Machine Learning

Lecture 3: Training Models

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Topics

- Direct approach: linear regression with ordinary least square
- Iterative approach
  - Gradient descent
  - Batch gradient descent
  - Stochastic gradient descent
  - Mini-batch gradient descent
- Logistic regression

Model training

Two different ways

- Using a direct “closed-form” equation.
- Using an iterative optimization approach.

Direct approach

Linear regression with Ordinary Least Square (OLS)

- Linear regression model can be expressed by the following formula

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$$

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n + \varepsilon$$

where

$\hat{y}$ is the predicted value

n is the number of features

x_i is the ith feature value

Simple linear regression

$$Y_i = \alpha + \beta X_i + \varepsilon_i$$
$$e_i \sim N(0, \sigma^2) \quad i.i.d.$$
$$\varepsilon_i \text{ is independent of } X_i$$

- The intercept is α
- The slope is β
- We use the normal distribution to describe the "error"

Method of least squares

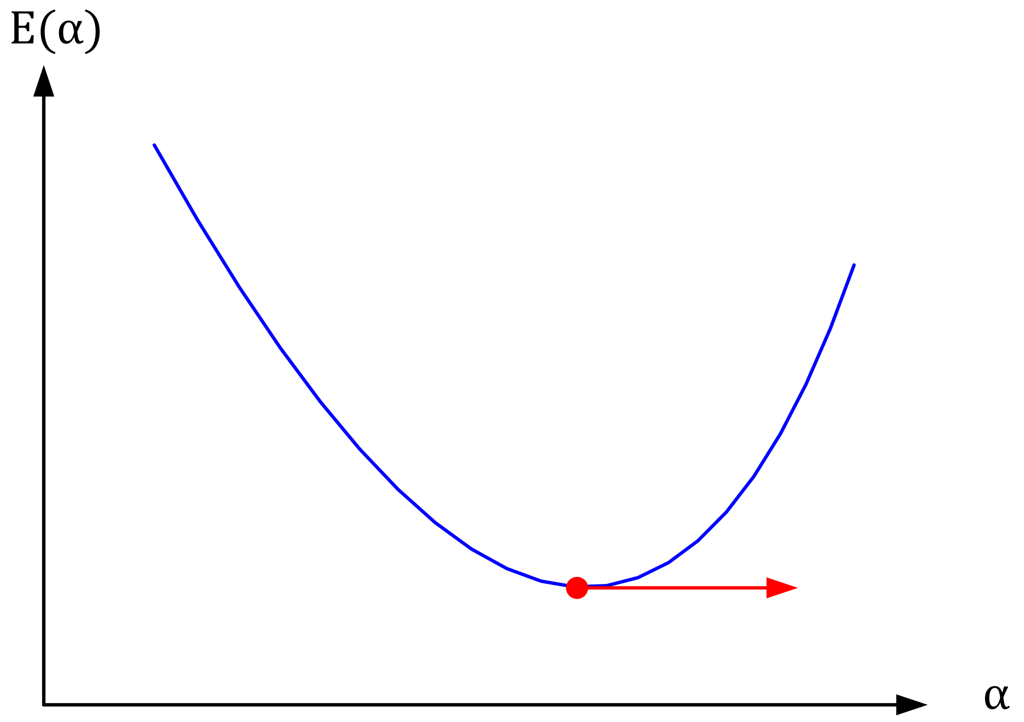
- Choose the β's so that the sum of the squares of the errors, ε_i, are minimized
- The least squares function is

$$S = \sum_{i=1}^{n} \varepsilon_i^2$$

$$= \sum_{i=1}^{n} \left(y_i - \alpha - \beta x_i \right)^2$$

OLS solution

Minimum of a function is the point where the slope is zero



Derivative of the error functions

The function S is to be minimized with respect to β_0, β_1

and

$$\frac{\partial S}{\partial \alpha} = -2\sum_{i=1}^{n}\left(y_i - \alpha - \beta x_i\right) = 0$$

$$\frac{\partial S}{\partial \beta} = -2\sum_{i=1}^{n}\left(y_i - \alpha - \beta x_i\right)x_i = 0$$

Least square normal equation

$$n\alpha + \beta\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$

$$\alpha\sum_{i=1}^{n} x_i + \beta\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i$$

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Find alpha (intercept)

$$\alpha = \frac{\begin{vmatrix} \sum_{i=1}^{n} y_i & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i y_i & \sum_{i=1}^{n} x_i^2 \end{vmatrix}}{\begin{vmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{vmatrix}} = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i y_i \sum_{i=1}^{n} x_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i \right)^2}$$

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Find beta (slope)

$$\beta = \frac{\begin{vmatrix} n & \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i y_i \end{vmatrix}}{\begin{vmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{vmatrix}} = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

Example: Multiple regression

x_1	x_2	y
1	2	12
2	1	9
3	2	19
1	1	8

$$y = c_1x_1 + c_2x_2 + c_3$$

$$\begin{aligned} c_1 + 2c_2 + c_3 &= 12 \\ 2c_1 + c_2 + c_3 &= 9 \\ 3c_1 + 2c_2 + c_3 &= 19 \\ c_1 + c_2 + c_3 &= 8 \end{aligned}$$

$$\begin{bmatrix} 1 & 2 & 1 \\ 2 & 1 & 1 \\ 3 & 2 & 1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 12 \\ 9 \\ 19 \\ 8 \end{bmatrix}$$

Pseudoinverse

Y $N \times 1$ vector

A $N \times M$ matrix, where M is the number of parameters

B $M \times 1$ vector

$$\mathbf{Y} = \mathbf{AB}$$

$$\mathbf{AB} = \mathbf{Y}$$

$$\mathbf{A}^{\mathrm{T}}\mathbf{AB} = \mathbf{A}^{\mathrm{T}}\mathbf{Y}$$

$$\underbrace{\left(\mathbf{A}^{\mathrm{T}}\mathbf{A}\right)^{-1}}\mathbf{A}^{\mathrm{T}}\mathbf{AB} = \left(\mathbf{A}^{\mathrm{T}}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{Y}$$

$$\mathbf{B} = \left(\mathbf{A}^{\mathrm{T}}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{Y}$$

Python: pseudoinverse

```
A = np.array([[1,2,1],
              [2,1,1],
              [3,2,1],
              [1,1,1]])
print(A)
```

```
[[1 2 1]
 [2 1 1]
 [3 2 1]
 [1 1 1]]
```

```
B = np.array([12,9,19,8])
B.shape = (-1,1)
print(B)
```

```
[[12]
 [ 9]
 [19]
 [ 8]]
```

```
np.matmul(np.linalg.pinv(A),B)
```

```
array([[ 3. ],
       [ 5.5],
       [-1.5]])
```

Iterative approach
Gradient descent

- A very generic optimization algorithm capable of finding optimal solutions to a wide range of problems.

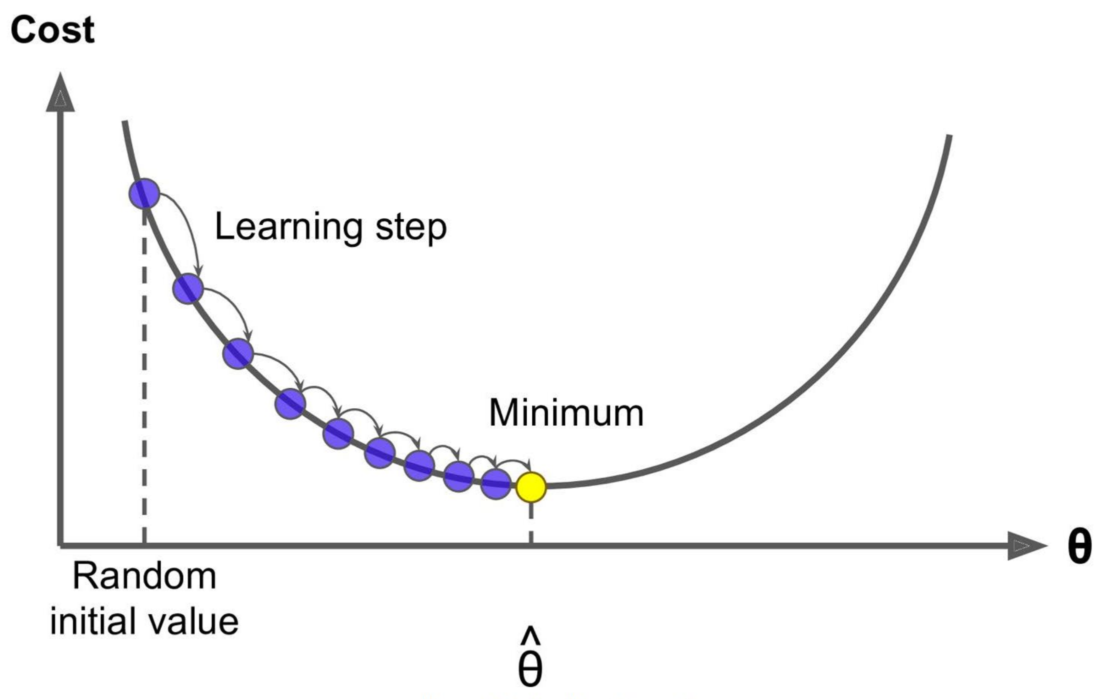


Figure 4-3. Gradient Descent

Suppose you are lost in the mountains in a dense fog; you can only feel the slope of the ground below your feet.

A good strategy to get to the bottom of the valley quickly is to go downhill in the direction of the steepest slope.

Nonlinear Least Square

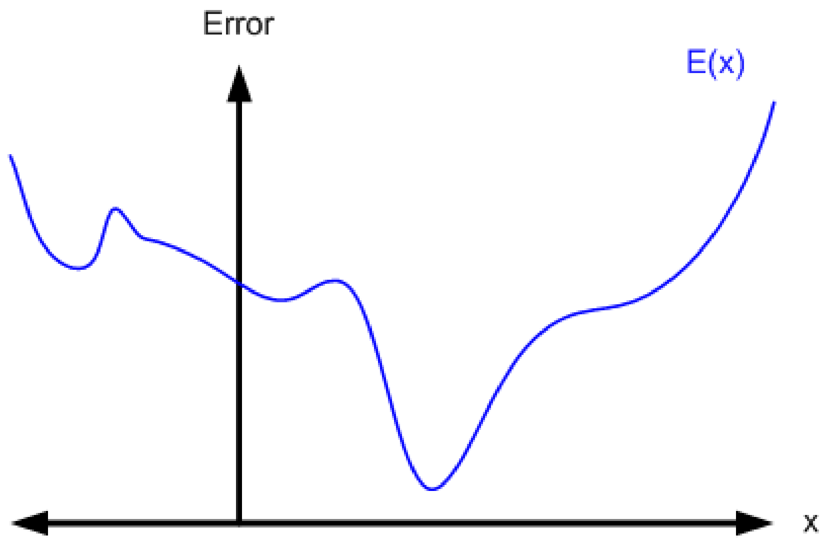
- Suppose that we have a sample of n observations on the response and the regressor, say, y_i, x_{i1}, x_{i2}, …, x_{ik} for i=1,2,…,n

- The least square method involves minimizing the least square function

$$S(\boldsymbol{\beta}) = \sum_{i=1}^{n} \left[y_i - f\left(\mathbf{x_i}, \boldsymbol{\beta}\right) \right]^2$$

Nonlinear objective function

Non-linear
objective function

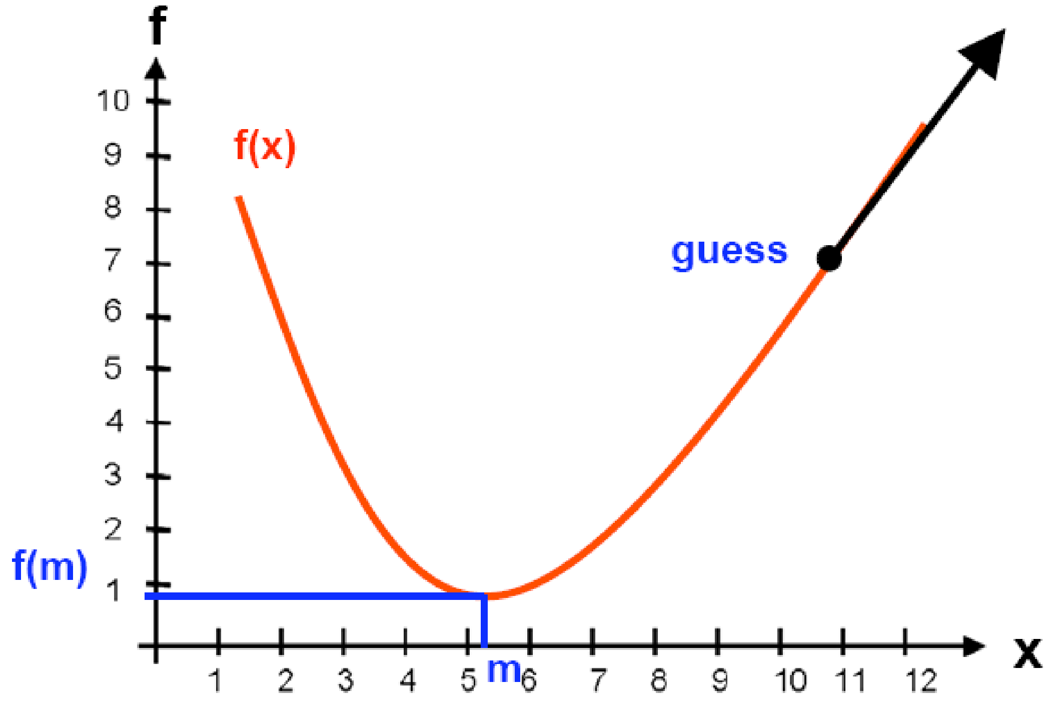


Unsolvable for roots
of derivative of error

$$\frac{dE}{dx} = e^{-x}$$

Gradient Descent Basic 1
Objective function

Minimum of a function is found by following the slope of the function



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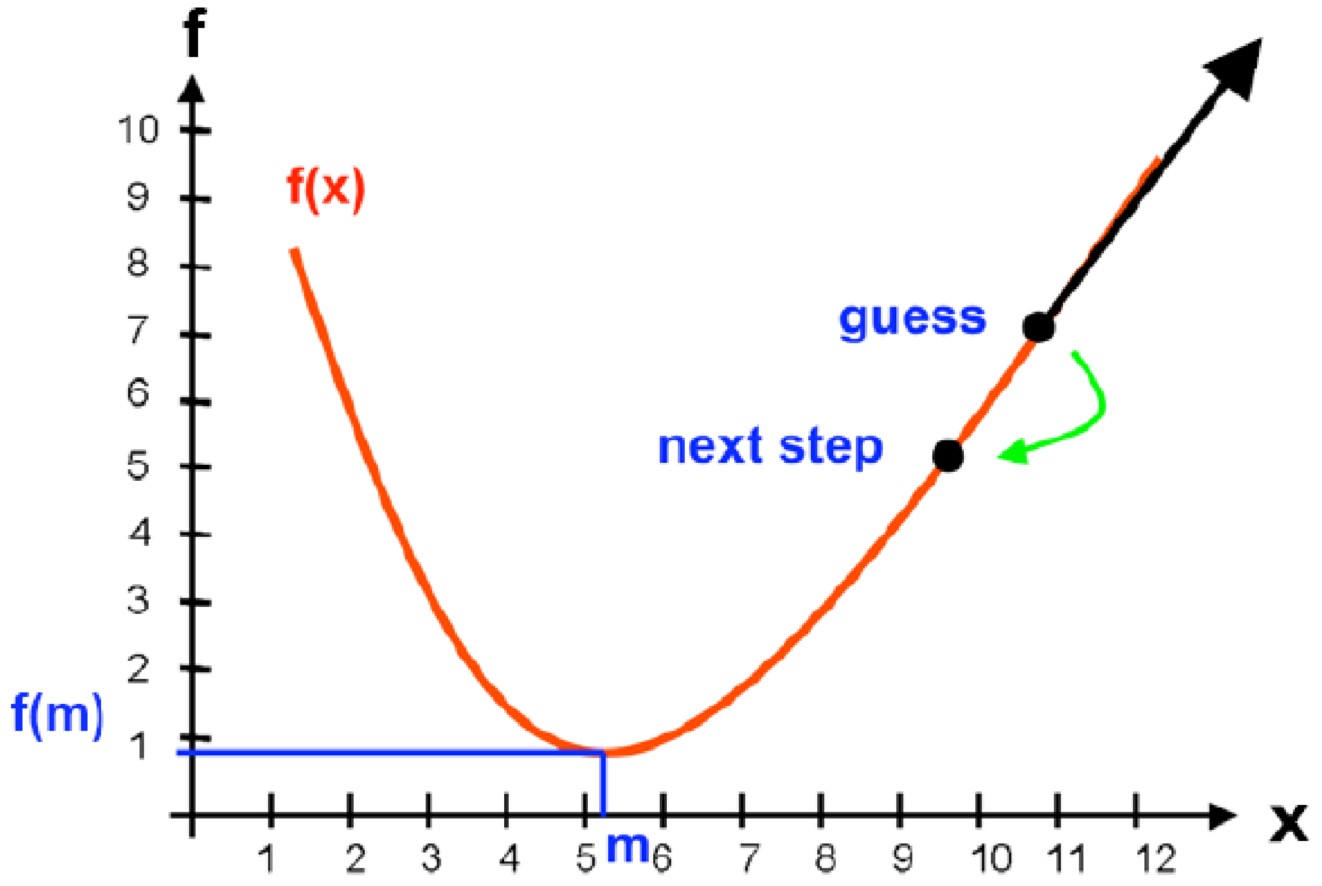
Gradient Descent Basic 2
Moving opposite to gradient



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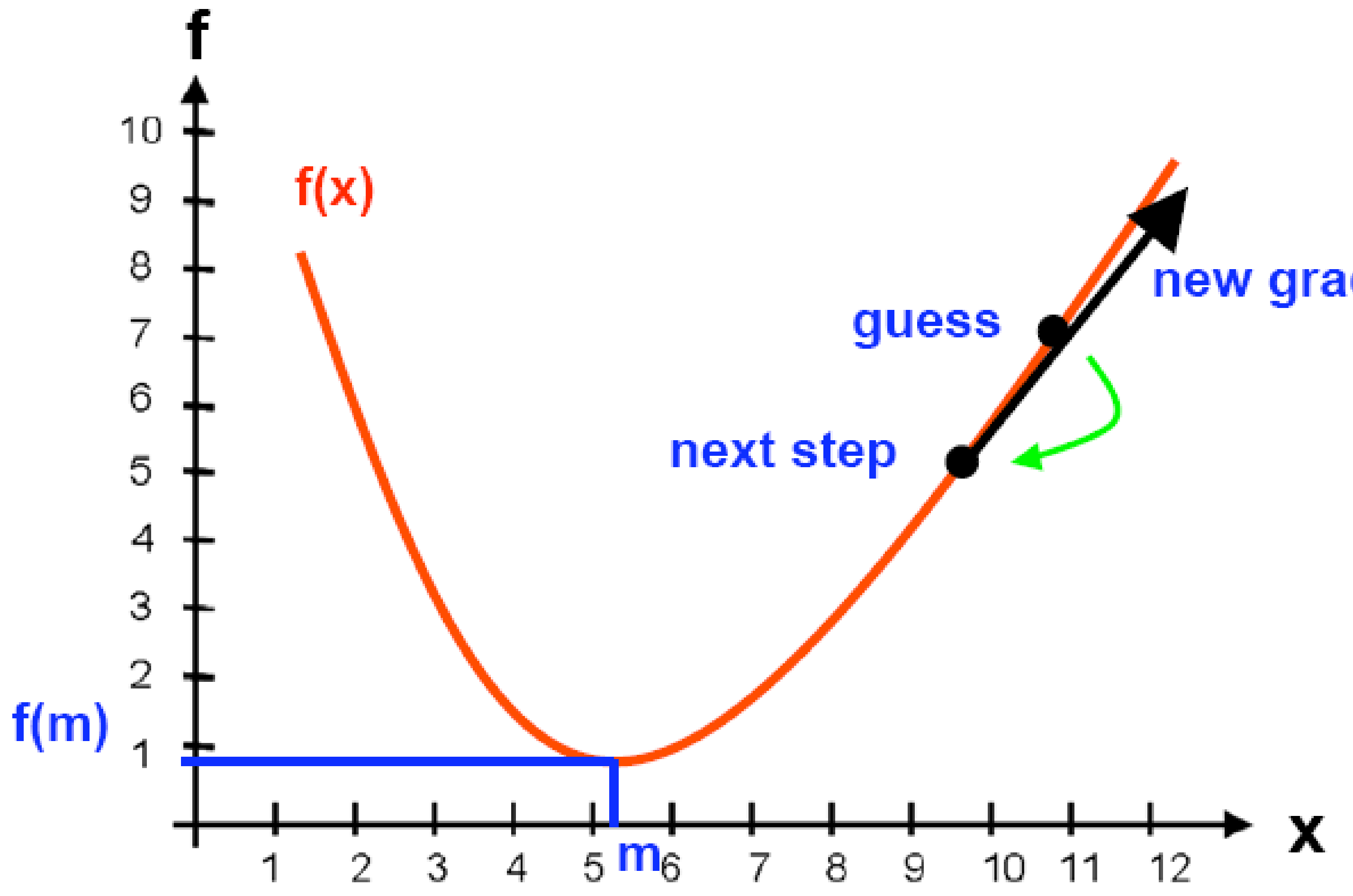
Gradient Descent Basic 3
Iterative gradient evaluation



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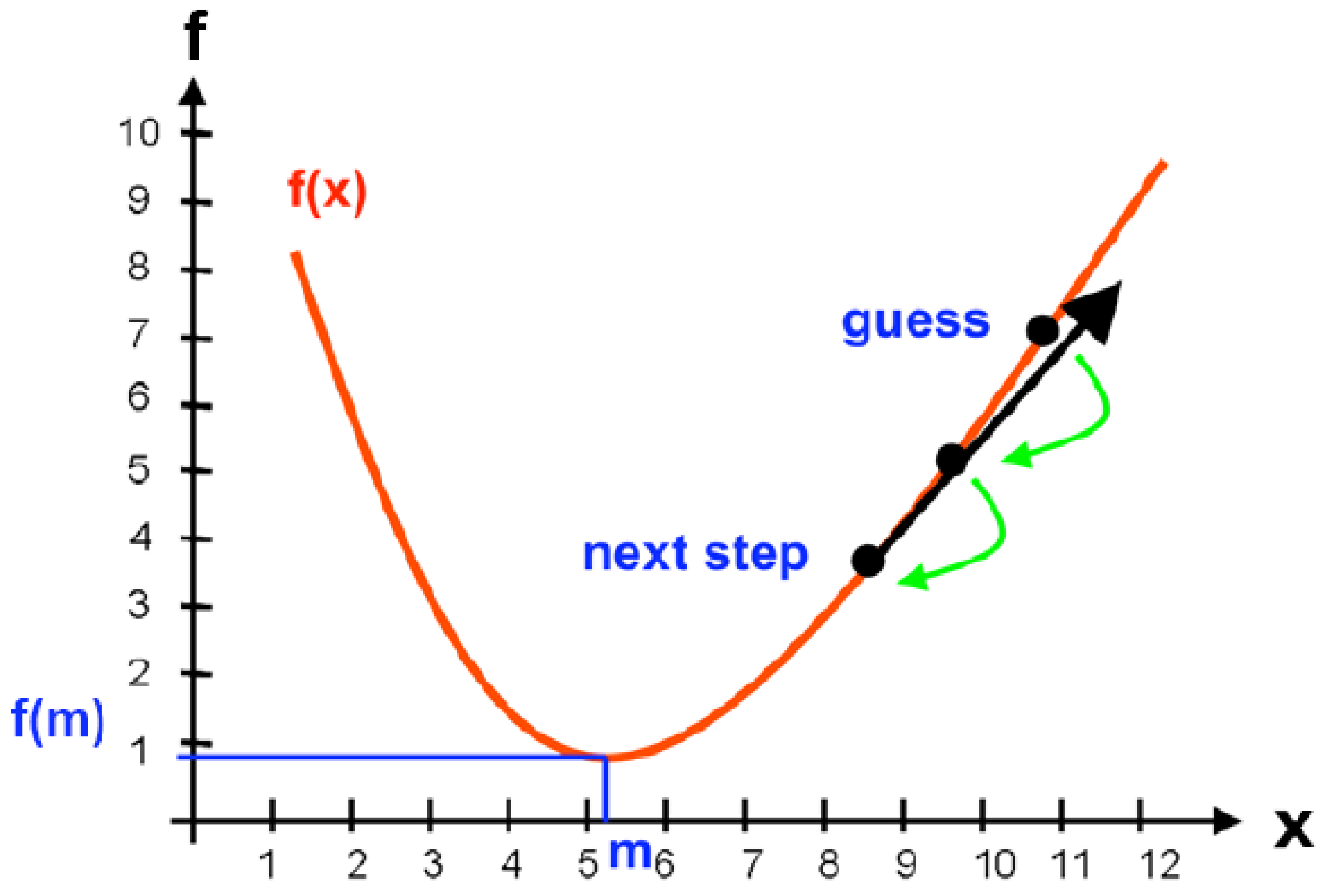
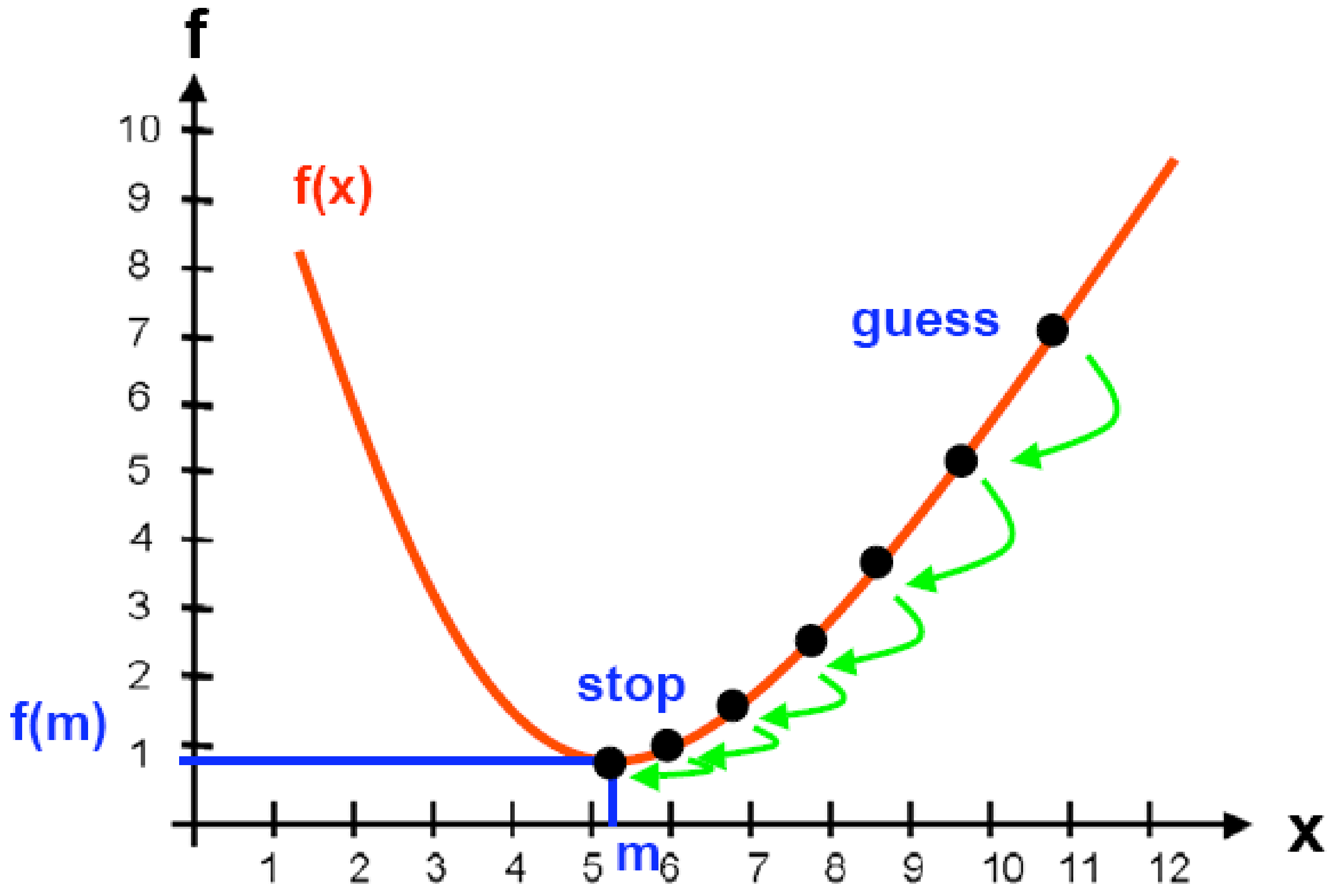
Gradient Descent Basic 4
Moving opposite to gradient



Gradient Descent Basic 5

Iteratively descent opposite to the gradient



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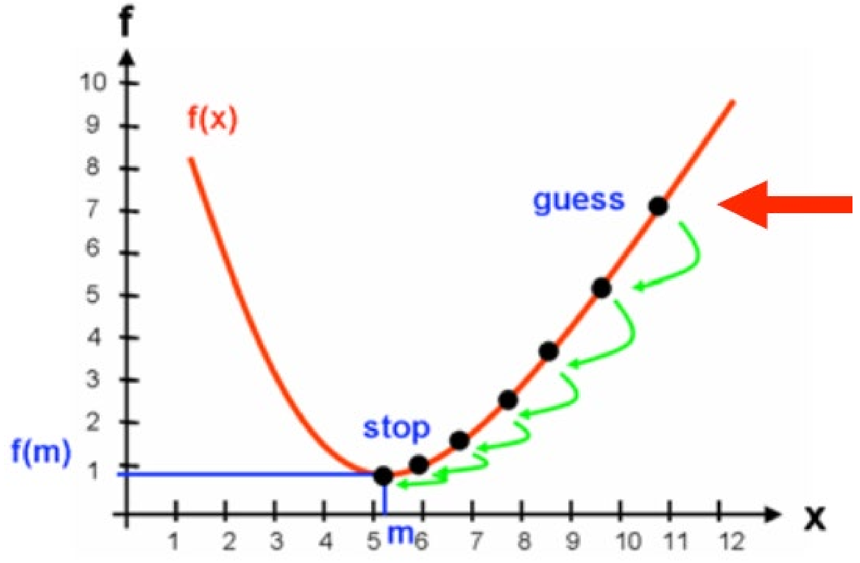
Gradient Descent – algorithm

- Start with a point (randomly guessing)
- Repeat
  - Determine a descent direction
  - Choose a step
  - Update
- Until stopping criterion is satisfied



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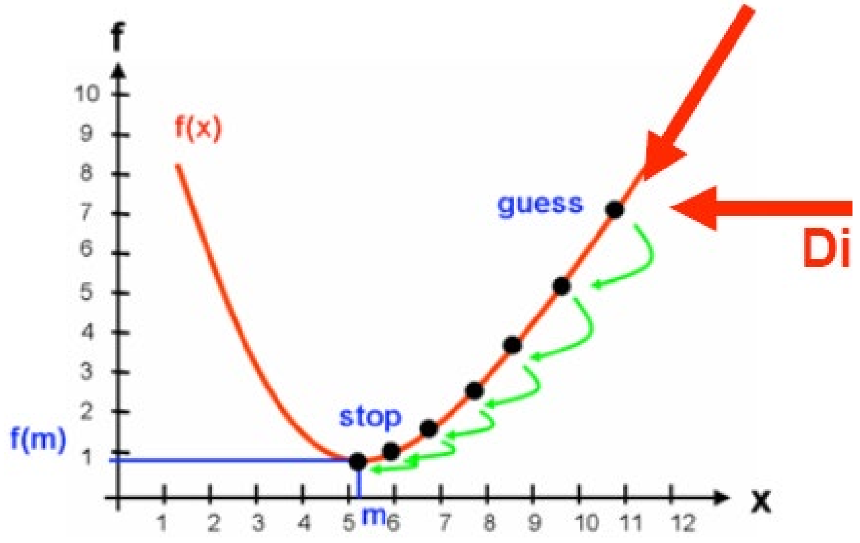

Gradient Descent – algorithm

- Start with a point (randomly guessing)
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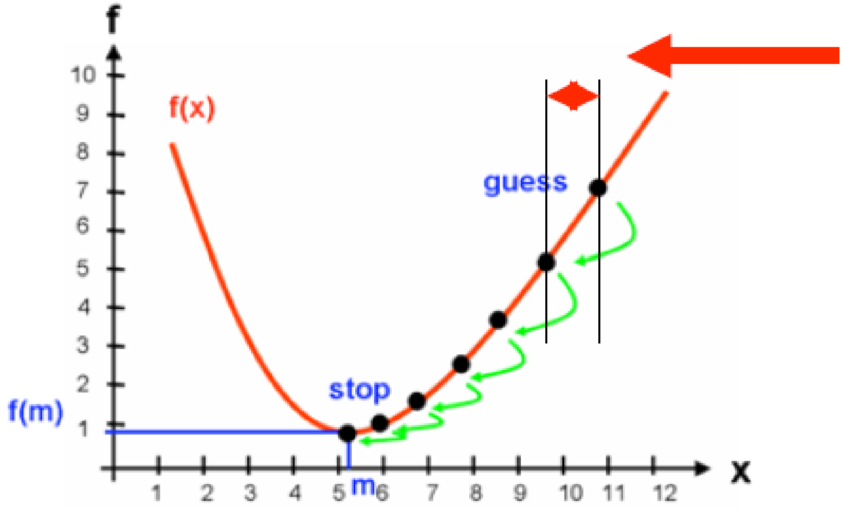

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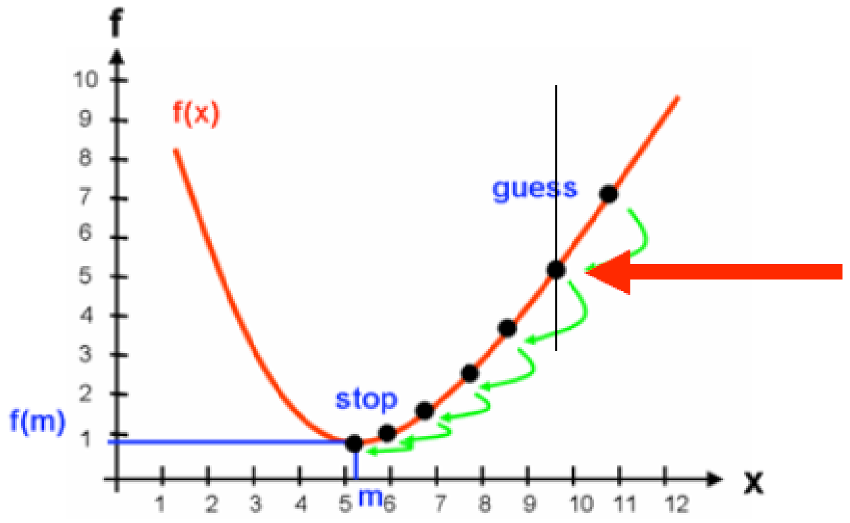

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Gradient Descent – algorithm

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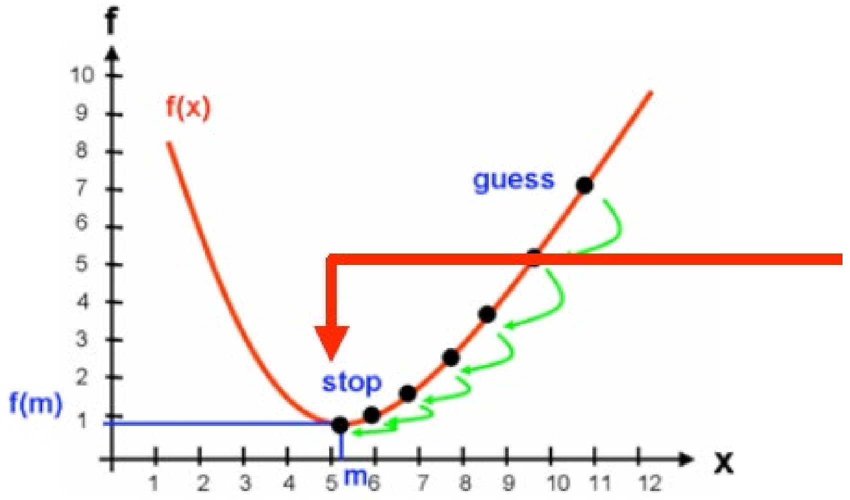

Gradient Descent – algorithm

- Start with a point (randomly guessing) → Randomly guessing β
- Repeat
  - Determine a descent direction → $\text{direction} = -\frac{dS(\beta)}{d\beta}$
  - Choose a step → $\text{step} > 0$
  - Update → $\beta^{t+1} = \beta^{t} - step\,\frac{dS(\beta)}{d\beta}$
- Until stopping criterion is satisfied → $\frac{dS(\beta)}{d\beta} \approx 0$

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Batch Gradient Descent

- To implement Gradient Descent, you need to compute the gradient of the cost function with regards to each model parameter θ_j.
- Batch gradient descent uses data of the whole batch to compute gradient

$$\frac{\partial}{\partial \theta_j} \mathrm{MSE}(\boldsymbol{\theta}) = \frac{2}{m} \sum_{i=1}^{m} \left(\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}\right) x_j^{(i)}$$

$$\boldsymbol{\theta}^{(\text{next step})} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \, \mathrm{MSE}(\boldsymbol{\theta})$$

Stochastic gradient descent

- Batch Gradient Descent uses the whole training set to compute the gradients at every step, which makes it very slow when the training set is large.
- Stochastic gradient descent samples random instances for training at each training step

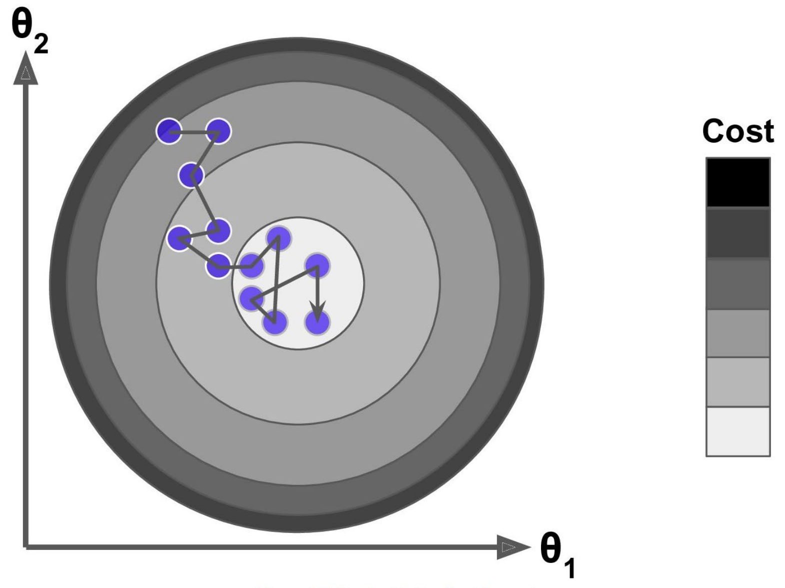
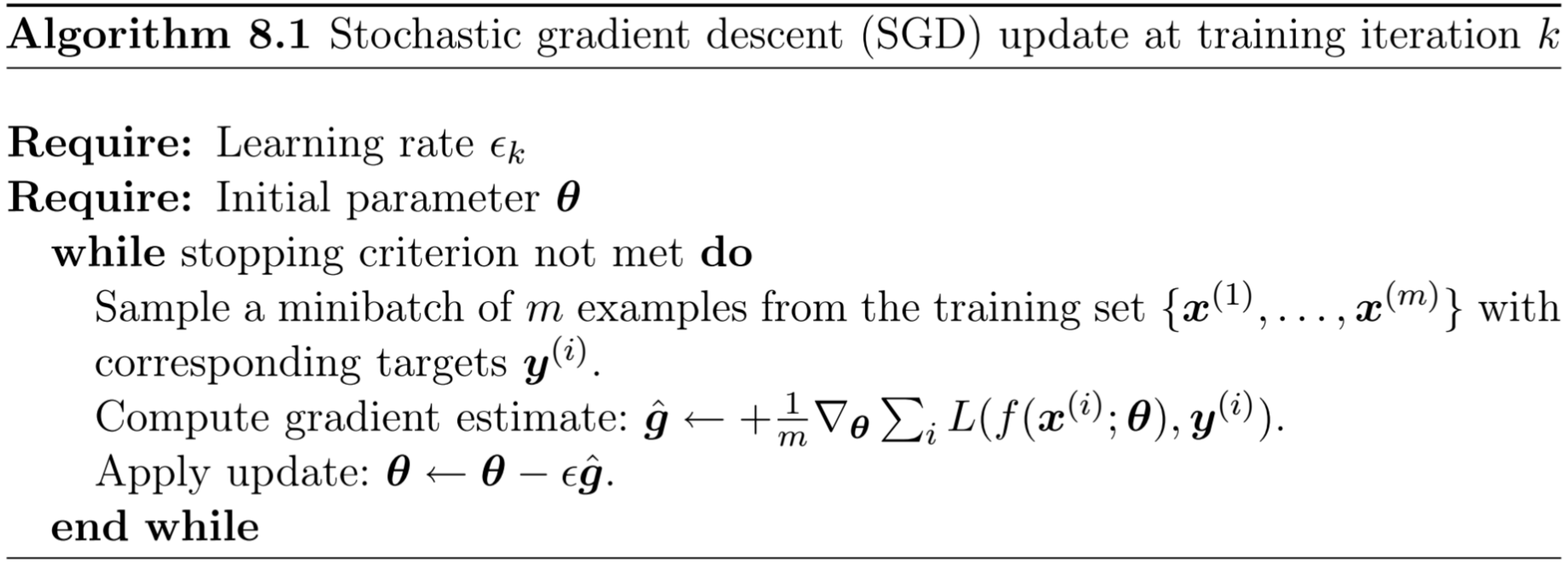


Figure 4-9. Stochastic Gradient Descent

Mini-Batch Gradient Descent

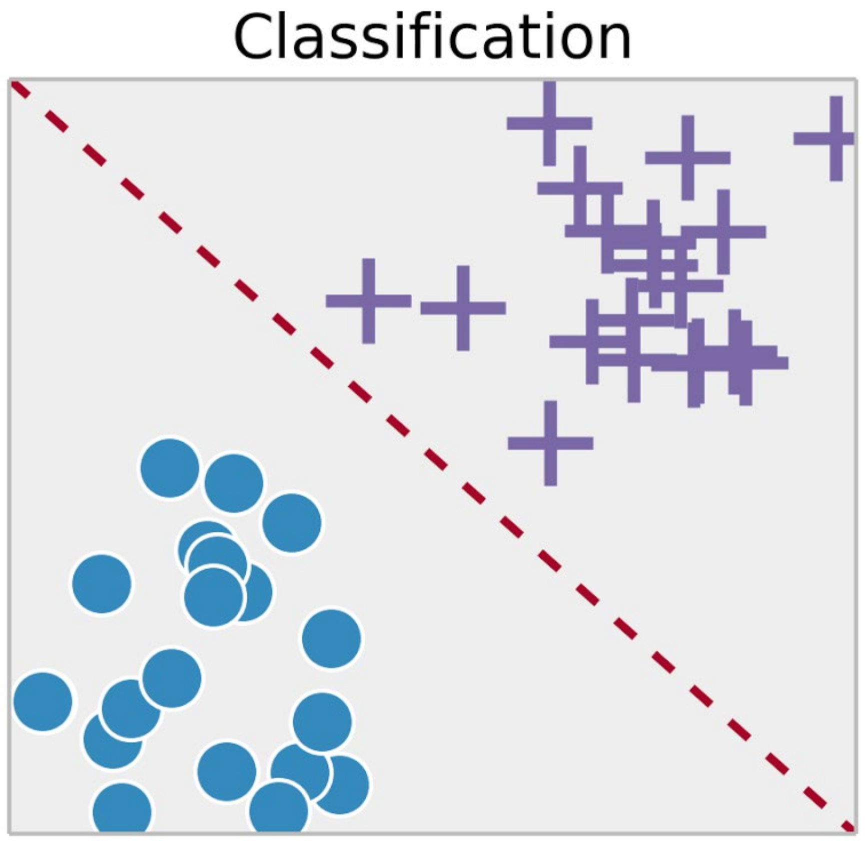
- Both stochastic and use small batch
- Apply for small batch instead of an instance.
- Faster by GPU computing



Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration k

```
Require: Learning rate $\epsilon_k$
Require: Initial parameter $\boldsymbol{\theta}$
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ with
    corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow +\frac{1}{m}\nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$.
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \hat{\boldsymbol{g}}$.
  end while
```

Example: Logistic Regression



Logistic regression

Logistic regression has the following mathematical formulae,

$$(\frac{H_{\boldsymbol{\theta}}(x_i)}{1 - H_{\boldsymbol{\theta}}(x_i)}) = f(x_i) = \theta_0 + \sum_{i=1}^{n} \theta_i x_i$$

and

$$H_{\boldsymbol{\theta}}(x_i) = \frac{1}{1 + e^{-f(x)}}.$$

Loss function

This function has a nice property that,

$$\frac{\partial}{\partial \boldsymbol{\theta}} H_{\boldsymbol{\theta}}(x_i) = H_{\boldsymbol{\theta}}(x_i)(1 - H_{\boldsymbol{\theta}}(x_i))x_i.$$

For logistic regression, we can formulate the loss function as follows,

$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}[-y_i \log H_{\boldsymbol{\theta}}(x_i) - (1 - y_i) \log (1 - H_{\boldsymbol{\theta}}(x_i))].$$

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Gradient

$$
\begin{aligned}
\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} &= \frac{\partial}{\partial \boldsymbol{\theta}}\left(\frac{1}{n}\sum_{i=1}^{n}(-y_i \log H_{\boldsymbol{\theta}}(x_i) - (1-y_i)\log(1-H_{\boldsymbol{\theta}}(x_i)))\right) \\
&= \frac{1}{n}\sum_{i=1}^{n}(-y_i \frac{\partial}{\partial \boldsymbol{\theta}} \log H_{\boldsymbol{\theta}}(x_i) - (1-y_i)\frac{\partial}{\partial \boldsymbol{\theta}}\log(1-H_{\boldsymbol{\theta}}(x_i))) \\
&= \frac{1}{n}\sum_{i=1}^{n}(-\frac{y_i}{H_{\boldsymbol{\theta}}(x_i)}\frac{\partial}{\partial \boldsymbol{\theta}}H_{\boldsymbol{\theta}}(x_i) - \frac{1-y_i}{1-H_{\boldsymbol{\theta}}(x_i)}\frac{\partial}{\partial \boldsymbol{\theta}}(1-H_{\boldsymbol{\theta}}(x_i))) \\
&= \frac{1}{n}\sum_{i=1}^{n}(-\frac{y_i}{H_{\boldsymbol{\theta}}(x_i)}H_{\boldsymbol{\theta}}(x_i)(1-H_{\boldsymbol{\theta}}(x_i))x_i \\
&\quad - \frac{1-y_i}{1-H_{\boldsymbol{\theta}}(x_i)}H_{\boldsymbol{\theta}}(x_i)(1-H_{\boldsymbol{\theta}}(x_i))(-x_i)) \\
&= \frac{1}{n}\sum_{i=1}^{n}(-y_i(1-H_{\boldsymbol{\theta}}(x_i))x_i - (1-y_i)H_{\boldsymbol{\theta}}(x_i)(-x_i)) \\
&= \frac{1}{n}\sum_{i=1}^{n}(-y_i(1-H_{\boldsymbol{\theta}}(x_i)) + (1-y_i)H_{\boldsymbol{\theta}}(x_i))x_i \\
&= \frac{1}{n}\sum_{i=1}^{n}(-y_i + y_iH_{\boldsymbol{\theta}}(x_i) + H_{\boldsymbol{\theta}}(x_i) - y_iH_{\boldsymbol{\theta}}(x_i))x_i \\
&= \frac{1}{n}\sum_{i=1}^{n}(H_{\boldsymbol{\theta}}(x_i) - y_i)x_i
\end{aligned}
$$

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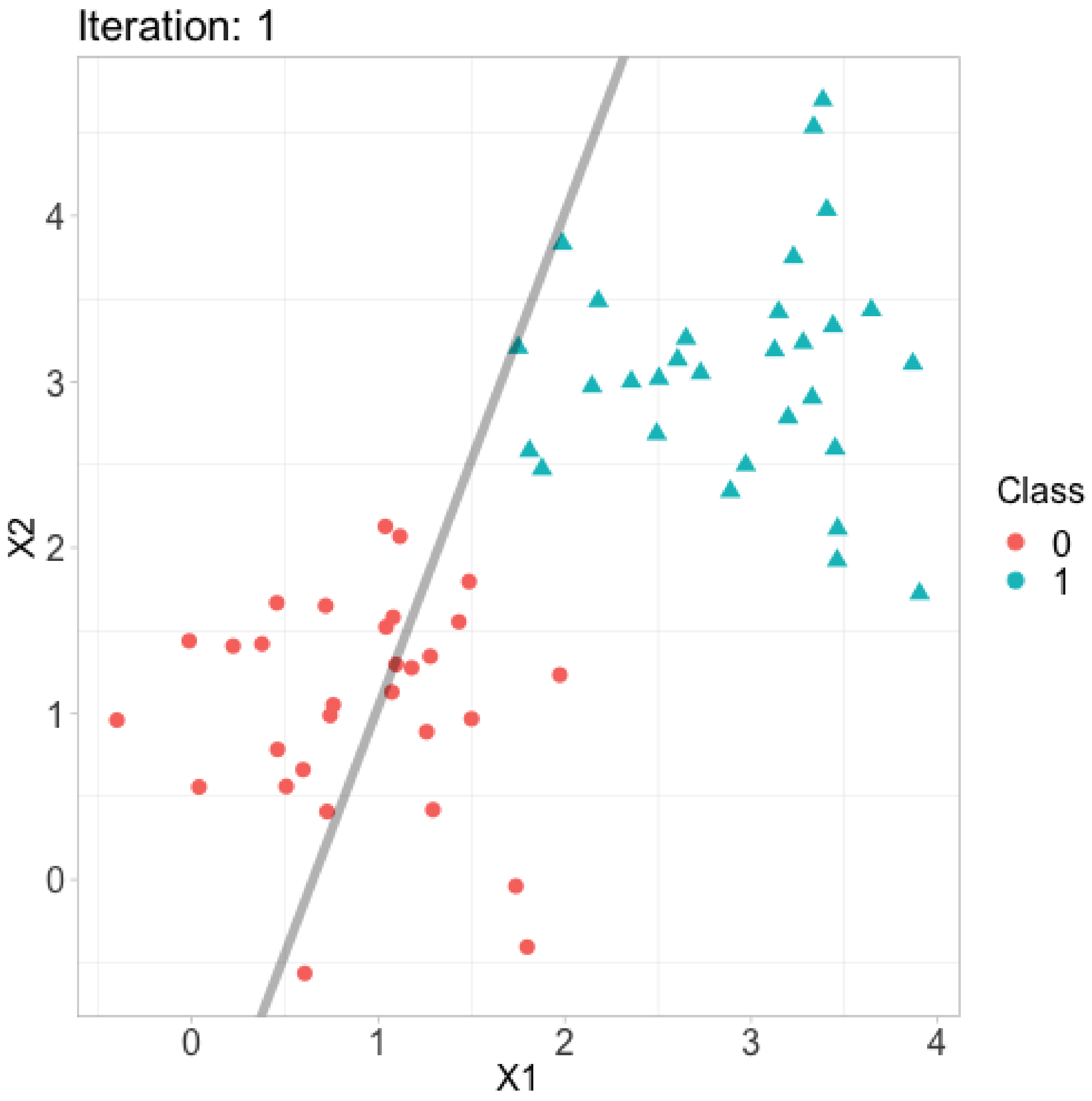
Gradient descent

We can then iteratively update the parameters using the gradient descent approach,

$$\begin{aligned}\boldsymbol{\theta}^{(k+1)} &= \boldsymbol{\theta}^{(k)} - \alpha\frac{\partial J\boldsymbol{\theta}}{\partial\boldsymbol{\theta}} \\ &= \boldsymbol{\theta}^{(k)} - \alpha(\sum_{i=1}^{n}(H_{\boldsymbol{\theta}^{(k)}}(x_i) - y_i)x_i),\end{aligned}$$

where α is the learning rate. The initial parameters $\boldsymbol{\theta}^{(0)}$ can be randomized or set to any values as the loss function is convex.

Results



End of Lecture 3

Question?