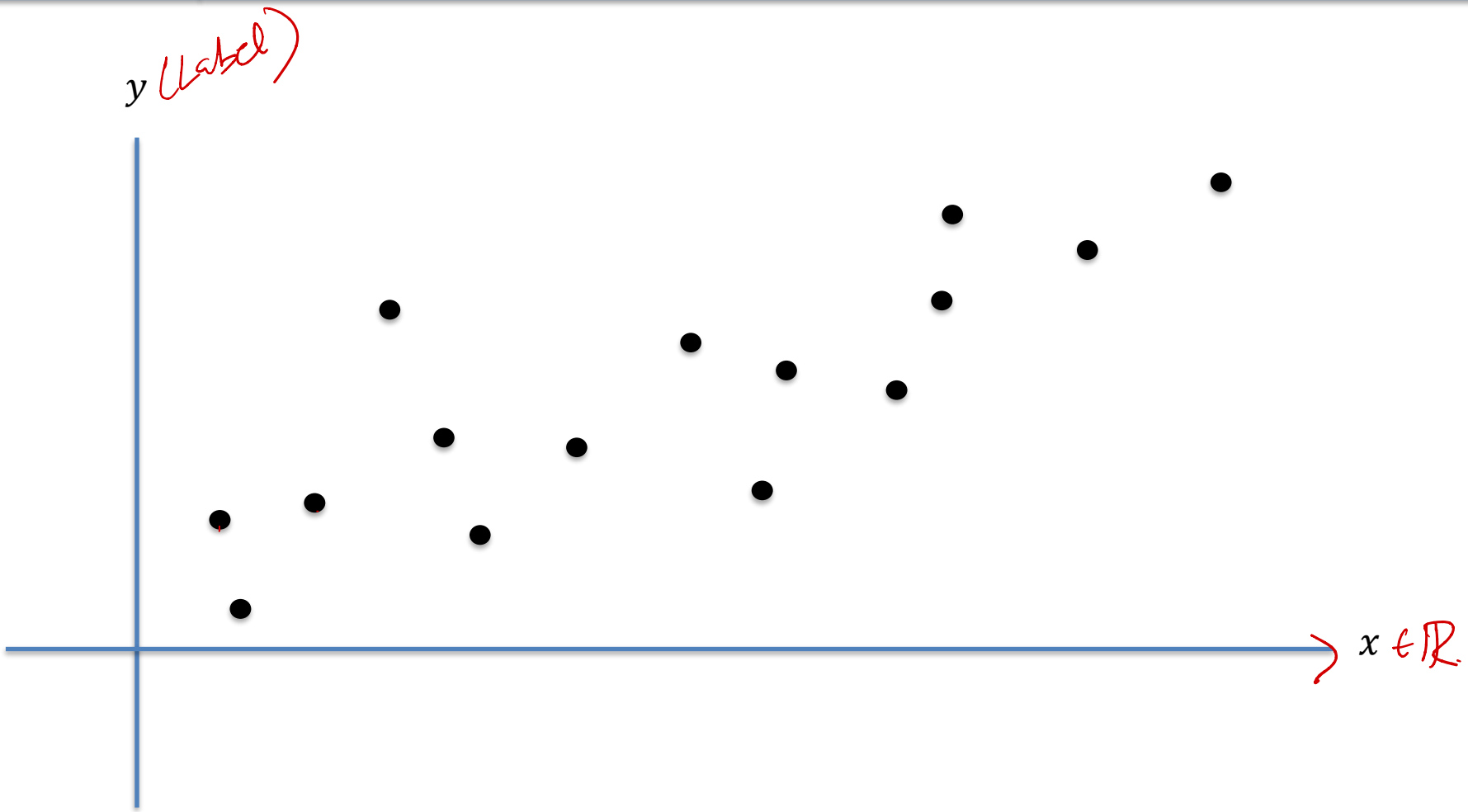
- Simple linear regression
  - Input: pairs of points $(x^{(1)}, y^{(1)}), \ldots, (x^{(M)}, y^{(M)})$ with $x^{(m)} \in \mathbb{R}^d$ and $y^{(m)} \in \mathbb{R}$ (Regression)
  - Hypothesis space: set of linear functions $f(x) = a^T x + b$ with $a \in \mathbb{R}^d, b \in \mathbb{R}$ (a, b) → Parameters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

$$L(f(x), y) = (f(x) - y)^2$$

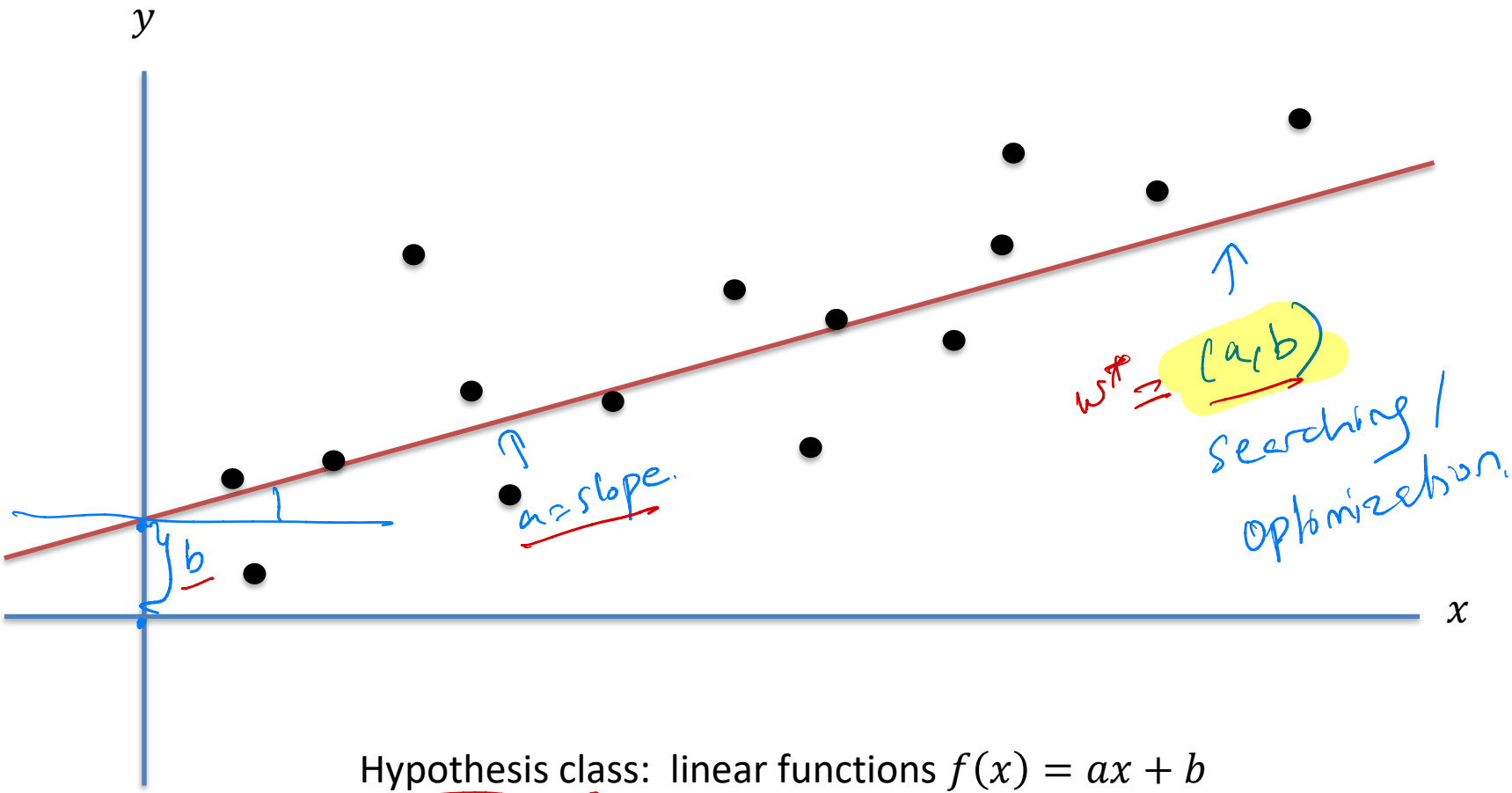
pred, true

$$(23 - 25)^2 = 4$$

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

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

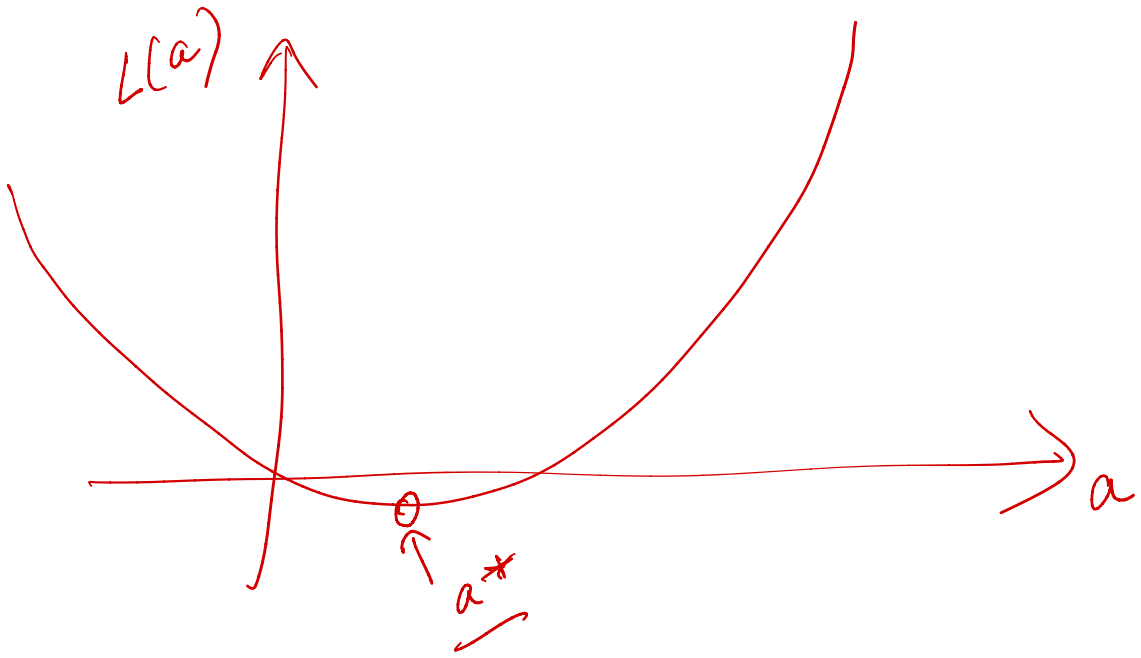
- Want to minimize the average loss on the training data
- The optimal linear hypothesis is then given by

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

Linear Regression [optimization / searching]

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

- How do we find the optimal a and b?



Linear Regression

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

$a \in \mathbb{R}^d, b \in \mathbb{R}$

$L(a,b)$

- 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

$\min_{a,b} L(a,b)$

$a^*: \nabla L(a^*) = 0$

$\nabla L(b) = 0$

Solve $\nabla L \begin{pmatrix} a^* \\ b \end{pmatrix} = 0$

Linear Regression Workflow

1. Model $f: a^T x + b$
2. Loss $L: [a^T x + b - y]^2$ (x: feat, y: label)
3. OPT $: \min_{a,b} \sum_m (a^T x^{(m)} + b - y^{(m)})^2$
   - ↳ opt algo: gradient descent.
4. Eval — RMSE, R2

features $x \in \mathbb{R}^d$

$y \in \mathbb{R}$

Poly $(x, 3)$ ← Too complex model

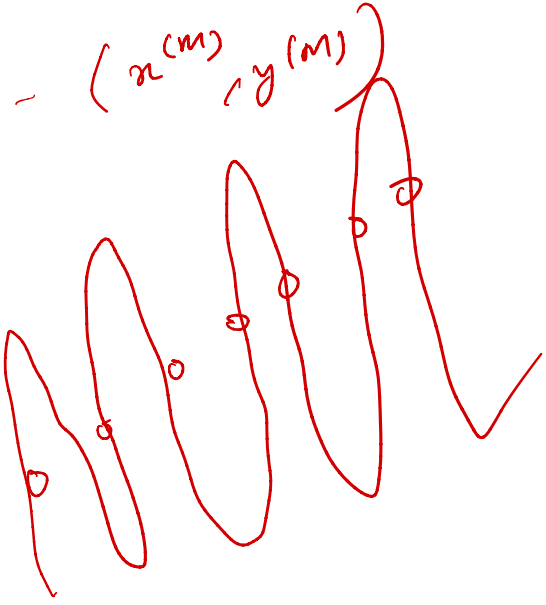
Training : $[(x^{(1)}, y^{(1)}), \ldots (x^{(m)}, y^{(m)})$

$d >>> M$

200K 500

↑

too many Degrees of freedom



Linear Regression

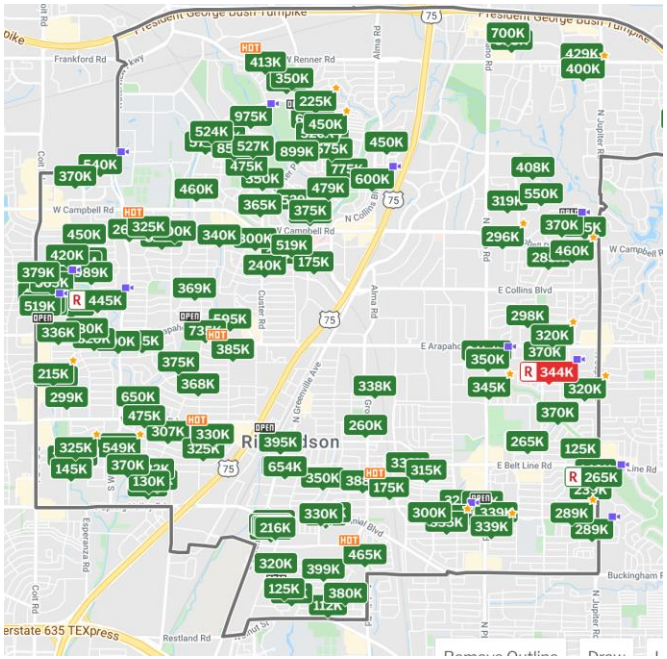
$$\min_{a,b} \frac{1}{M} \sum_{m} \left(ax^{(m)} + b - y^{(m)} \right)^2$$

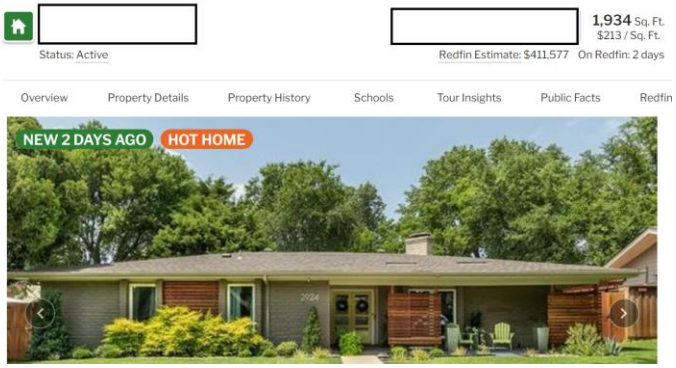
- How do we find the optimal a and b?
  - Solution 1: take derivatives and solve (there is a closed form solution!)
  - Solution 2: use gradient descent

Part II

    - 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		

y = Price of home

x = features

[Loc^n, Size, Bd(Bath), HOA, Prop Tax, Crime, ...)

[Zipcode]

Feature Engg

Searching Problem

Part II: Gradient Descent and Optimization

Continuous

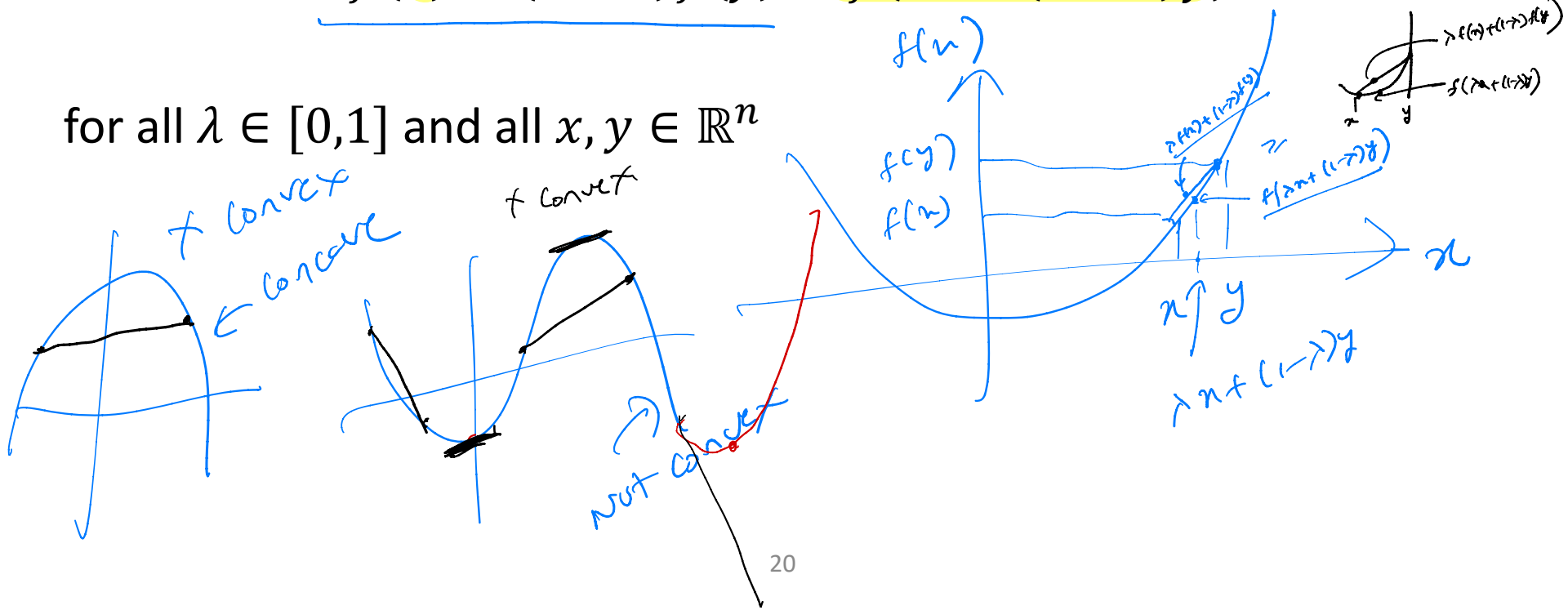
Gradient Descent

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)

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

θ_0

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

Convex

Hyper-param

Pick a_0, b_0 random / zeros

$$a_{t+1} = a_t - \gamma_t \nabla L(a_t)$$
$$b_{t+1} = b_t - \gamma_t \nabla L(b_t)$$

repeat k times until convergence.

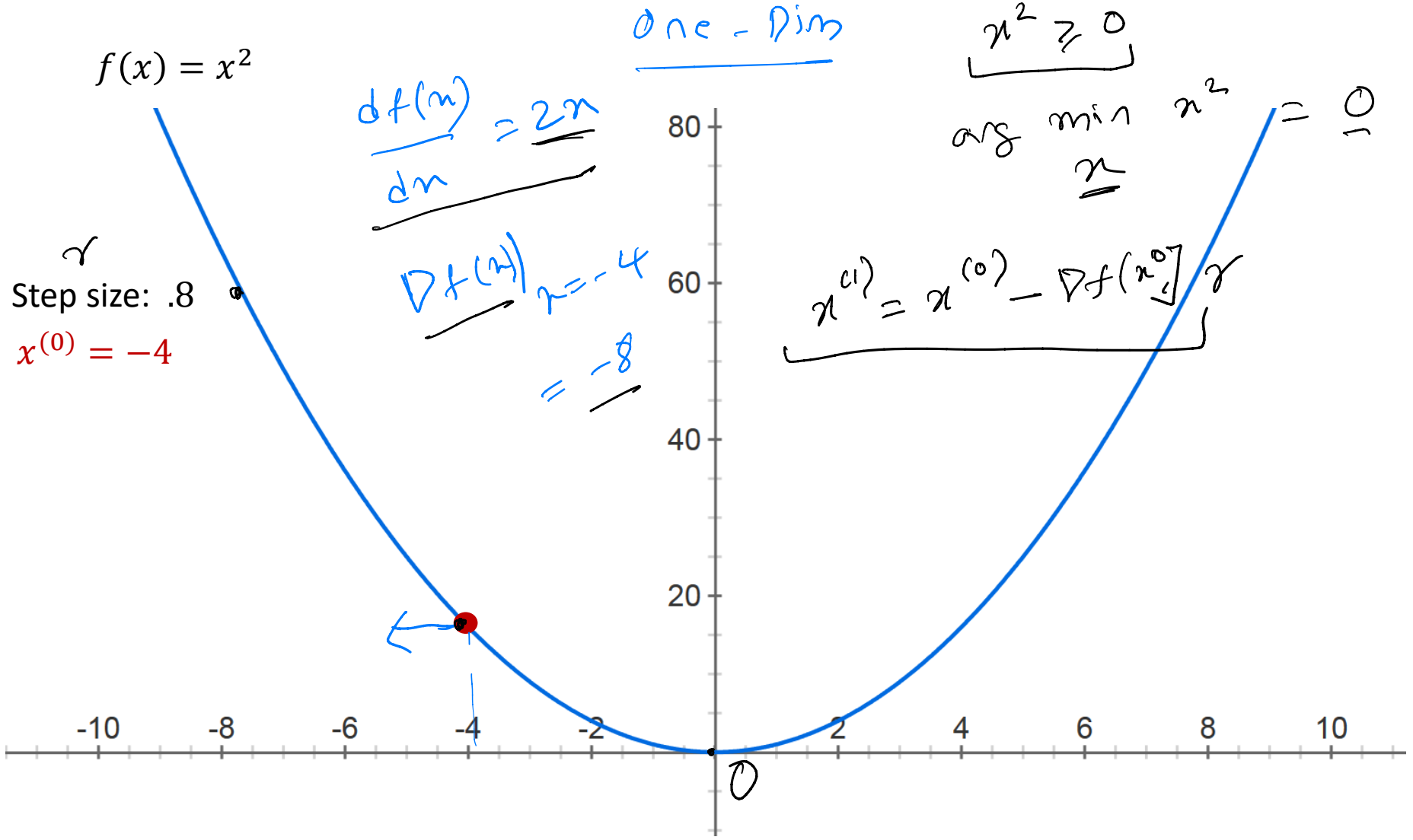
$$\theta_{t+1} = \theta_t - \gamma_t \nabla f(\theta_t)$$

Learning Rate.

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



Gradient Descent

$f(x) = x^2$

$x^{(1)} = x^{(0)} - \gamma(-2x)$

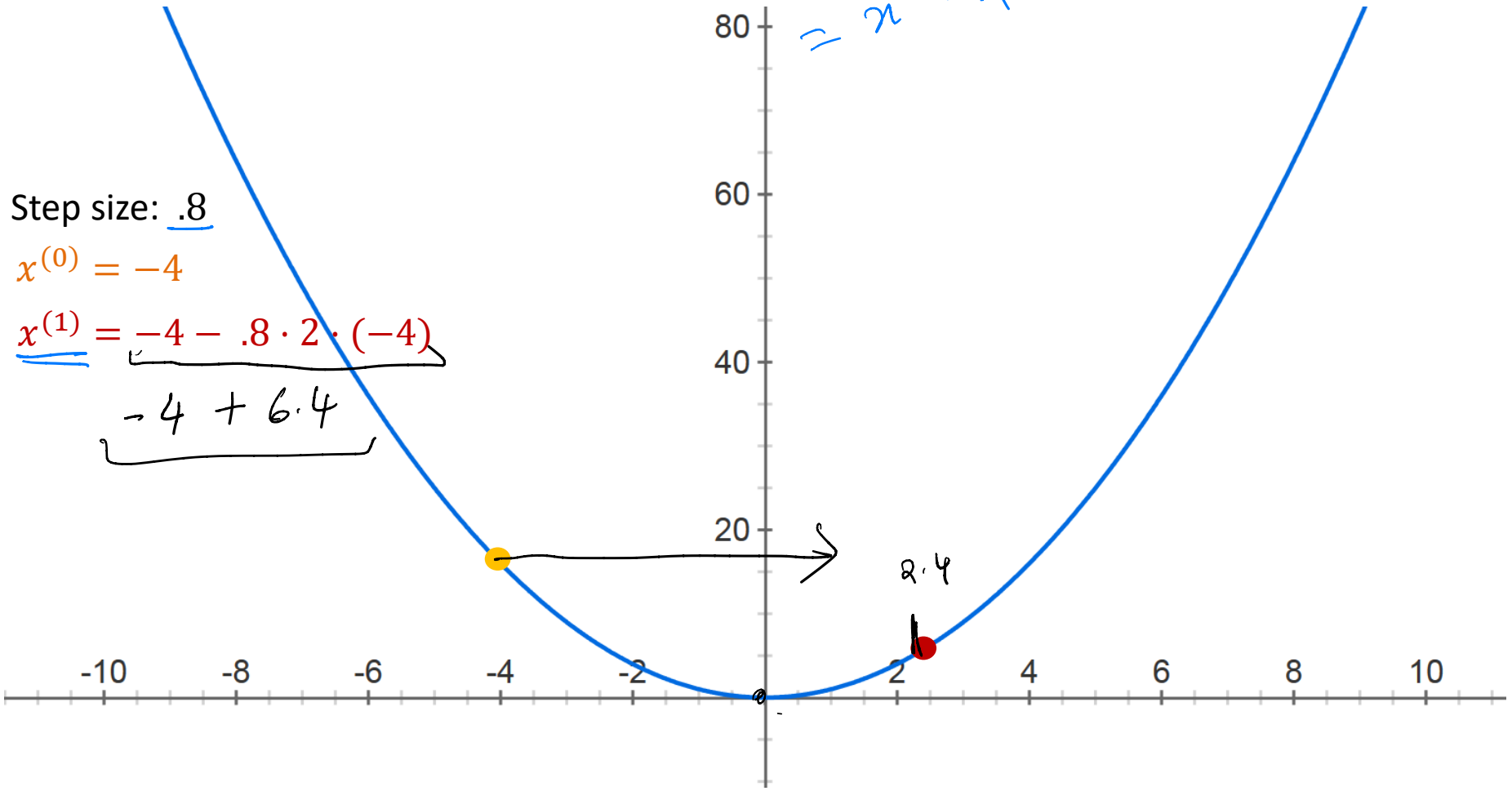
$= x^{(0)} + \gamma \cdot 2x$

Step size: .8

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

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

$-4 + 6.4$



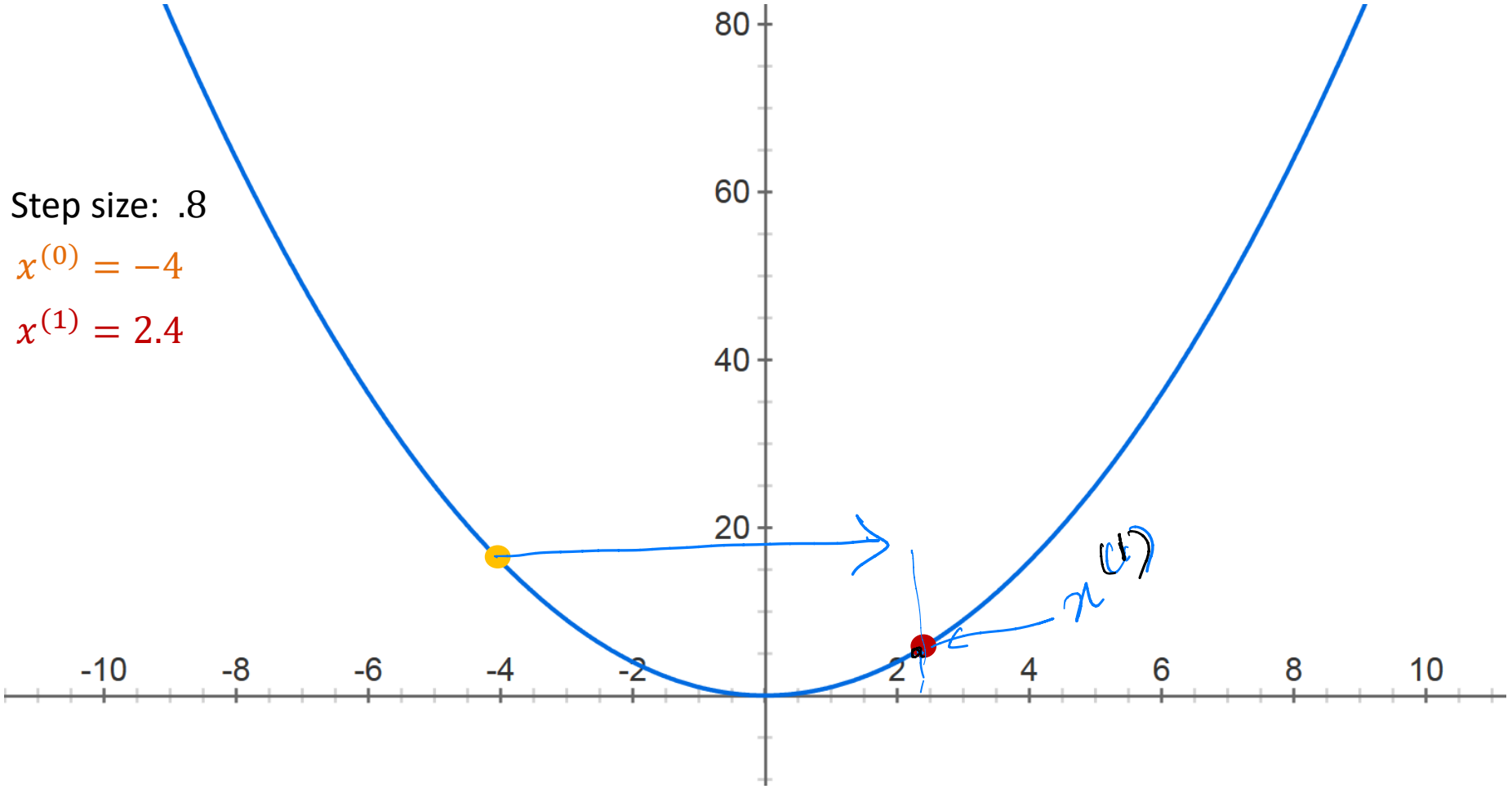
Gradient Descent

$f(x) = x^2$

Step size: .8

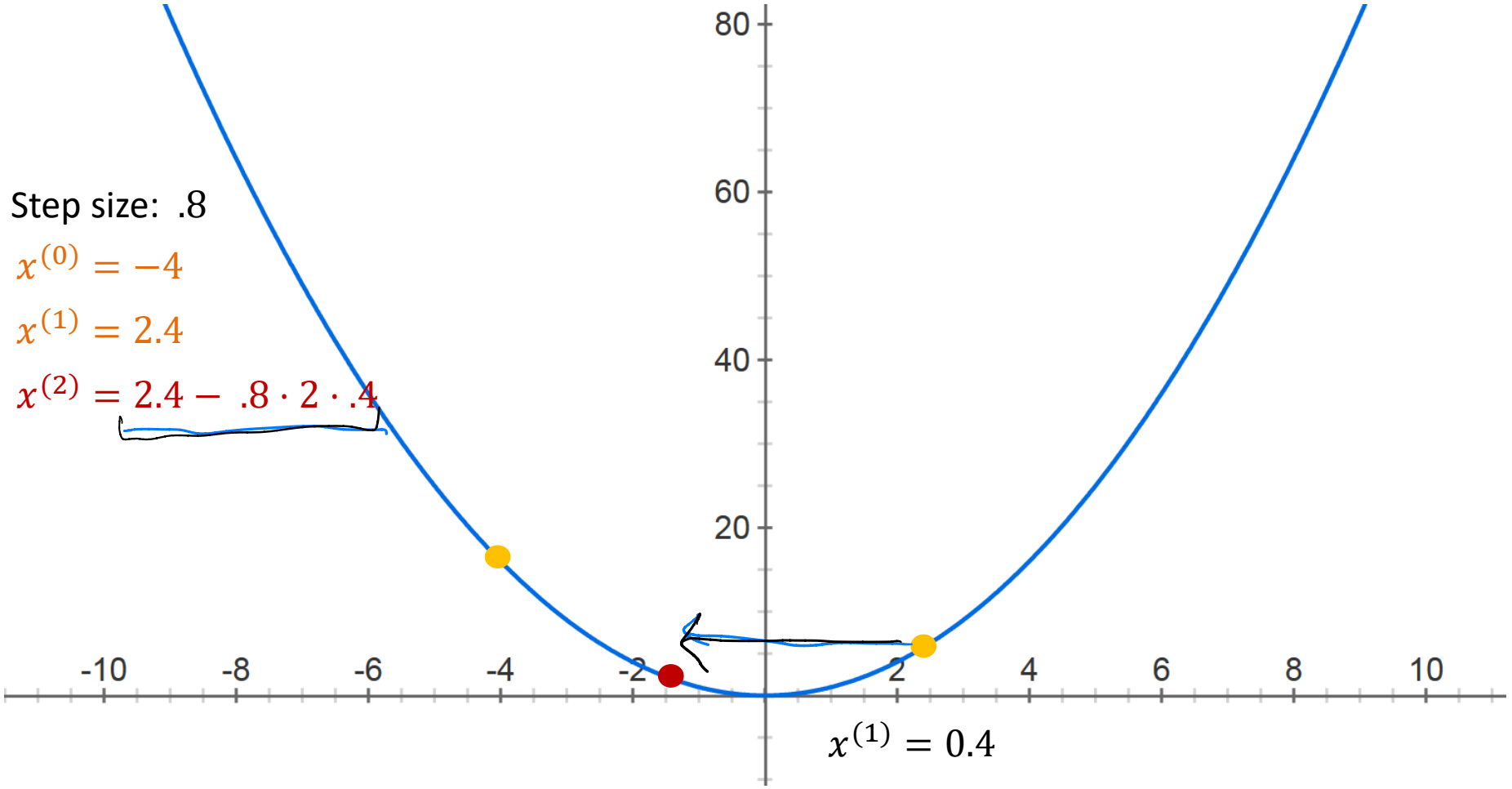
$x^{(0)} = -4$

$x^{(1)} = 2.4$



Gradient Descent

$f(x) = x^2$



Step size: .8

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

$x^{(1)} = 2.4$

$x^{(2)} = 2.4 - .8 \cdot 2 \cdot .4$

Gradient Descent

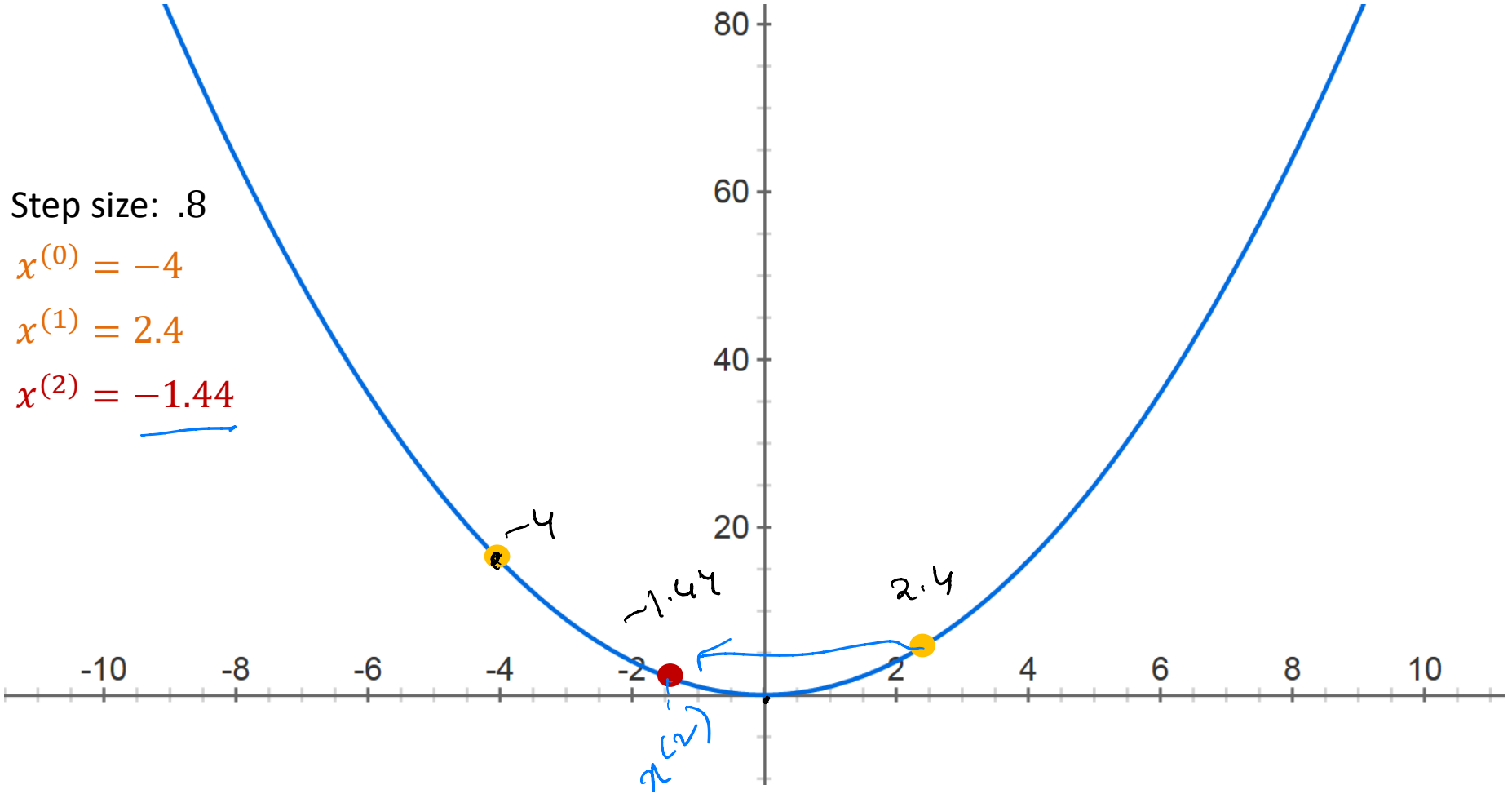
$f(x) = x^2$

Step size: .8

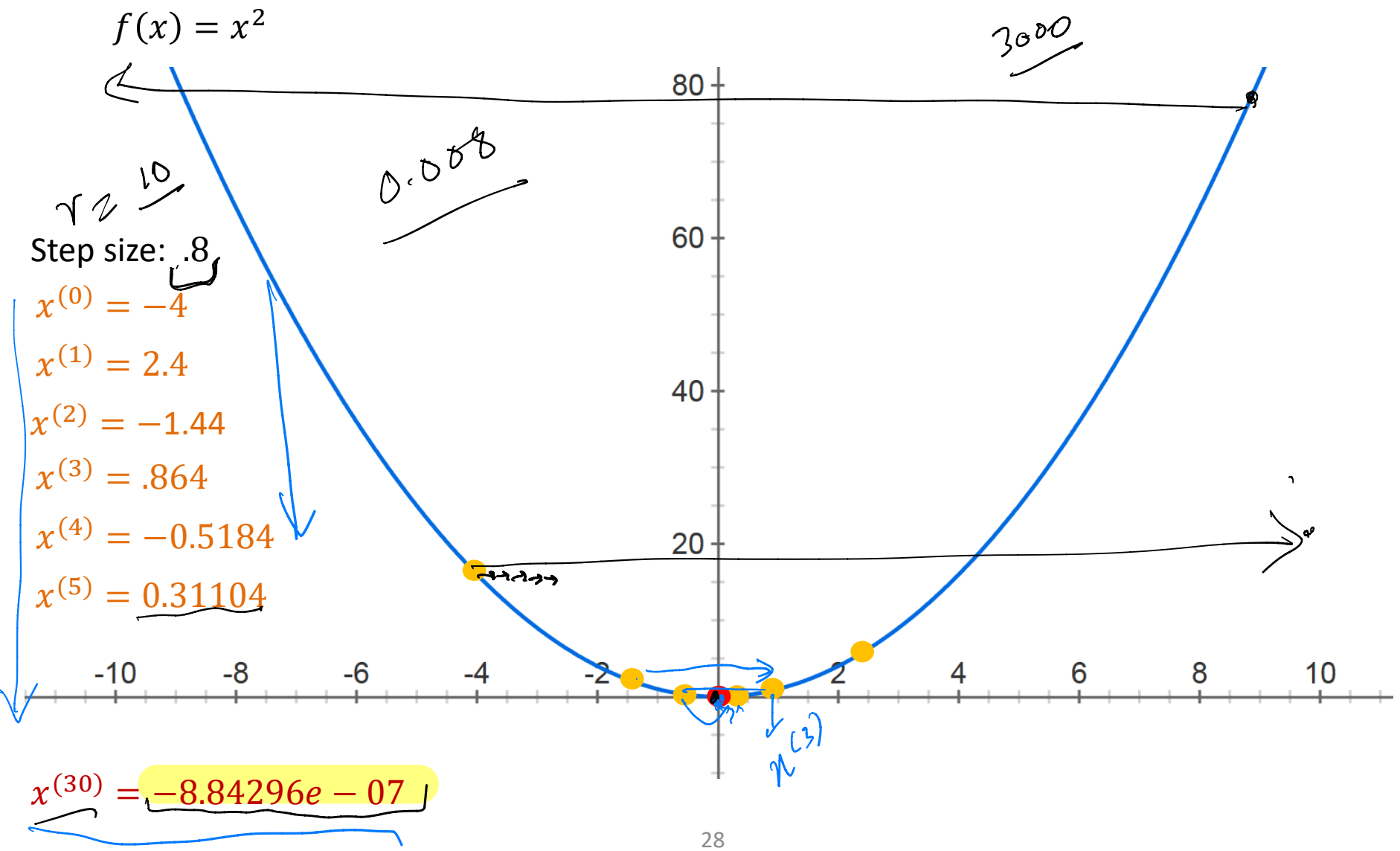
$x^{(0)} = -4$

$x^{(1)} = 2.4$

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



Gradient Descent (Numerical Algo)



Gradient Descent

$a, x^{(m)} \in \mathbb{R}$

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

- What is the gradient of this function?

- What does a gradient descent iteration look like for this simple regression problem?

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

Derivation of the Gradient (one dim)

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

$a \in \mathbb{R}$, $b \in \mathbb{R}$

$$\frac{df}{da} = \nabla f(a) = \frac{1}{M}\sum_{m=1}^{M} 2\left[a \cdot x^{(m)} + b - y^{(m)}\right] x^{(m)}$$

$$\nabla f(b) = \frac{1}{M}\sum_{m=1}^{M} 2\left(a x^{(m)} + b - y^{(m)}\right]$$

$$a^{(t+1)} = a^{(t)} - \gamma_t \nabla f(a)\Big|_{a=a^t}$$

$$b^{(t+1)} = b^{(t)} - \gamma_t \nabla f(b)\Big|_{b=b^t}$$

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)

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

$$\underbrace{\nabla f(a)}_{\in \mathbb{R}^n} = \frac{1}{M}\sum_{m=1}^{M} \underbrace{2\left[a^T x^{(m)} + b - y^{(m)}\right]}_{\text{scalar}} \underbrace{x^{(m)}}_{\mathbb{R}^n}$$

$\nabla f(b)$: same as 1d case.

$g(a) = a^T x^{(m)}$

$\nabla g(a) = x^{(m)}$

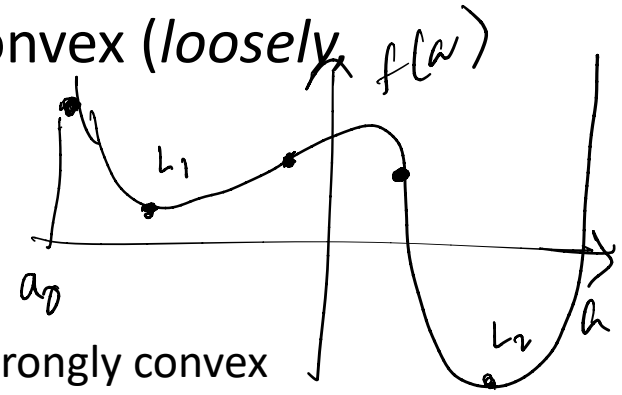
$$\nabla g(a) = \begin{bmatrix} \partial g/\partial a_1 \\ \partial g/\partial a_2 \\ \vdots \\ \partial g/\partial a_n \end{bmatrix} = x^{(m)}$$

$$g(a) = \sum_{i=1}^{n} a_i x_i^{(m)}$$

$$\frac{\partial g}{\partial a_i} = x_i^{(m)}$$

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

Polynomial Regression

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

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

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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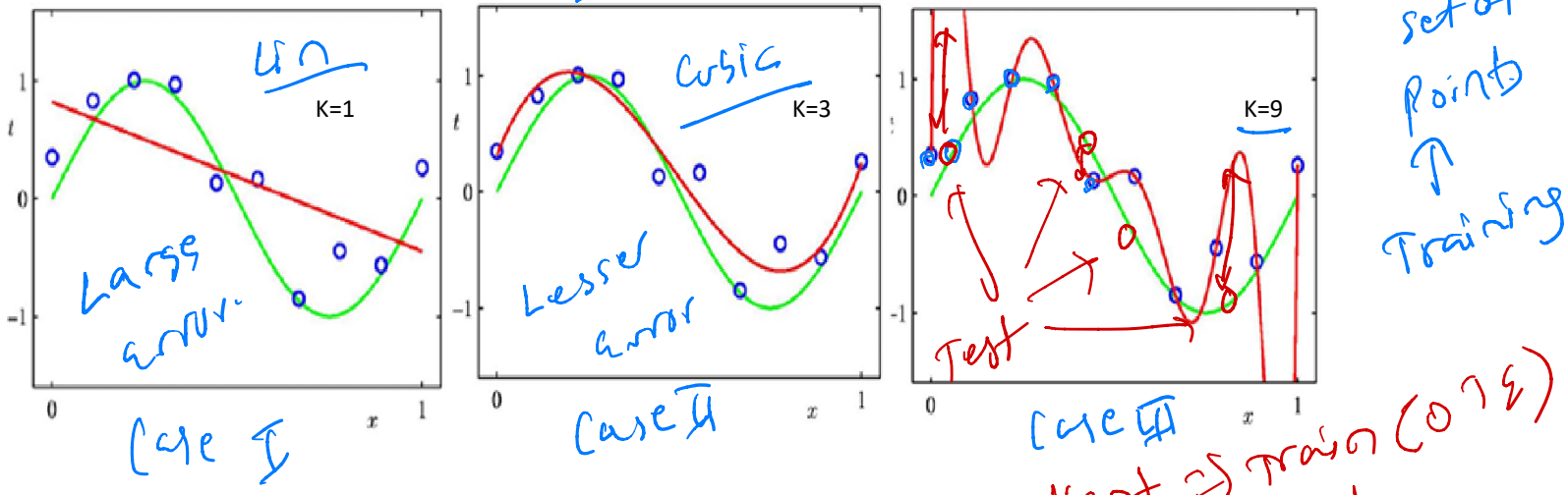
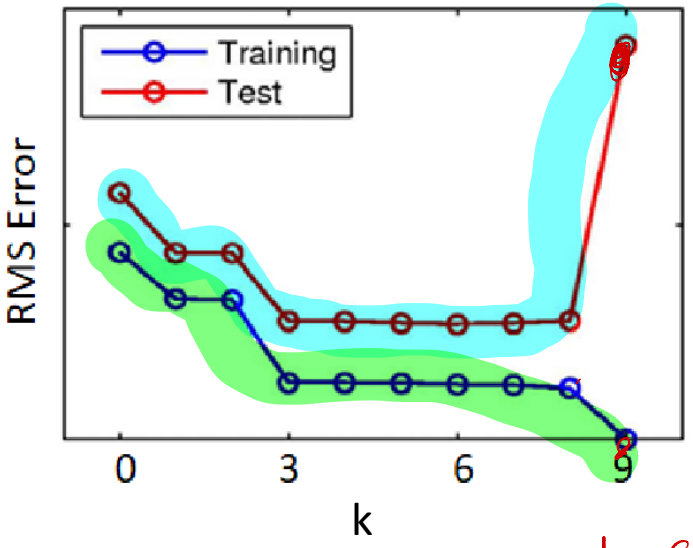


Caveats with Polynomial Regression

- 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)



Too many parameters

"Regularization"

Part IV: Hands On

House Price Prediction

- Boston House Price Dataset

CRIM: Per capita crime rate by town (crime)
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 → Label / Target

Feat

Summary of the Hands On Portion

- Load the Dataset (sk-learn)
- Exploratory Data Analysis (numpy)
- Training a Linear Regression Model
- Training a Polynomial Regression Model

→ inbuilt LR in sk-learn

- Training a Linear/Poly Regression from scratch using gradient descent

Contrast to inbuilt LR