EE2211 Tutorial 8

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Q1

Suppose we are minimizing $f(x) = x^4$ with respect to x. We initialize x to be 2. We perform gradient descent with learning rate 0.1. What is the value of x after the first iteration?

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Q1

Suppose we are minimizing $f(x) = x^4$ with respect to x. We initialize x to be 2. We perform gradient descent with learning rate 0.1. What is the value of x after the first iteration?

- The gradient of $f(x)$ is $4x^3$
- At x = 2, the gradient is $4 \times 2^3 = 32$
- After first iteration of gradient descent, value of x will be $x = 2 - 0.1 \times 32 = -1.2$

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Q2

(Python)

Please consider the csv file (government-expenditure-on-education.csv), which depicts the government's educational expenditure over the years. We would like to predict expenditure as a function of year. To do this, fit an exponential model $f(x, w) = \exp(-x^T w)$ with squared error loss to estimate w based on the csv file and gradient descent.

a) Plot the cost function $C(w)$ as a function of the number of iterations

b) Use the fitted parameters to plot the predicted educational expenditure from year 1981 to year 2023

c) Repeat (a) using a learning rate of 0.1 and learning rate of 0.001. What do you observe relative to (a)?

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Q2

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \nabla_{\mathbf{w}} \sum_{i=1}^{m} (f(\mathbf{x}_i, \mathbf{w}) - y_i)^2$$

$$= \sum_{i=1}^{m} \nabla_{\mathbf{w}} (f(\mathbf{x}_i, \mathbf{w}) - y_i)^2 \qquad g(x) \qquad f(x, w) = \exp(-x^T w)$$

$$= \sum_{i=1}^{m} 2(f(\mathbf{x}_i, \mathbf{w}) - y_i) \nabla_{\mathbf{w}} f(\mathbf{x}_i, \mathbf{w}) \qquad \text{chain rule}$$

$$= \sum_{i=1}^{m} 2(f(\mathbf{x}_i, \mathbf{w}) - y_i) \nabla_{\mathbf{w}} \exp(-\mathbf{x}_i^T \mathbf{w}) \qquad g(x)$$

$$= -\sum_{i=1}^{m} 2(f(\mathbf{x}_i, \mathbf{w}) - y_i) \exp(-\mathbf{x}_i^T \mathbf{w}) \nabla_{\mathbf{w}} (\mathbf{x}_i^T \mathbf{w}) \qquad \text{chain rule}$$

$$= -\sum_{i=1}^{m} 2(f(\mathbf{x}_i, \mathbf{w}) - y_i) \exp(-\mathbf{x}_i^T \mathbf{w}) \mathbf{x}_i \qquad \frac{d(b^T x)}{dx} = b$$

$$= -\sum_{i=1}^{m} 2(f(\mathbf{x}_i, \mathbf{w}) - y_i) f(\mathbf{x}_i, \mathbf{w}) \mathbf{x}_i$$

Chain Rule:
If we define $h(x) = f(g(x))$, then derivative of $h(x)$ is
$h'(x) = f'\big(g(x)\big) g'(x)$

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Q2

Load and Normalize Data

- Load CSV data from government-expenditure-on-education.csv using pandas.
- Extract expenditure and years data as NumPy arrays.
- Normalize both the expenditure and years:
  - y = expenditure / max_expenditure (normalized expenditure)
  - X (feature matrix) contains ones for bias and normalized years.

```
# load data
df = pd.read_csv("government-expenditure-on-education.csv")
expenditure = df['total_expenditure_on_education'].to_numpy()
years = df['year'].to_numpy()

# create normalized variables
max_expenditure = max(expenditure)
max_year = max(years)
y = expenditure/max_expenditure
X = np.ones([len(y), 2])
X[:, 1] = years/max_year
```

Q2

```
# Gradient descent
    learning_rate = 0.1
    w = np.zeros(2)
    pred_y, cost, gradient = exp_cost_gradient(X, w, y)
    num_iters = 2000000
    cost_vec = np.zeros(num_iters)
    print('Initial Cost =', cost)

    for i in range(0, num_iters):

        # update w
        w = w - learning_rate*gradient

        # compute updated cost and new gradient
        pred_y, cost, gradient = exp_cost_gradient(X, w, y)
        cost_vec[i] = cost

        if(i % 200000 == 0):
            print('Iter', i, ': cost =', cost)

    pred_y, cost, gradient = exp_cost_gradient(X, w, y)
    print('Final Cost =', cost)
```

Initialize Gradient Descent

- Set learning rate to 0.1 and initialize the weights w to zeros.
- Set number of iterations to 2,000,000.
- Compute the initial cost, predictions, and gradient using the exp_cost_gradient() function.
- Initialize an array cost_vec to store the cost values over iterations.

Perform Gradient Descent

Run a loop for 2,000,000 iterations:

- Update weights using gradient descent: w = w - learning_rate * gradient.
- Compute new predictions, cost, and gradient after each update.
- Store the cost after each iteration.

Q2

The function exp_cost_gradient() calculates:

- Predicted values using the exponential model.
- Cost (mean squared error) between predicted and true values.
- Gradient of the cost function with respect to the weights.

```
def exp_cost_gradient(X, w, y):

    # Compute prediction, cost and gradient based on mean square error loss
    pred_y = np.exp(-X @ w)
    cost   = np.sum((pred_y - y)*(pred_y - y))
    gradient = -2 * (pred_y - y) * pred_y @ X

    return pred_y, cost, gradient
```

$$\nabla_{\mathrm{w}} C(\mathrm{w}) = -\sum_{i=1}^{m} 2(f(\mathrm{x}_i, \mathrm{w}) - y_i) f(\mathrm{x}_i, \mathrm{w}) \mathrm{x}_i$$

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Q2

Extrapolate government expenditure until the year 2023:

- Create new feature matrix ext_X for the years up to 2023.
- Use the final weights w to predict expenditure values for these future years.

```
# Extrapolate until year 2023
  ext_years = np.arange(min(years), 2024, 1)
  ext_X = np.ones([len(ext_years), 2])
  ext_X[:, 1] = ext_years/max_year
  pred_y = np.exp(-ext_X @ w)
```

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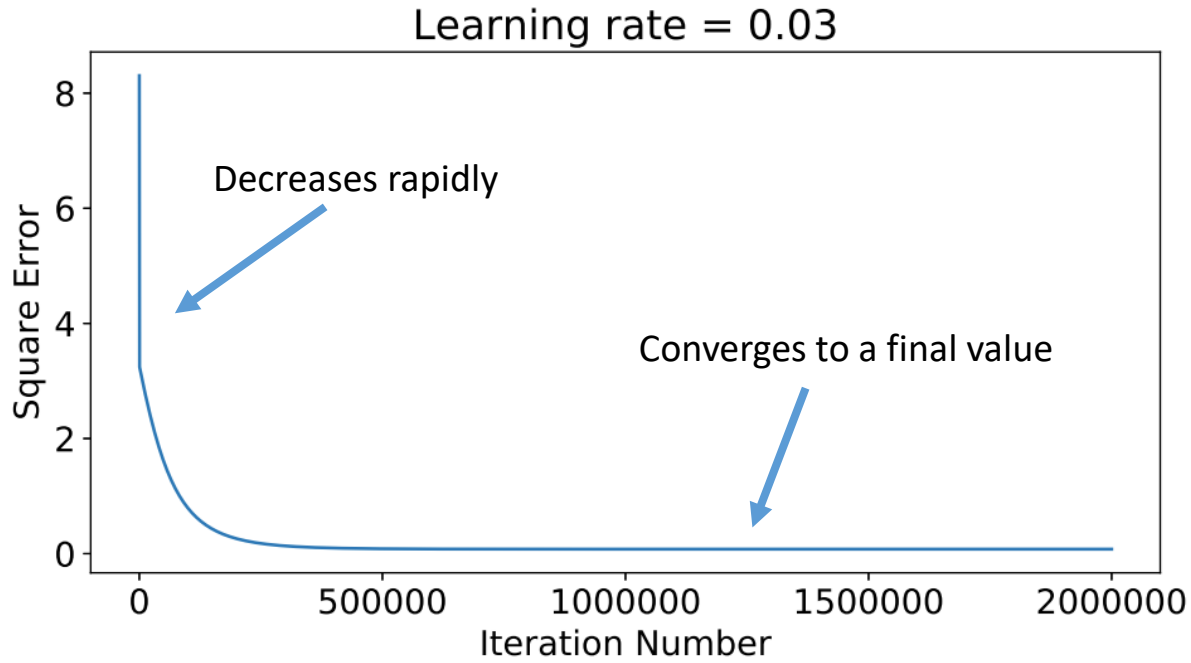
Q2

a) Plot the cost function $C(w)$ as a function of the number of iterations



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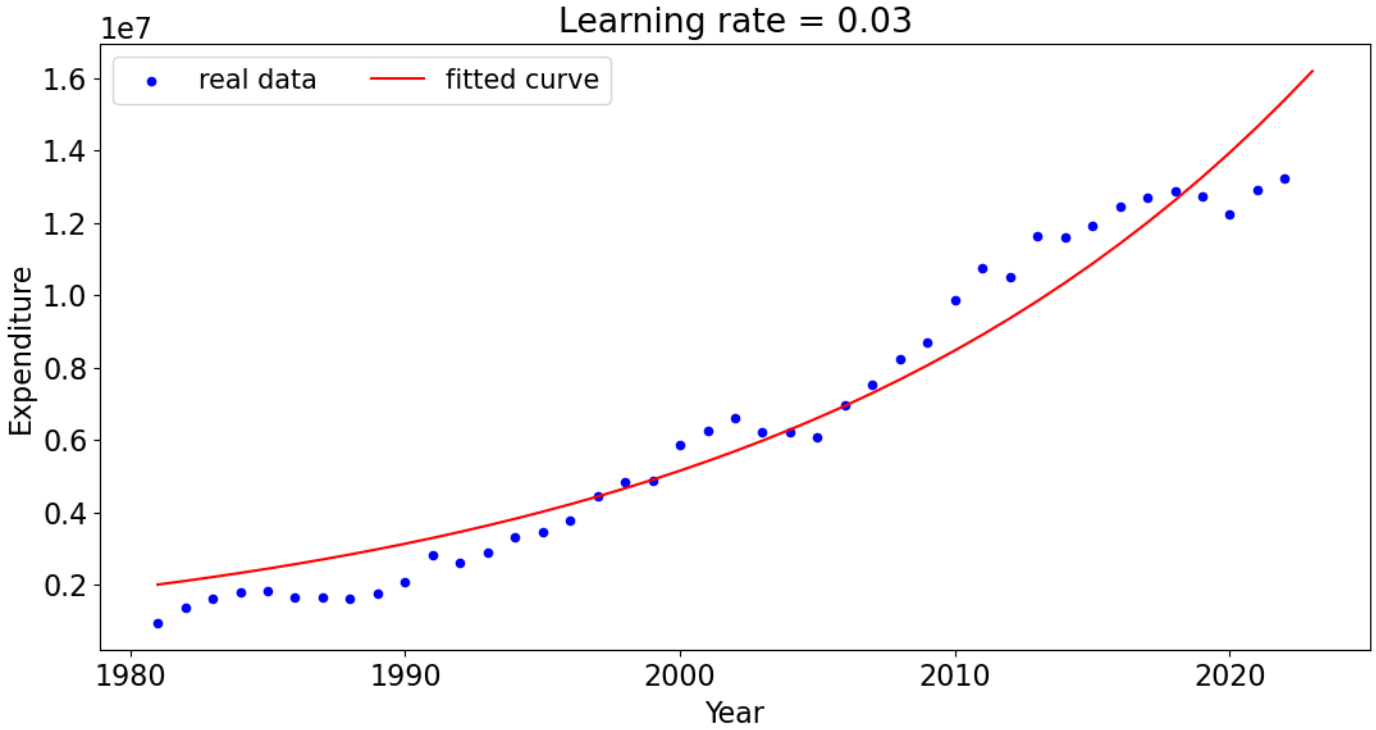
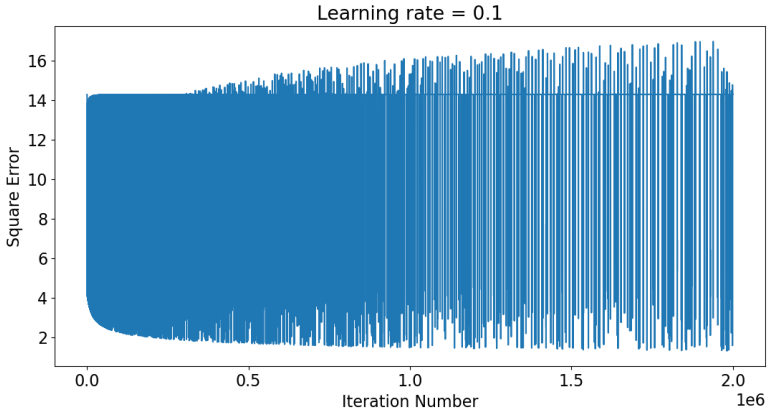
Q2

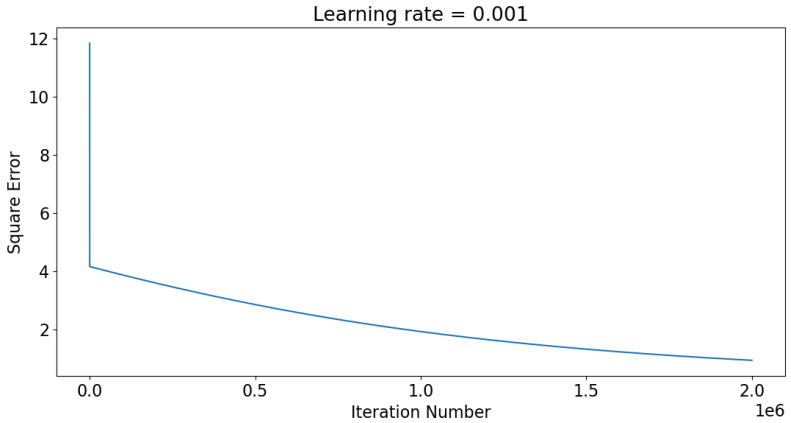
b) Use the fitted parameters to plot the predicted educational expenditure from year 1981 to year 2023



Q2

c) Repeat (a) using a learning rate of 0.1 and learning rate of 0.001. What do you observe relative to (a)?





A learning rate of 0.1 is too big, so the cost function does not decrease monotonically with increasing iterations, but instead fluctuate a lot without convergence. The final cost function value is much worse.

A learning rate of 0.001 is too small. So even though the cost function decreases monotonically with increasing iterations, gradient descent has not converged even after 2000000 iterations. The final cost function value is much worse.

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Q3

Given the linear learning model $f(x, w) = x^T w$, where $x \in \mathbb{R}^d$. Consider the loss function $L(f(x_i, w), y_i) = (f(x_i, w) - y_i)^4$, where i indexes the i-th training sample. The final cost function is $C(w) = \sum_{i=1}^{m} L(f(x_i, w), y_i)$, where m is the total number of training samples. Derive the gradient of the cost function with respect to w.

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Q3

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \nabla_{\mathbf{w}} \sum_{i=1}^{m} (f(\mathbf{x}_i, \mathbf{w}) - y_i)^4$$

$$= \sum_{i=1}^{m} \nabla_{\mathbf{w}} (f(\mathbf{x}_i, \mathbf{w}) - y_i)^4$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \nabla_{\mathbf{w}} f(\mathbf{x}_i, \mathbf{w})$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \nabla_{\mathbf{w}} (\mathbf{x}_i^T \mathbf{w})$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \mathbf{x}_i$$

Chain Rule:

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$$

$f(x, w) = x^T w$

Let $f(x_i, w) - y_i$ be a

Let $f(x_i, w)$ be u

$$\frac{da}{dw} = \frac{da}{du} \times \frac{du}{dw}$$

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$$\frac{d(b^T x)}{dx} = b$$

Q4

Repeat Question 3 using $f(x, w) = \sigma(x^T w)$,

where $\sigma\ (a) = \frac{1}{1+\exp(-\beta a)}$

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Q4

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \nabla_{\mathbf{w}} \sum_{i=1}^{m} (f(\mathbf{x}_i, \mathbf{w}) - y_i)^4$$

$$= \sum_{i=1}^{m} \nabla_{\mathbf{w}} (f(\mathbf{x}_i, \mathbf{w}) - y_i)^4$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \nabla_{\mathbf{w}} f(\mathbf{x}_i, \mathbf{w}) \quad \text{chain rule}$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \nabla_{\mathbf{w}} \sigma(\mathbf{x}_i^T \mathbf{w})$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \frac{\partial \sigma(a)}{\partial a} \nabla_{\mathbf{w}} (\mathbf{x}_i^T \mathbf{w}) \quad \text{chain rule}$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \frac{\partial \sigma(a)}{\partial a} \mathbf{x}_i$$

$$f(x, w) = \sigma(x^T w)$$

$$\sigma\,(a) = \frac{1}{1 + \exp(-\beta a)}$$

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Q4

So we just have to evaluate $\frac{\partial \sigma(a)}{\partial a}$ and plug it into the above equation. Note that $\frac{\partial \sigma(a)}{\partial a}$ is evaluated at $a = \mathbf{x}_i^T \mathbf{w}$, so

$$\begin{aligned}
\frac{\partial \sigma(a)}{\partial a} &= \frac{\partial}{\partial a}\left(\frac{1}{1+\exp(-\beta a)}\right) \\
&= -\frac{1}{(1+e^{-\beta a})^2}\frac{\partial(1+e^{-\beta a})}{\partial a} \\
&= \frac{\beta}{(1+e^{-\beta a})^2}e^{-\beta a} \\
&= \frac{\beta}{(1+e^{-\beta a})^2}(1+e^{-\beta a}-1) \\
&= \beta\left(\frac{1}{1+e^{-\beta a}} - \frac{1}{(1+e^{-\beta a})^2}\right) \\
&= \beta\left(\sigma(a) - \sigma^2(a)\right) \\
&= \beta\sigma(a)(1-\sigma(a)) \\
&= \beta\sigma(\mathbf{x}_i^T\mathbf{w})(1-\sigma(\mathbf{x}_i^T\mathbf{w}))
\end{aligned}$$

From previous slide

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \frac{\partial \sigma(a)}{\partial a}\mathbf{x}_i$$

Quotient Rule Formula

$$\frac{d}{dx}\left[\frac{f(x)}{g(x)}\right] = \frac{g(x)f'(x) - f(x)g'(x)}{(g(x))^2}$$

Therefore,

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \beta\sigma(\mathbf{x}_i^T\mathbf{w})(1-\sigma(\mathbf{x}_i^T\mathbf{w}))\mathbf{x}_i$$

Q5

Repeat Question 3 using $f(x, w) = \sigma(x^T w)$, where $\sigma\ (a) = \max(0, a)$

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Q5

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \nabla_{\mathbf{w}} \sum_{i=1}^{m} (f(\mathbf{x}_i, \mathbf{w}) - y_i)^4$$

First part is the same as Q4

$$= \sum_{i=1}^{m} \nabla_{\mathbf{w}} (f(\mathbf{x}_i, \mathbf{w}) - y_i)^4$$

$\sigma(a) = \max(0, a)$

$a = \mathrm{x}_i^{\mathrm{T}} \mathrm{w}$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \nabla_{\mathbf{w}} f(\mathbf{x}_i, \mathbf{w}) \quad \text{chain rule}$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \nabla_{\mathbf{w}} \sigma(\mathbf{x}_i^T \mathbf{w})$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \frac{\partial \sigma(a)}{\partial a} \nabla_{\mathbf{w}} (\mathbf{x}_i^T \mathbf{w}) \quad \text{chain rule}$$

$$= \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \frac{\partial \sigma(a)}{\partial a} \mathbf{x}_i$$

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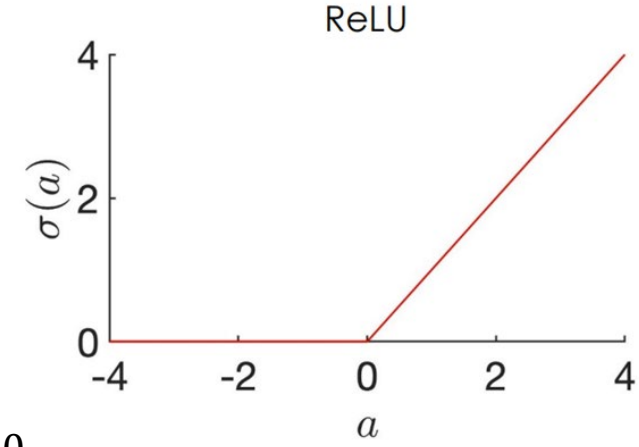
Q5

$$\sigma(a) = \max(0, a)$$
$$a = \mathrm{x}_i^{\mathrm{T}}\mathrm{w}$$



So we just have to evaluate $\frac{\partial \sigma(a)}{\partial a}$

$$\frac{\partial \sigma(a)}{\partial a} = \frac{\partial \max(0, a)}{\partial a} = \begin{cases} \frac{\partial a}{\partial a} = 1, & \text{if } a > 0 \\ \frac{\partial 0}{\partial a} = 0, & \text{if } a < 0 \end{cases}$$

Since $a = \mathrm{x}_i^T\mathrm{w}$, we can obtain

$$\frac{\partial \sigma(a)}{\partial a} = \begin{cases} 1, & \text{if } \mathrm{x}_i^{\mathrm{T}}\mathrm{w} > 0 \\ 0, & \text{if } \mathrm{x}_i^{\mathrm{T}}\mathrm{w} < 0 \end{cases}$$

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Q5

$$\frac{\partial \sigma(a)}{\partial a} = \begin{cases} 1, & \text{if } \mathrm{x}_i^{\mathrm{T}}\mathrm{w} > 0 \\ 0, & \text{if } \mathrm{x}_i^{\mathrm{T}}\mathrm{w} < 0 \end{cases}$$

Let us define $\delta(\mathrm{x}_i^T\mathrm{w} > 0) = \begin{cases} 1 & \text{if } \mathrm{x}_i^T\mathrm{w} > 0 \\ 0 & \text{if } \mathrm{x}_i^T\mathrm{w} < 0 \end{cases}$, so we get

$$\frac{\partial \sigma(a)}{\partial a} = \delta(\mathbf{x}_i^T\mathbf{w} > 0)$$

From previous slide

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \frac{\partial \sigma(a)}{\partial a} \mathbf{x}_i$$

Therefore, $$\nabla_{\mathbf{w}} C(\mathbf{w}) = \sum_{i=1}^{m} 4(f(\mathbf{x}_i, \mathbf{w}) - y_i)^3 \mathbf{x}_i \delta(\mathbf{x}_i^T\mathbf{w} > 0),$$

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THANK YOU

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