CS 260: Foundations of Data Science

Prof. Thao Nguyen

Fall 2024

HAVERFORD
COLLEGE

Materials by Sara Mathieson

Outline for today

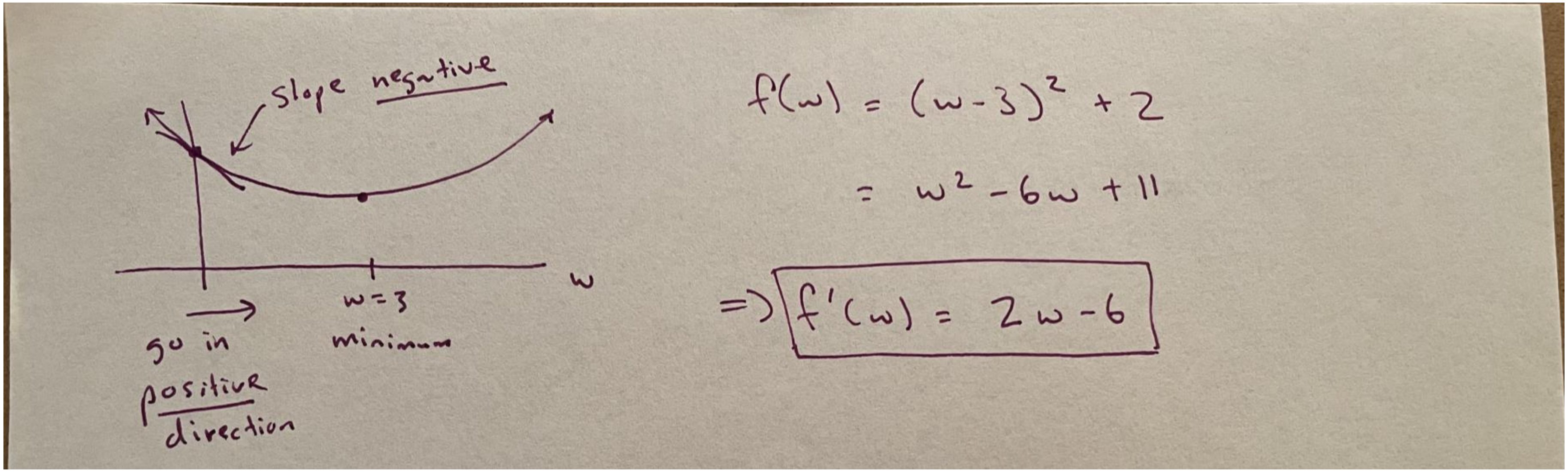
- SGD (Stochastic Gradient Descent)
- Handout 6 (SGD solution example)
- Analytic vs. SGD (pros and cons)
- (if time) Polynomial regression

Outline for today

- SGD (Stochastic Gradient Descent)
- Handout 6 (SGD solution example)
- Analytic vs. SGD (pros and cons)
- (if time) Polynomial regression

Stochastic gradient descent example

Goal: minimize the function $f(w) = w^2 - 6w + 11$

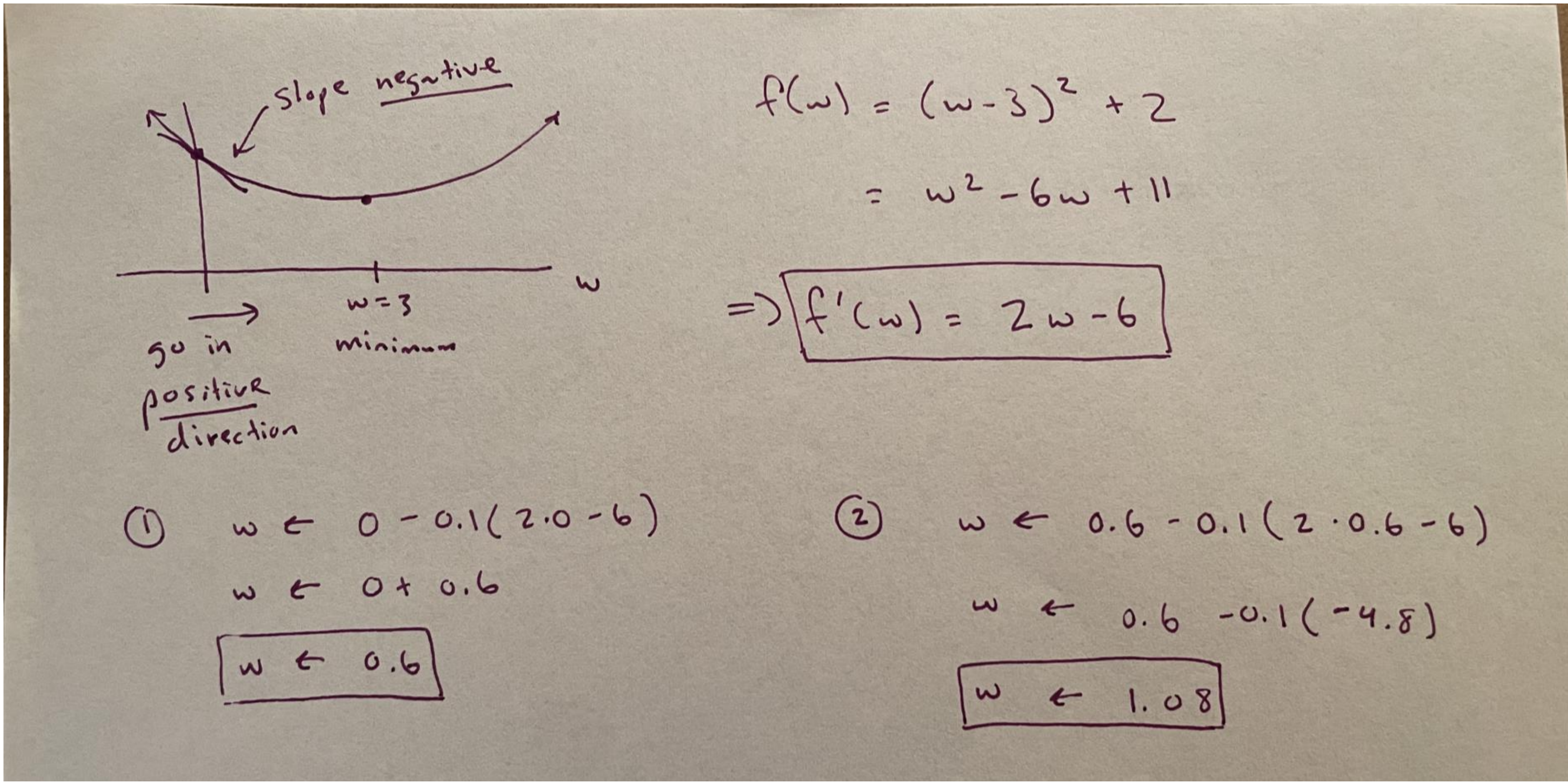


$$w \leftarrow w - \alpha f'(w)$$

step size

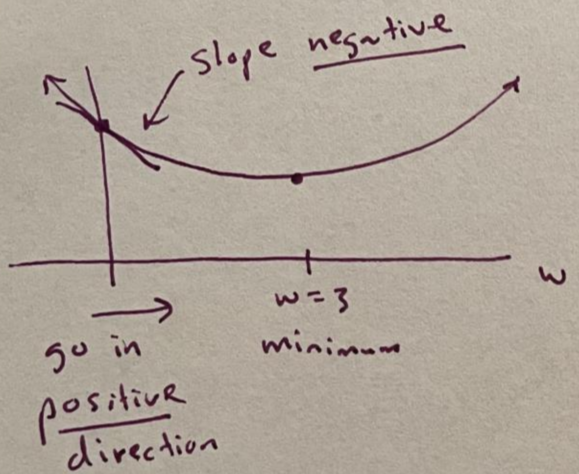
Stochastic gradient descent example

Goal: minimize the function $f(w) = w^2 - 6w + 11$



Stochastic gradient descent example

Goal: minimize the function $f(w) = w^2 - 6w + 11$



$$f(w) = (w-3)^2 + 2$$
$$= w^2 - 6w + 11$$
$$\Rightarrow \boxed{f'(w) = 2w - 6}$$

① $w \leftarrow 0 - 0.1(2\cdot 0 - 6)$

$w \leftarrow 0 + 0.6$

$\boxed{w \leftarrow 0.6}$

② $w \leftarrow 0.6 - 0.1(2 \cdot 0.6 - 6)$

$w \leftarrow 0.6 - 0.1(-4.8)$

$\boxed{w \leftarrow 1.08}$

Stop when:

$$|f(w^t) - f(w^{t-1})| < \varepsilon \quad , \quad \varepsilon = 1 \times 10^{-8}$$

(for example)

Stochastic Gradient Descent for Linear Regression

Key Idea: take the derivative of **one datapoint** at a time and use that to update w

$$J(\vec{w}) = \frac{1}{2} \sum_{i=1}^{n} (\vec{w} \cdot \vec{x}_i - y_i)^2$$

gradient with respect to <u>one</u> datapoint: (i.e. $\vec{x}_i$)

$$\nabla J_{\vec{x}_i} = \frac{\partial J(\vec{w})_{\vec{x}_i}}{\partial \vec{w}} = (\vec{w} \cdot \vec{x}_i - y_i)\, \vec{x}_i$$

Stochastic Gradient Descent for Linear Regression

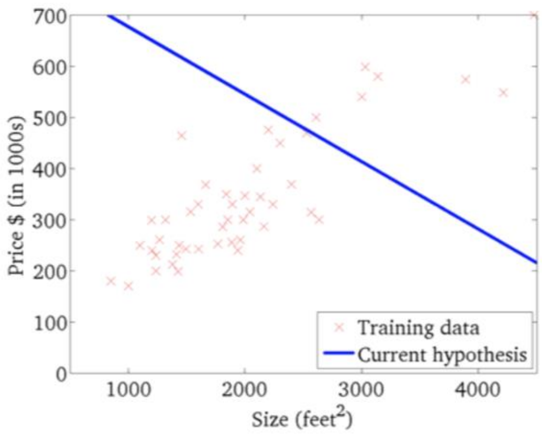
for (epoch) iteration t :

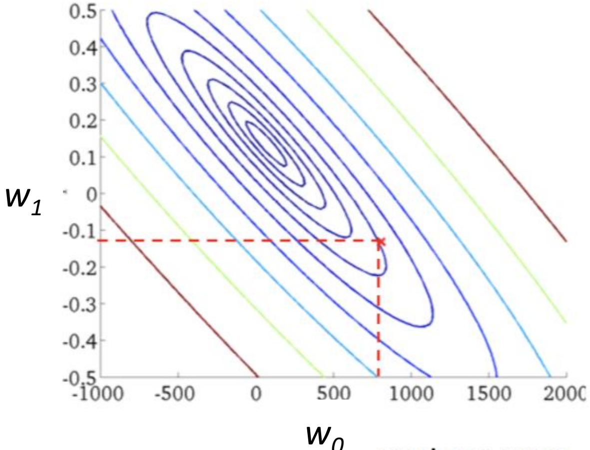
for $i = 1, 2, 3 \cdots n$: } usually shuffle

$$\vec{w} \leftarrow \vec{w} - \alpha(\vec{w} \cdot \vec{x}_i - y_i)\vec{x}_i$$

check for convergence : $|J(\vec{w}^{t}) - J(\vec{w}^{t-1})| < \varepsilon$

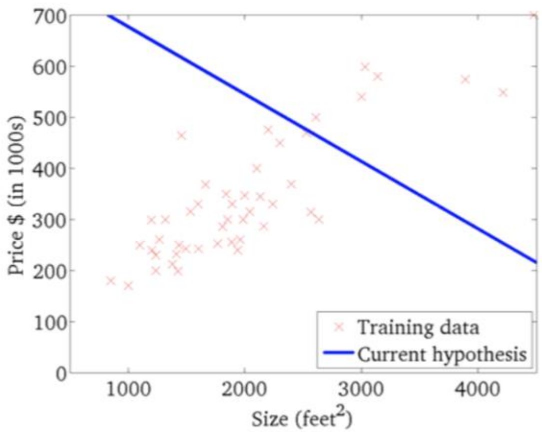
Linear Model and Cost Function J

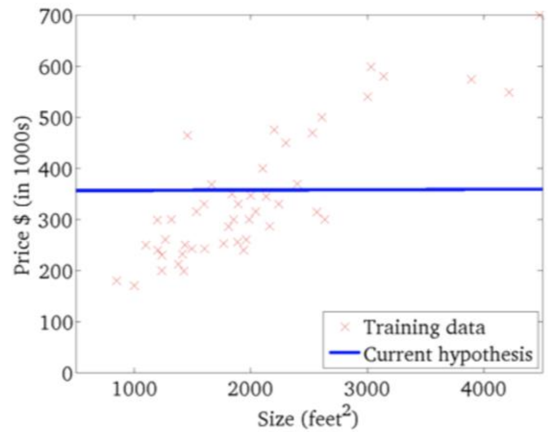


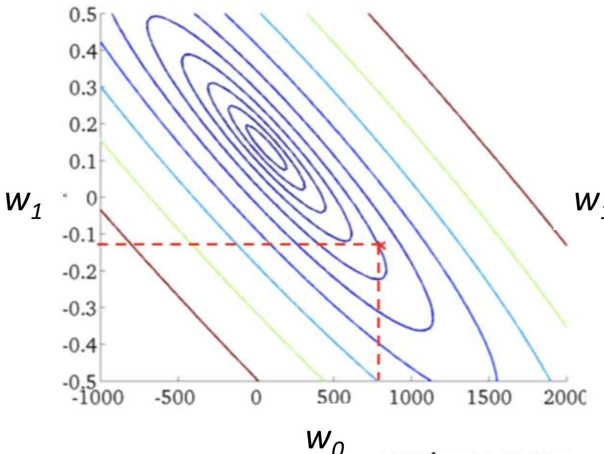


contour map

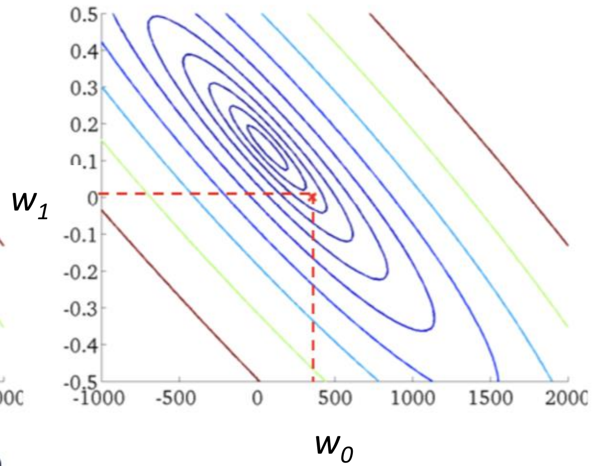
Linear Model and Cost Function J





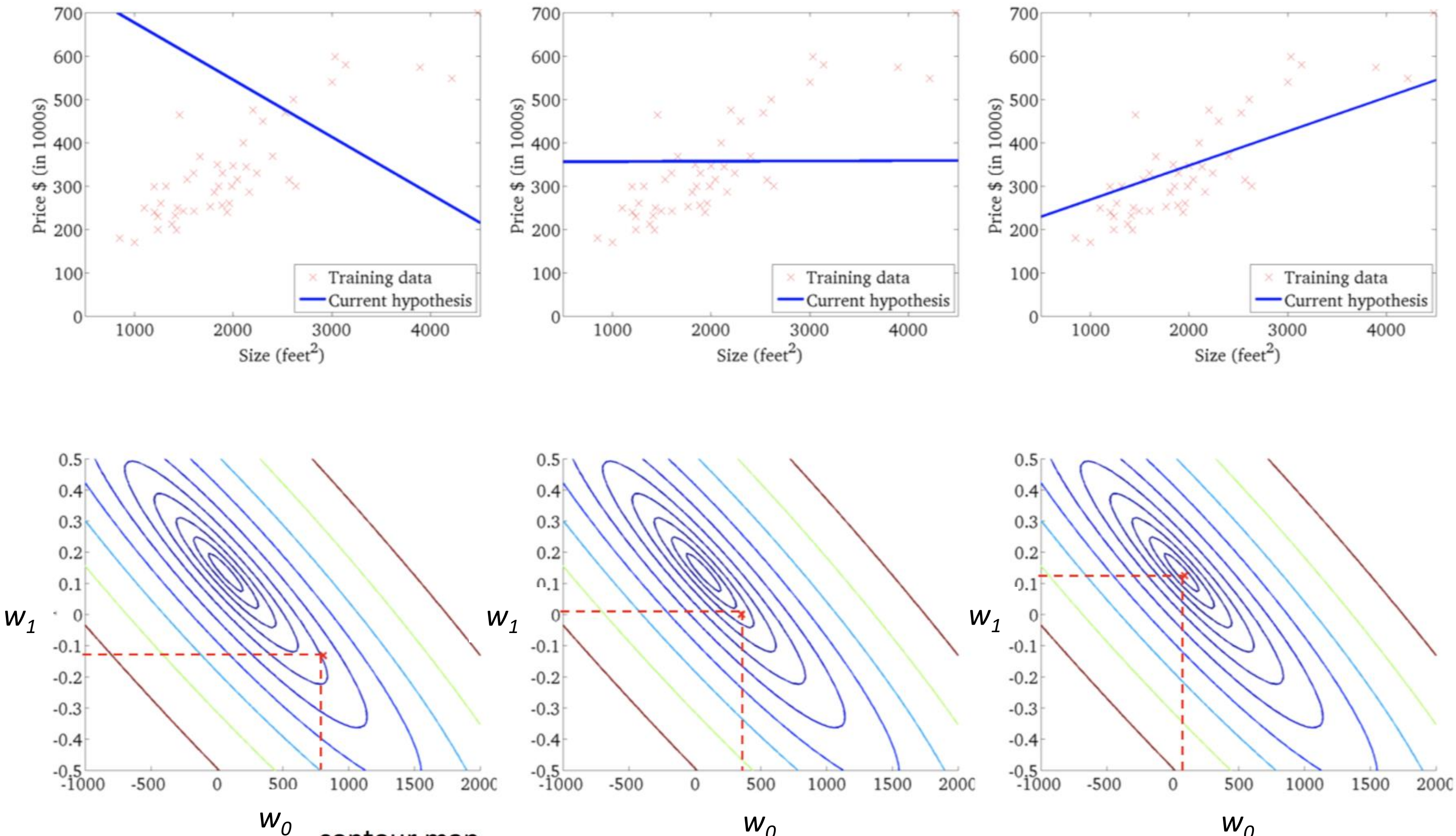


contour map



Slide: modified from Jessica Wu
Based on slide by Andrew Ng

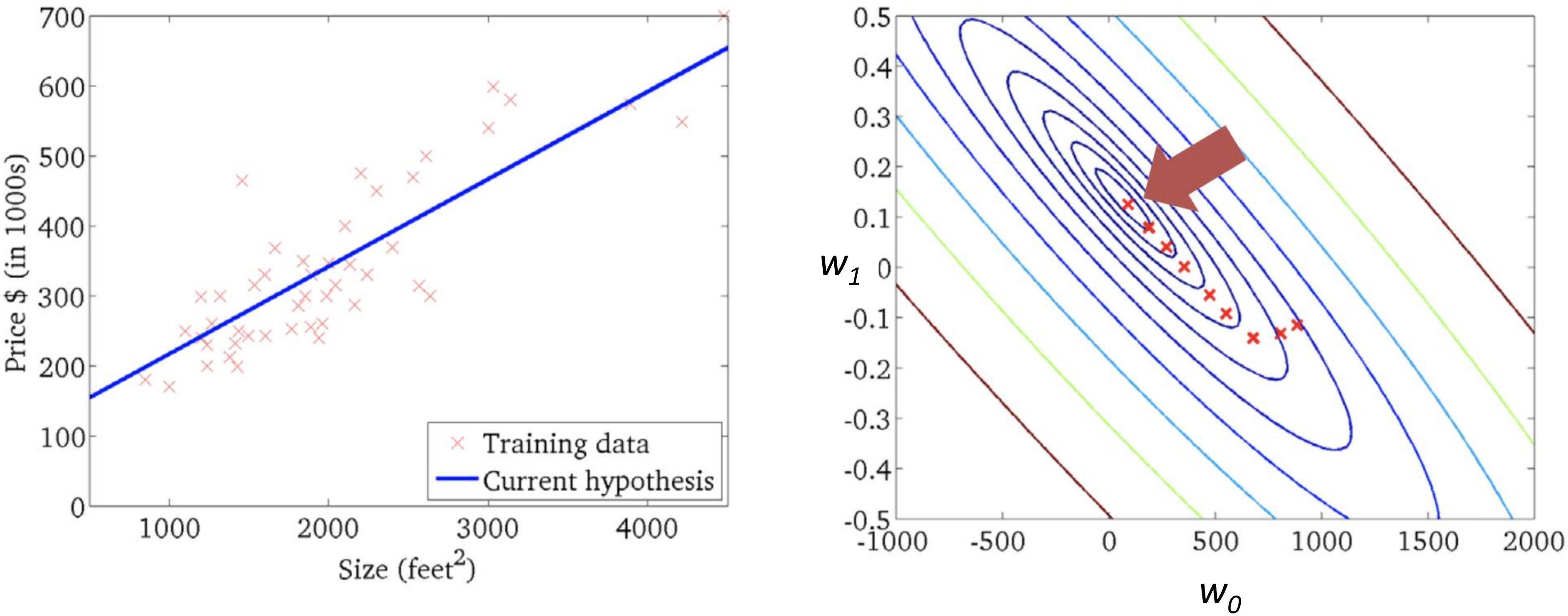
Linear Model and Cost Function J



contour map

Slide: modified from Jessica Wu
Based on slide by Andrew Ng

Gradient Descent: walking toward the minimum

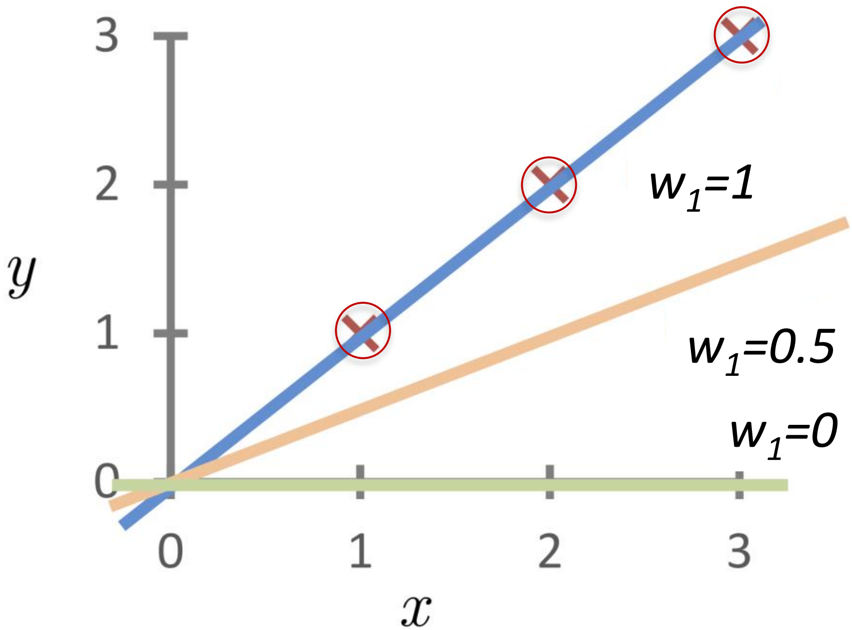


Slide: modified from Jessica Wu
Based on slide by Andrew Ng

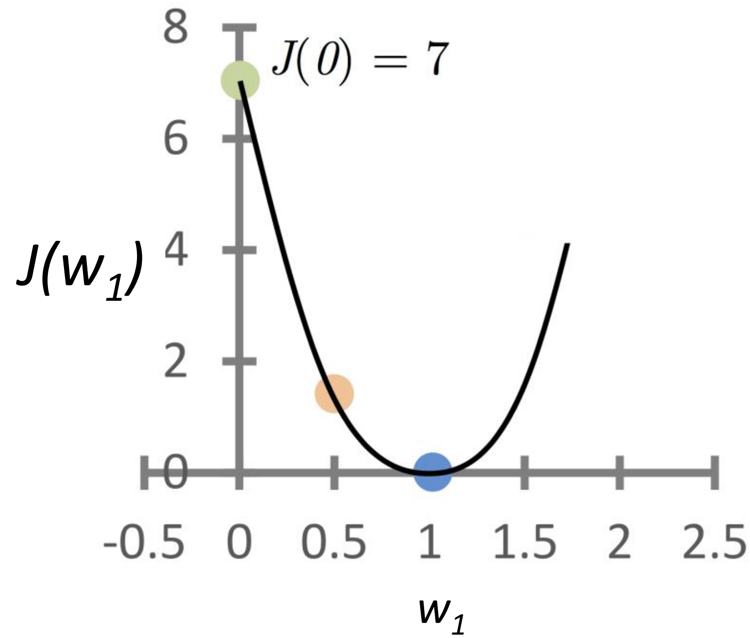
Cost Function (extra practice)

$h_w(x) = w_1 x$

(assume w_0=0 for this example)



$J(w_1)$

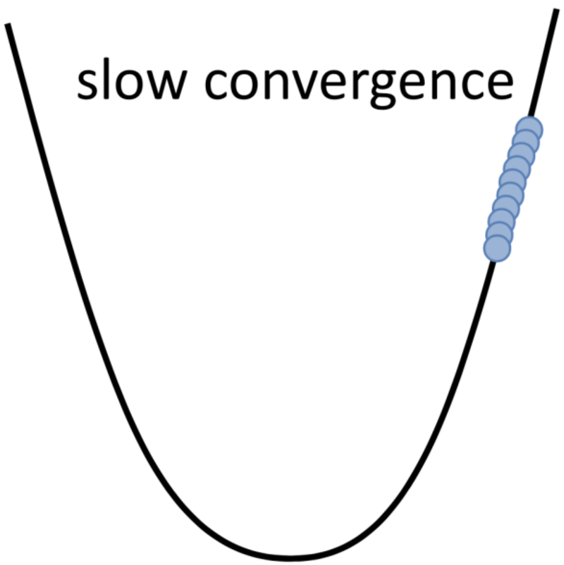


$$J(0.5) = \frac{1}{2}\left[(0.5-1)^2 + (1-2)^2 + (1.5-3)^2\right] = 1.75$$

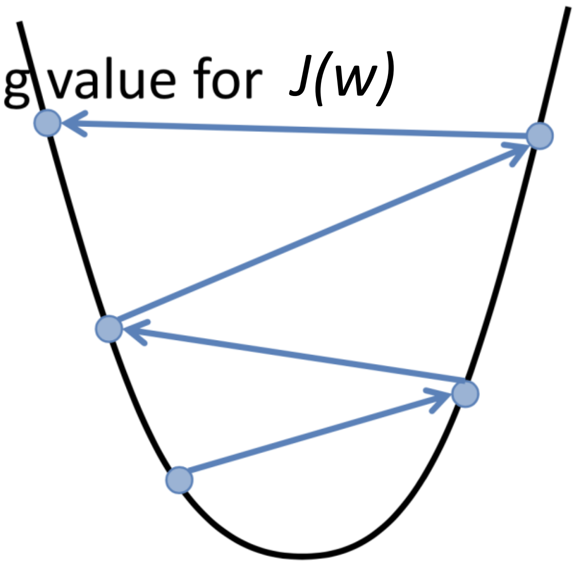
Slide: modified from Jessica Wu
Based on slide by Eric Eaton
[Example by Andrew Ng]

Choosing the step size alpha

α too small



α too large



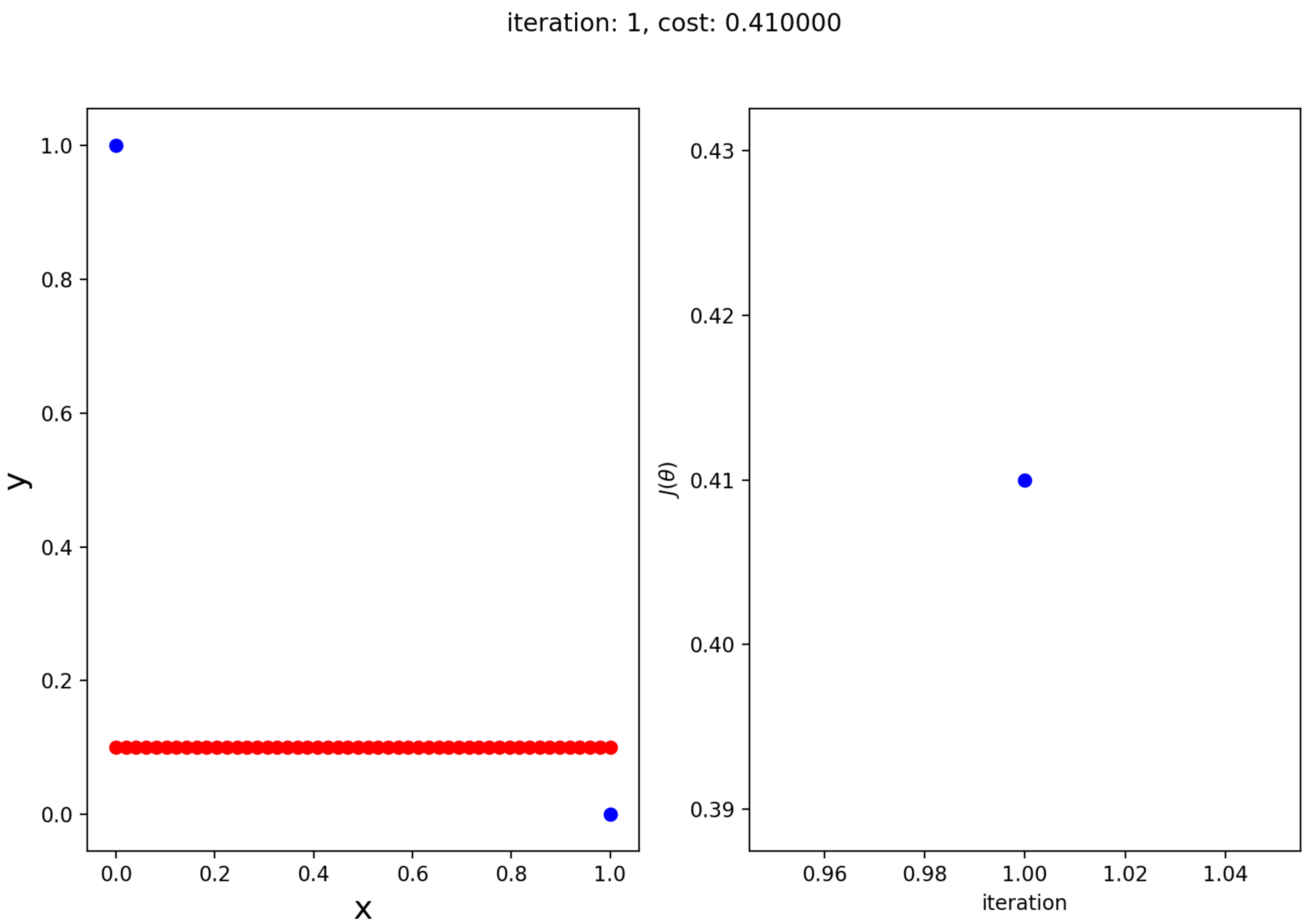
- may overshoot minimum
- may fail to converge (may even diverge)

Slide: modified from Jessica Wu
Based on slide by Eric Eaton
[Originally by Andrew Ng]

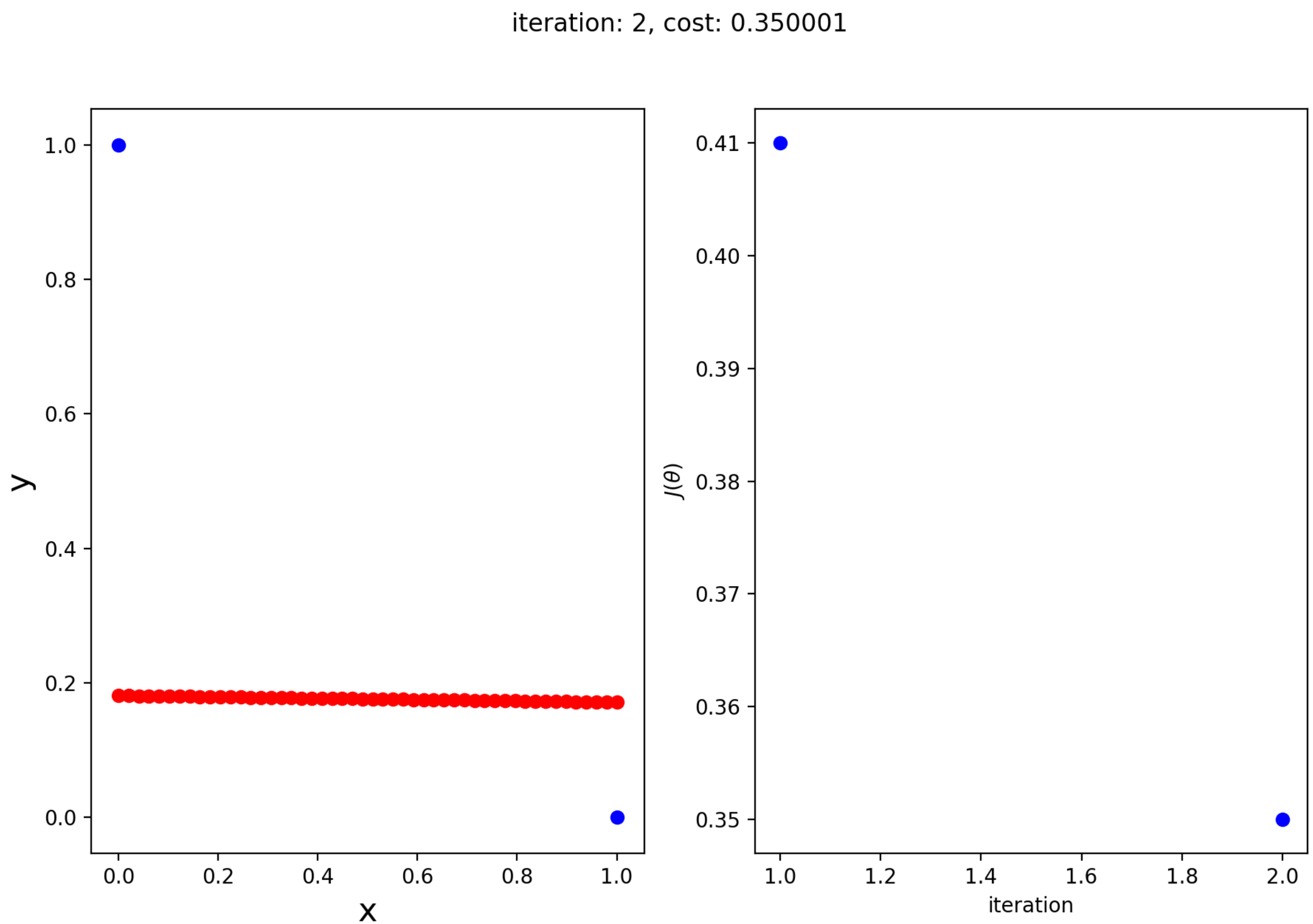
SGD with our small dataset from the handouts

Note: this is with the original order of the points

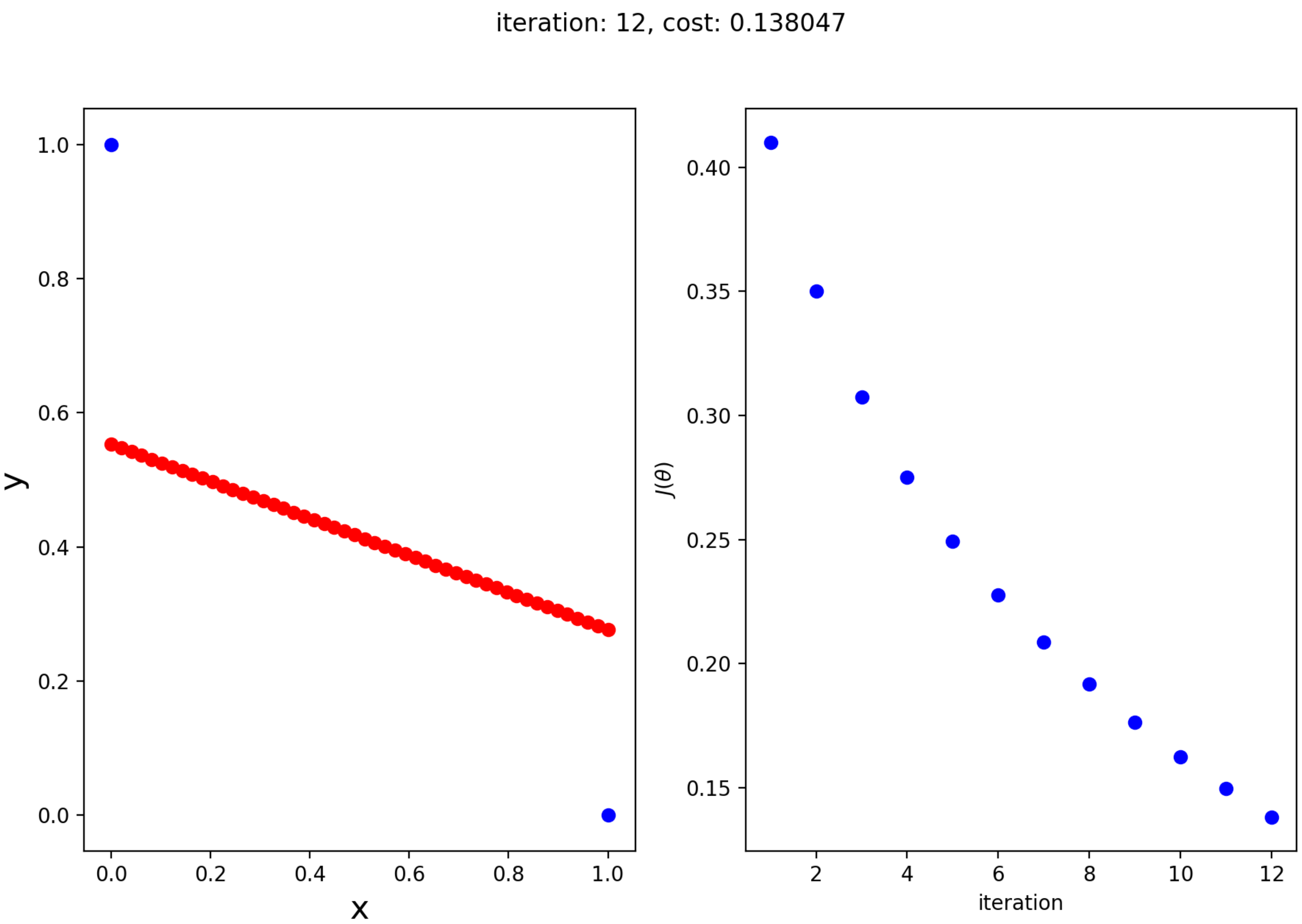
Small example, iteration 1



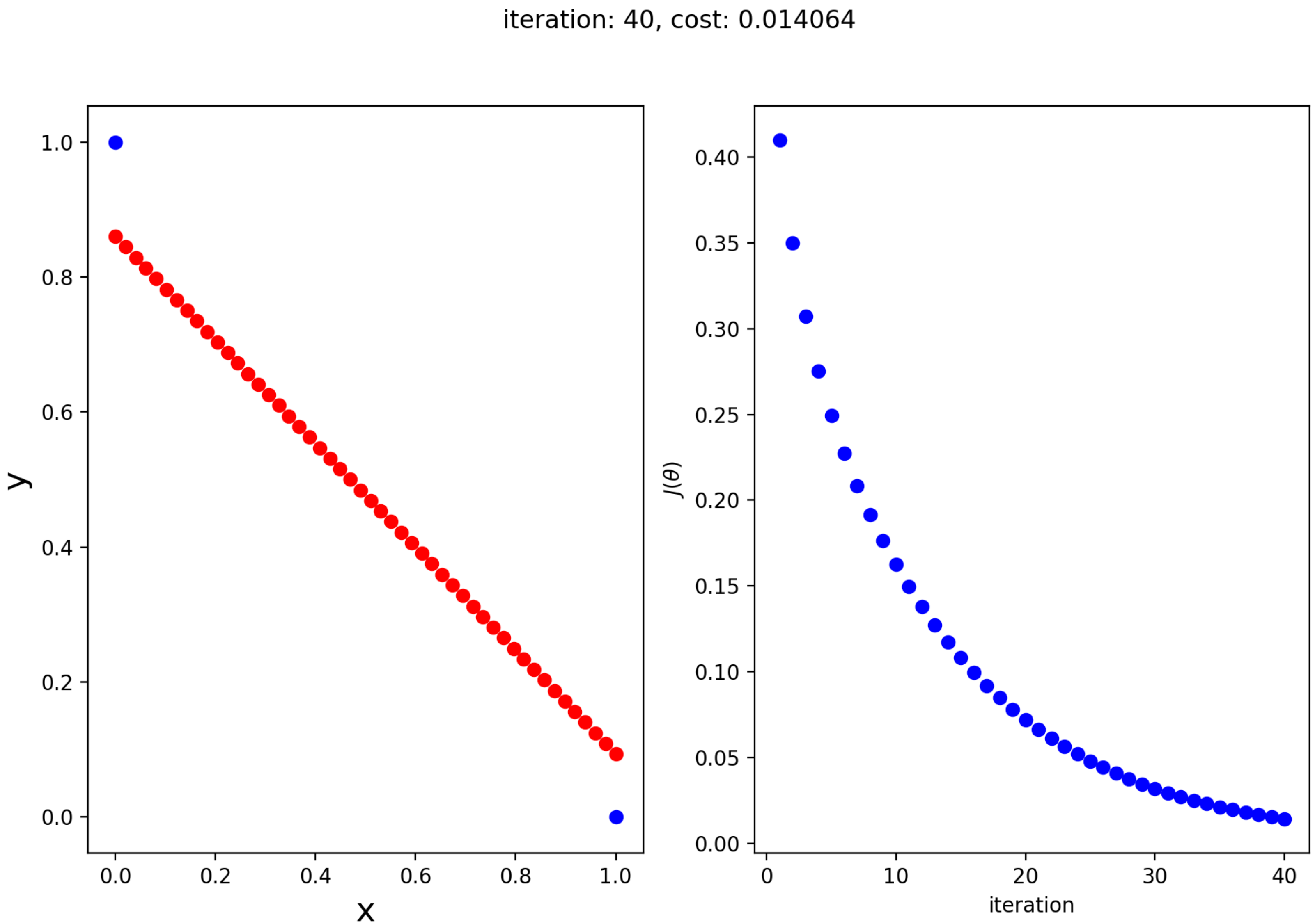
Small example, iteration 2



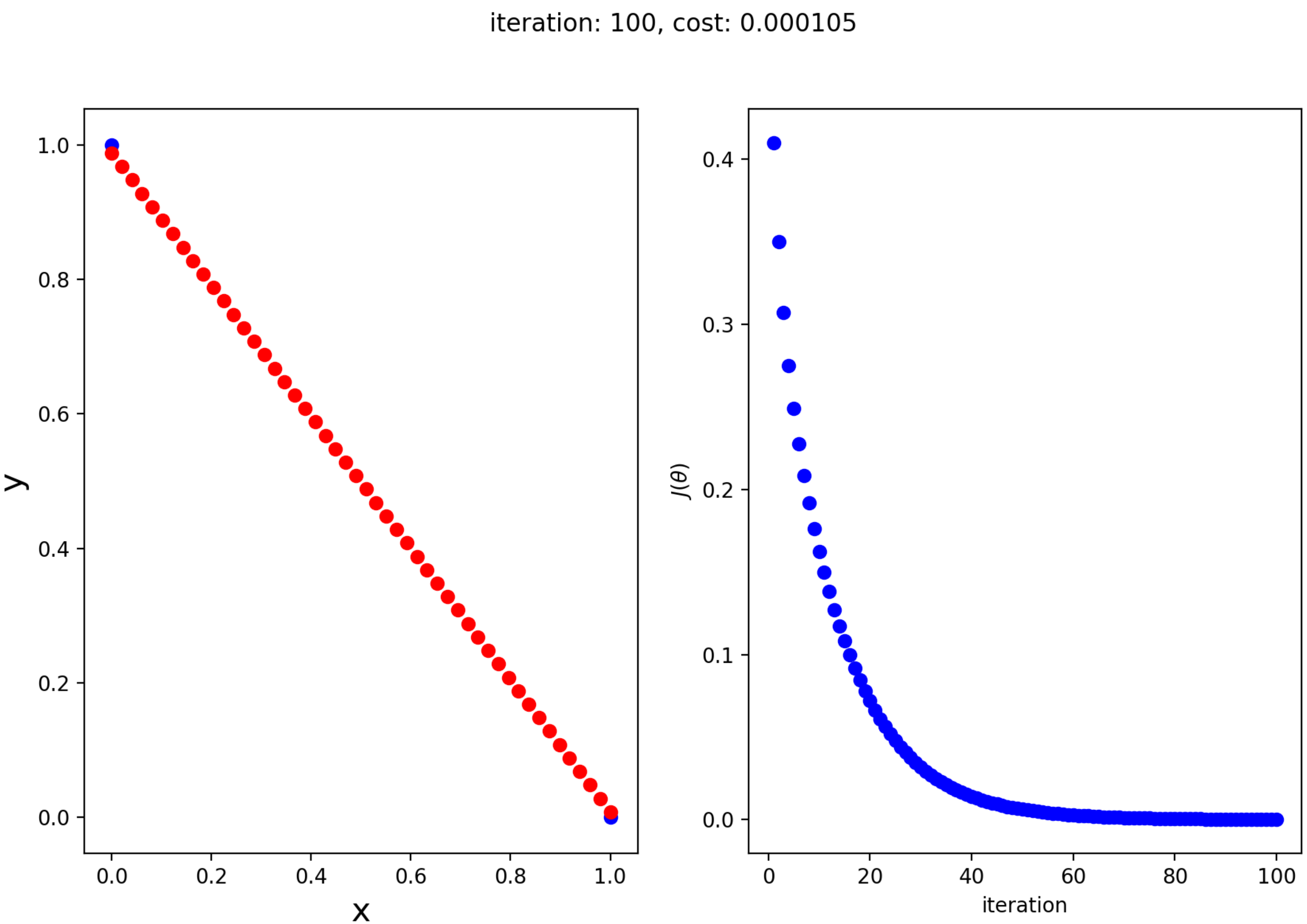
Small example, iteration 12



Small example, iteration 40



Small example, iteration 100



Outline for today

- SGD (Stochastic Gradient Descent)
- Handout 6 (SGD solution example)
- Analytic vs. SGD (pros and cons)
- (if time) Polynomial regression

Handout 6

Linear Regression: SGD solution *(find and work with a partner)*

In linear regression, we seek to minimize the sum of squared errors between the actual response and our prediction. We often call this RSS (residual sum of squares) or SSE (sum of squared errors). As an objective function, we often call it J and include a $\frac{1}{2}$ in front to make the derivatives work out nicely.

$$J(\boldsymbol{w}) = \frac{1}{2}\sum_{i=1}^{n}\left(h_{\boldsymbol{w}}(\boldsymbol{x_i}) - y_i\right)^2$$

For linear regression in general, one iteration of stochastic gradient descent includes the following updates (usually with the data points shuffled):

for i = 1,2,...,n:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \alpha(\boldsymbol{w} \cdot \boldsymbol{x}_i - y_i)\boldsymbol{x}_i$$

We will begin with our same data from the previous two handouts: $(x_1, y_1) = (0, 1)$ and $(x_2, y_2) = (1, 0)$, except we will reverse the order of the points to make the progress of gradient descent a bit clearer. So in this case our matrix/vector formulation is:

$$\boldsymbol{X} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}, \qquad \boldsymbol{y} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Handout 6

$$\boldsymbol{X} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}, \qquad \boldsymbol{y} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

1. Assuming $\alpha = 0.1$ and our initial values are $w_0 = 0$ and $w_1 = 0$, what are w_0 and w_1 after the just the first data point is used to update the gradient?

$$\vec{w} \leftarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix} - 0.1\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} - 1\right)\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\vec{w} \leftarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix} + 0.1\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\boxed{\vec{w} \leftarrow \begin{bmatrix} 0.1 \\ 0 \end{bmatrix}}$$

2. What are w_0 and w_1 after the second data point is used? Si

Handout 6

$$\boldsymbol{X} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}, \qquad \boldsymbol{y} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

1. Assuming $\alpha = 0.1$ and our initial values are $w_0 = 0$ and $w_1 = 0$, what are w_0 and w_1 after the just the first data point is used to update the gradient?

$$\vec{w} \leftarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix} - 0.1\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} - 1\right)\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\vec{w} \leftarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix} + 0.1 \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\boxed{\vec{w} \leftarrow \begin{bmatrix} 0.1 \\ 0 \end{bmatrix}}$$

2. What are w_0 and w_1 after the second data point is used? Since we only have two examples here, your result would be the weight vector after the first iteration of SGD.

$$\vec{w} \leftarrow \begin{bmatrix} 0.1 \\ 0 \end{bmatrix} - 0.1\left(\begin{bmatrix} 0.1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} - 0\right)\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\boxed{\vec{w} \leftarrow \begin{bmatrix} 0.09 \\ -0.01 \end{bmatrix}}$$

Handout 6

$$\boldsymbol{X} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}, \qquad \boldsymbol{y} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

1. Assuming $\alpha = 0.1$ and our initial values are $w_0 = 0$ and $w_1 = 0$, what are w_0 and w_1 after the just the first data point is used to update the gradient?

$$\vec{w} \leftarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix} - 0.1\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} - 1\right)\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\vec{w} \leftarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix} + 0.1 \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\boxed{\vec{w} \leftarrow \begin{bmatrix} 0.1 \\ 0 \end{bmatrix}}$$

2. What are w_0 and w_1 after the second data point is used? Since we only have two examples here, your result would be the weight vector after the first iteration of SGD.

$$\vec{w} \leftarrow \begin{bmatrix} 0.1 \\ 0 \end{bmatrix} - 0.1\left(\begin{bmatrix} 0.1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} - 0\right)\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\boxed{\vec{w} \leftarrow \begin{bmatrix} 0.09 \\ -0.01 \end{bmatrix}}$$

3. What is the value of the objective function (cost) after this initial iteration?

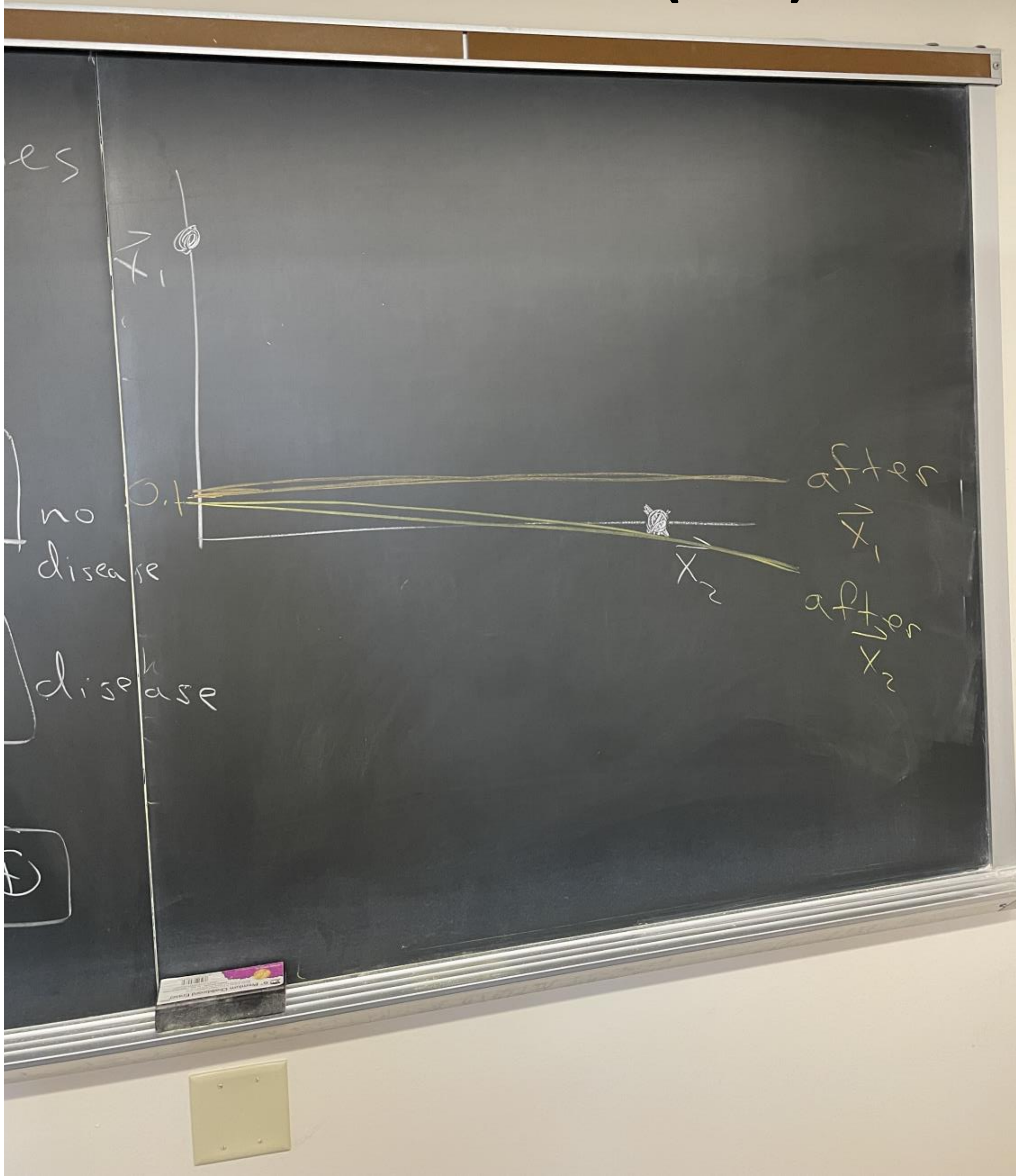
$$\hat{y} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 0.09 \\ -0.01 \end{bmatrix} = \begin{bmatrix} 0.09 \\ 0.08 \end{bmatrix}$$

$$\vec{y} - \hat{y} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \begin{bmatrix} 0.09 \\ 0.08 \end{bmatrix} = \begin{bmatrix} 0.91 \\ -0.08 \end{bmatrix}$$

$$J(\vec{w}) = \frac{1}{2}\begin{bmatrix} 0.91 \\ -0.08 \end{bmatrix} \cdot \begin{bmatrix} 0.91 \\ -0.08 \end{bmatrix}$$

$$\boxed{J(\vec{w}) = 0.417}$$

Handout 6 (#4)



Outline for today

- SGD (Stochastic Gradient Descent)
- Handout 6 (SGD solution example)
- Analytic vs. SGD (pros and cons)
- (if time) Polynomial regression

Pros and Cons

Gradient Descent

- requires multiple iterations
- need to choose α
- works well when p is large
- can support online learning

(Analytic Solution)

Normal Equations

- non-iterative
- no need for α
- slow if p is large
  - matrix inversion is $O(p^3)$

Linear Regression Runtime

- T = # iterations of SGD
- n = # examples
- p = # features

1) What is the runtime of SGD?
2) What is the runtime of the analytic solution?

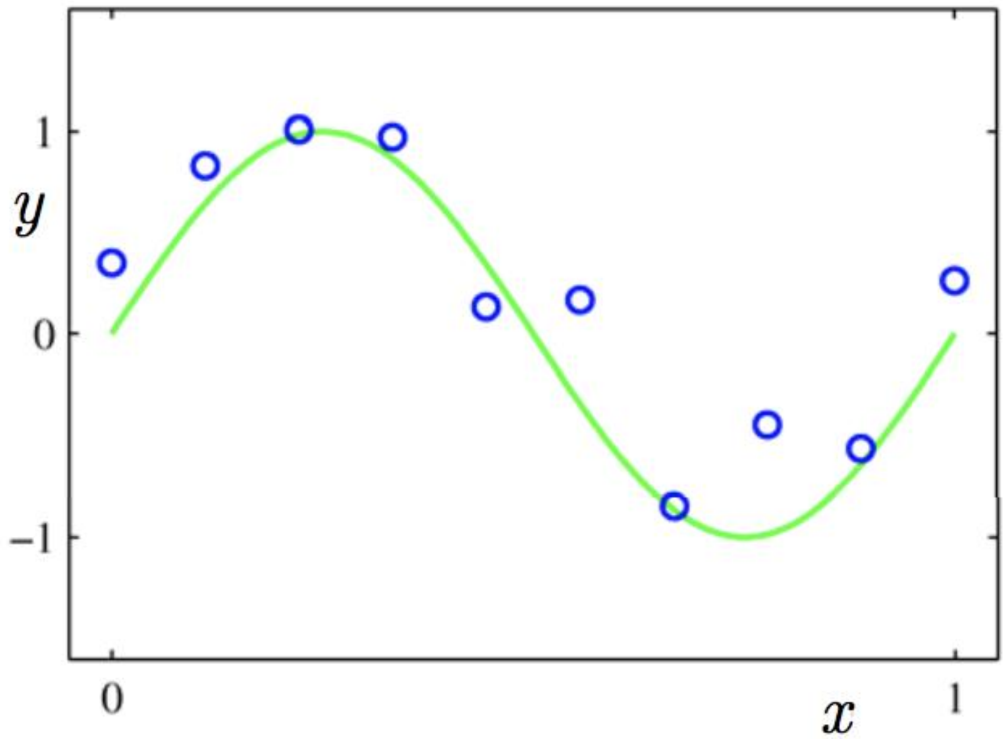
Challenge outside of class!

Outline for today

- SGD (Stochastic Gradient Descent)
- Handout 6 (SGD solution example)
- Analytic vs. SGD (pros and cons)
- (if time) Polynomial regression

Polynomial Regression

- Can be thought of as regular linear regression with a change of basis



Plot: Jessica Wu

Polynomial Regression

$$\boldsymbol{X} = \begin{bmatrix} x_1^0 & x_1^1 & x_1^2 & \cdots & x_1^d \\ & & \vdots & & \\ x_n^0 & x_n^1 & x_n^2 & \cdots & x_n^d \end{bmatrix}$$