# **Binary Classification**

Shusen Wang

### **Vector and Matrix Derivatives**

## Derivative of Scalar w.r.t. Scalar

#### **Examples:**

• 
$$y = x^2$$
;  $\frac{dy}{dx} = 2x$ .

• 
$$y = e^x$$
;  $\frac{dy}{dx} = e^x$ .

## Derivative of Vector w.r.t. Scalar

• The derivative of a vector  $\mathbf{y} \in \mathbb{R}^n$  w.r.t. a scalar  $x \in \mathbb{R}$ :

$$\frac{\partial \mathbf{y}}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x} \\ \frac{\partial y_2}{\partial x} \\ \vdots \\ \frac{\partial y_n}{\partial x} \end{bmatrix}$$

• Example:

$$\mathbf{y} = \begin{bmatrix} 3x^2 \\ x+1 \\ \log x \\ e^x \end{bmatrix}, \qquad \frac{\partial \mathbf{y}}{\partial x} = \begin{bmatrix} 6x \\ 1 \\ 1/x \\ e^x \end{bmatrix}$$

## Derivative of Scalar w.r.t. Vector

• The derivative of a scalar  $y \in \mathbb{R}$  w.r.t. a vector  $\mathbf{x} \in \mathbb{R}^m$ :

$$\left[ egin{array}{c} rac{\partial y}{\partial x_1} \ rac{\partial y}{\partial x_2} \ rac{\partial y}{\partial x_m} \end{array} 
ight]$$

• Example 1:

$$y = \|\mathbf{x}\|_2^2 = \sum_{i=1}^m x_i^2, \qquad \frac{\partial y}{\partial \mathbf{x}} = 2\mathbf{x}.$$

## Derivative of Scalar w.r.t. Vector

• The derivative of a scalar  $y \in \mathbb{R}$  w.r.t. a vector  $\mathbf{x} \in \mathbb{R}^m$ :

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_m} \end{bmatrix}$$

• Example 2:

$$y = \mathbf{x}^T \mathbf{z} = \sum_{i=1}^m x_i z_i, \qquad \frac{\partial y}{\partial \mathbf{x}} = \mathbf{z}.$$

## Derivative of Scalar w.r.t. Vector

• The derivative of a scalar  $y \in \mathbb{R}$  w.r.t. a vector  $\mathbf{x} \in \mathbb{R}^m$ :

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_m} \end{bmatrix}$$

• Example 3:

$$y = \sum_{i=1}^{m} \log(1 + e^{-x_i}), \qquad \frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial \log(1 + e^{-x_1})}{\partial x_1} \\ \vdots \\ \frac{\partial \log(1 + e^{-x_m})}{\partial x_m} \end{bmatrix} = \begin{bmatrix} -\frac{1}{1 + e^{x_1}} \\ \vdots \\ -\frac{1}{1 + e^{x_m}} \end{bmatrix}$$

### Derivative of Vector w.r.t. Vector

• The derivative of a vector  $\mathbf{y} \in \mathbb{R}^n$  w.r.t. a vector  $\mathbf{x} \in \mathbb{R}^m$ :

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_n}{\partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_m} & \frac{\partial y_2}{\partial x_m} & \cdots & \frac{\partial y_n}{\partial x_m} \end{bmatrix}$$

$$m \times n \text{ matrix}$$

• Example 1:

$$\frac{\partial \mathbf{x}}{\partial \mathbf{x}} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

$$m \times m$$

The (i, j)-th entry is  $\frac{\partial y_j}{\partial x_i}$ 

## Derivative of Vector w.r.t. Vector

• The derivative of a vector  $\mathbf{y} \in \mathbb{R}^n$  w.r.t. a vector  $\mathbf{x} \in \mathbb{R}^m$ :

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_n}{\partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_m} & \frac{\partial y_2}{\partial x_m} & \cdots & \frac{\partial y_n}{\partial x_m} \end{bmatrix}$$

$$m \times n \text{ matrix}$$

• Example 2:

$$\mathbf{y} = \begin{bmatrix} a_1 x_1^2 \\ a_2 x_2^2 \\ \vdots \\ a_m x_m^2 \end{bmatrix} \in \mathbb{R}^m, \qquad \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \underbrace{\begin{bmatrix} 2a_1 x_1 & 0 & \cdots & 0 \\ 0 & 2a_2 x_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 2a_m x_m \end{bmatrix}}_{m \times m}$$

### Derivative of Vector w.r.t. Vector

• The derivative of a vector  $\mathbf{y} \in \mathbb{R}^n$  w.r.t. a vector  $\mathbf{x} \in \mathbb{R}^m$ :

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_n}{\partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_m} & \frac{\partial y_2}{\partial x_m} & \cdots & \frac{\partial y_n}{\partial x_m} \end{bmatrix}$$

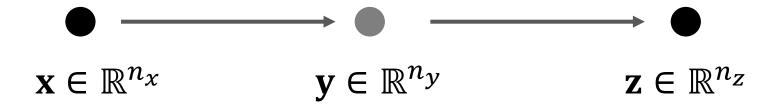
$$m \times n \text{ matrix}$$

• Example 3:

$$\mathbf{A} \in \mathbb{R}^{n imes m}, \qquad \mathbf{y} = \mathbf{A}\mathbf{x} \in \mathbb{R}^n, \qquad \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \mathbf{A}^T \in \mathbb{R}^{m imes n}$$

# **Chain Rule**

• Let  $\mathbf{z} \in \mathbb{R}^{n_z}$  be a function of  $\mathbf{y} \in \mathbb{R}^{n_y}$  and  $\mathbf{y}$  be a function of  $\mathbf{x} \in \mathbb{R}^{n_x}$ .



$$\frac{d\mathbf{z}}{d\mathbf{x}} = \underbrace{\frac{d\mathbf{y}}{d\mathbf{x}}}_{n_x \times n_z} \underbrace{\frac{d\mathbf{z}}{d\mathbf{y}}}_{n_x \times n_y} \underbrace{\frac{d\mathbf{z}}{n_y \times n_z}}_{n_y \times n_z}$$

### Derivative of Scalar w.r.t. Matrix

- The derivative of a scalar  $y \in \mathbb{R}$  w.r.t. a matrix  $\mathbf{Z} \in \mathbb{R}^{p \times q}$ :
  - 1. Vectorization:  $\mathbf{x} = \text{vec}(\mathbf{Z}) \in \mathbb{R}^{pq \times 1}$ .
  - 2. Compute  $\frac{\partial y}{\partial x} \in \mathbb{R}^{pq \times 1}$ .
  - 3. Reshape the resulting  $pq \times 1$  vector to  $p \times q$  matrix.

### Derivative of Vector w.r.t. Matrix

- The derivative of a vector  $\mathbf{y} \in \mathbb{R}^n$  w.r.t. a matrix  $\mathbf{Z} \in \mathbb{R}^{p \times q}$ :
  - 1. Vectorization:  $\mathbf{x} = \text{vec}(\mathbf{Z}) \in \mathbb{R}^{pq \times 1}$ .
  - 2. Compute  $\frac{\partial \mathbf{y}}{\partial \mathbf{x}} \in \mathbb{R}^{pq \times n}$ .
  - 3. Reshape the resulting  $pq \times n$  matrix to  $p \times q \times n$  tensor.

# **Binary Classification**

**Tasks** 

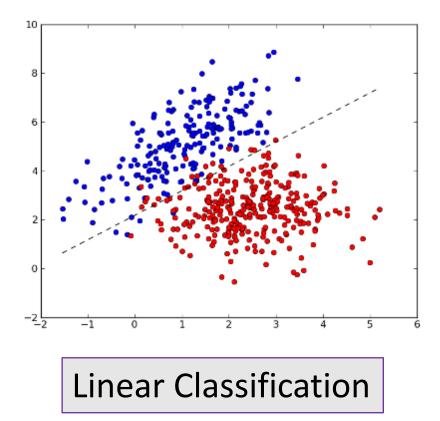
Methods

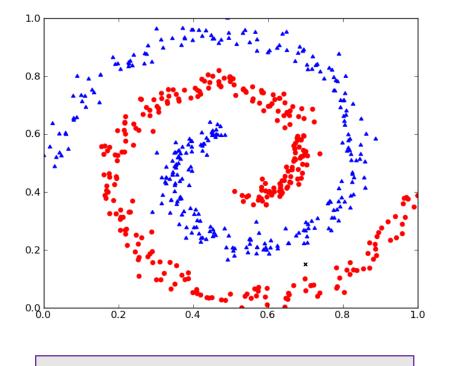
Algorithms

# **Binary Classification**

**Input:** feature vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  and labels  $y_1, \dots, y_n \in \{-1, +1\}$ .

**Output:** a function  $f: \mathbb{R}^d \mapsto \{-1, +1\}$ .





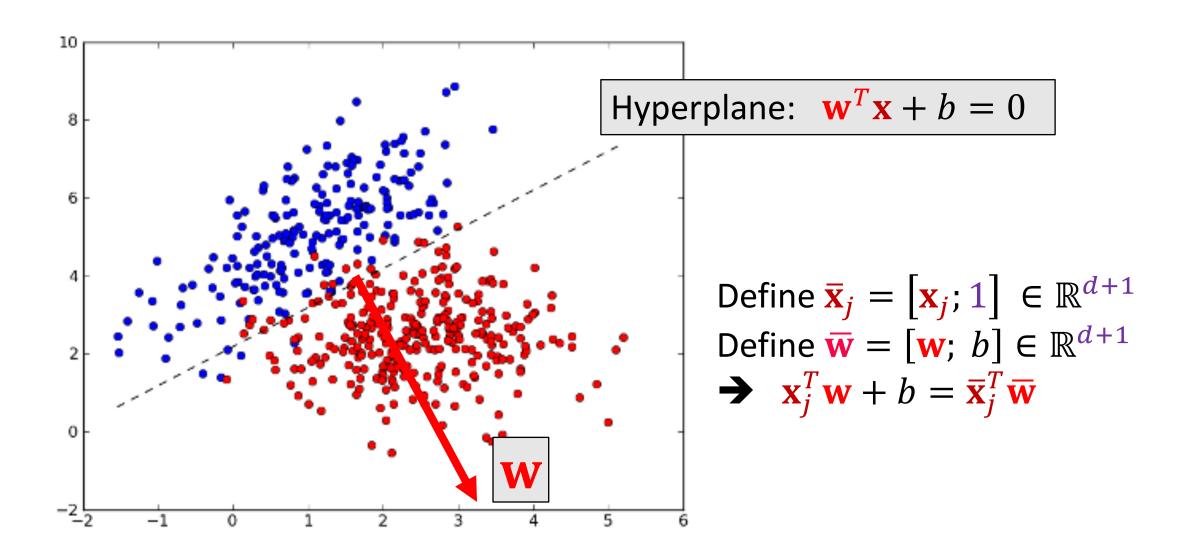
**Nonlinear Classification** 

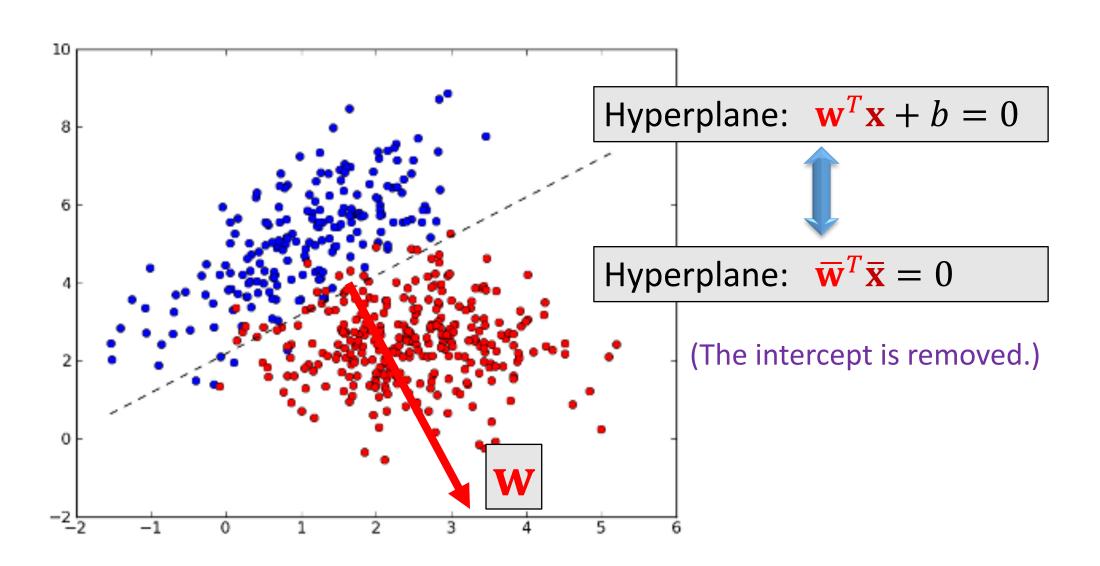
# Logistic Regression (Linear Classifier)

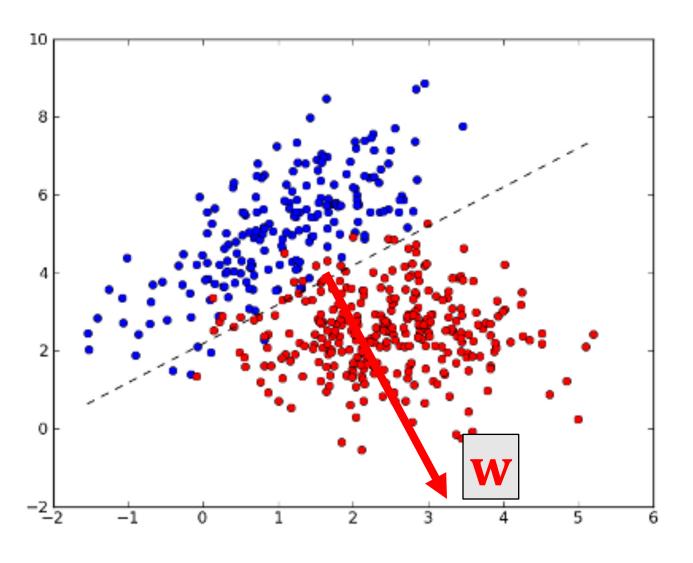
Tasks

Methods

Algorithms

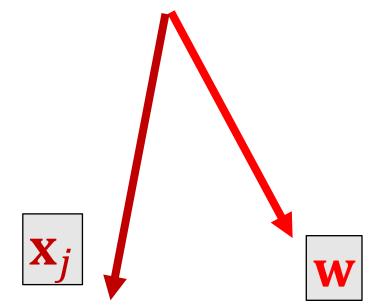


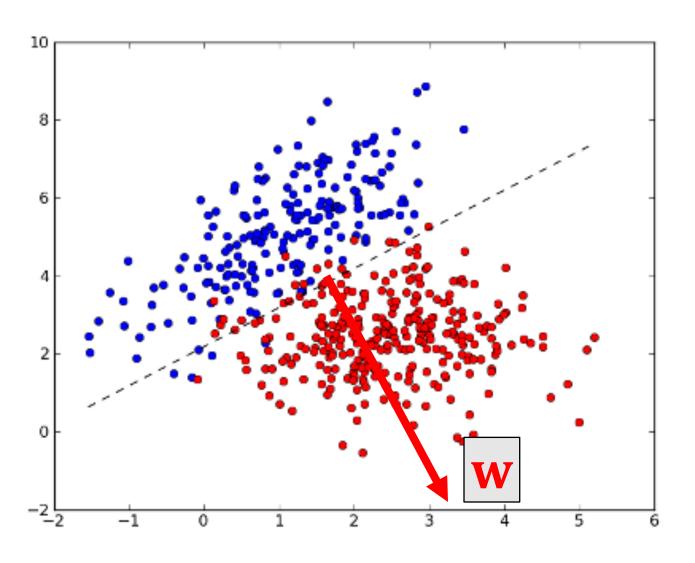




Learn a vector w such that

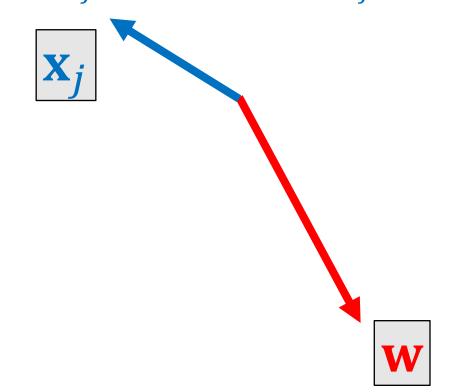
• If  $y_j = +1$ , then  $\mathbf{w}^T \mathbf{x}_j > 0$ .

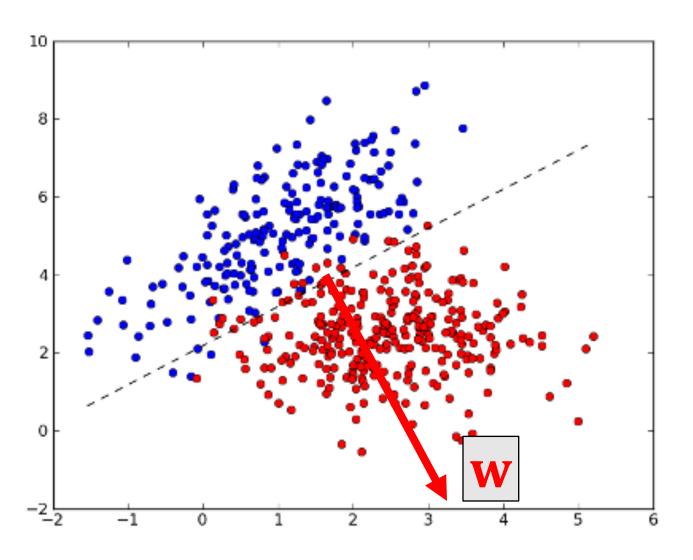




Learn a vector w such that

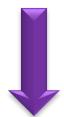
- If  $y_i = +1$ , then  $\mathbf{w}^T \mathbf{x}_i > 0$ .
- If  $y_j = -1$ , then  $\mathbf{w}^T \mathbf{x}_j < 0$ .





Learn a vector w such that

- If  $y_i = +1$ , then  $\mathbf{w}^T \mathbf{x}_i > 0$ .
- If  $y_i = -1$ , then  $\mathbf{w}^T \mathbf{x}_i < 0$ .

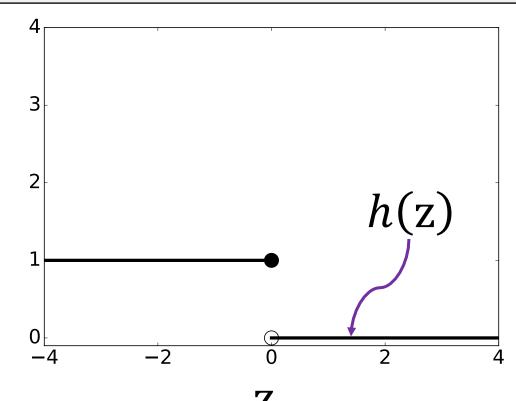


#### **Key Idea:**

Encourage  $y_i \mathbf{w}^T \mathbf{x}_i$  to be positive

# Directly Minimize the Classification Error?

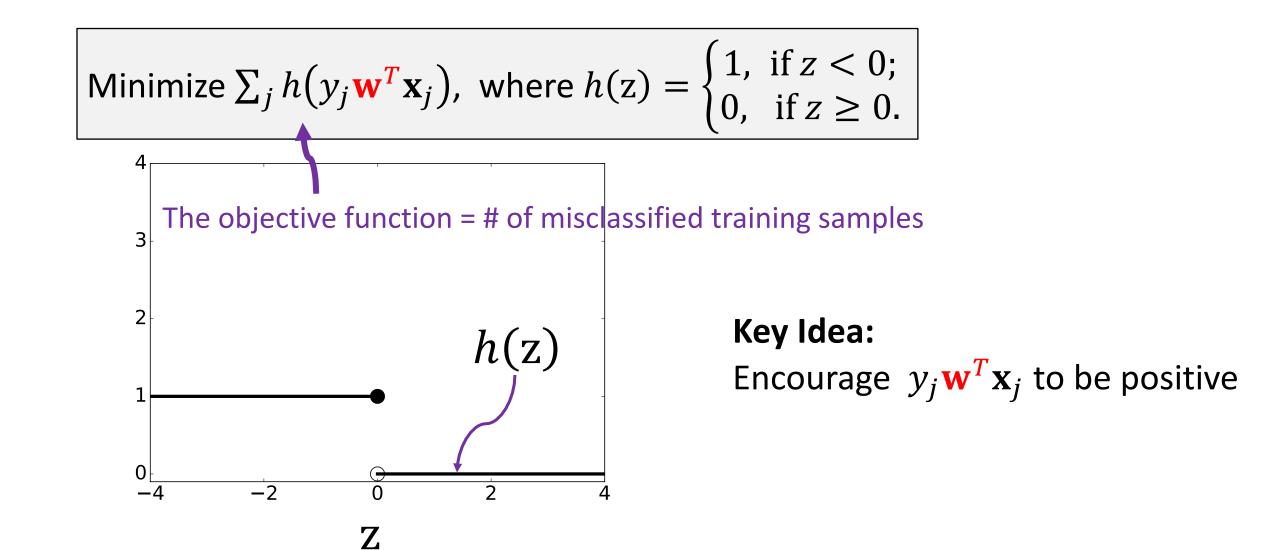
Minimize 
$$\sum_{j} h(y_{j} \mathbf{w}^{T} \mathbf{x}_{j})$$
, where  $h(z) = \begin{cases} 1, & \text{if } z < 0; \\ 0, & \text{if } z \geq 0. \end{cases}$ 



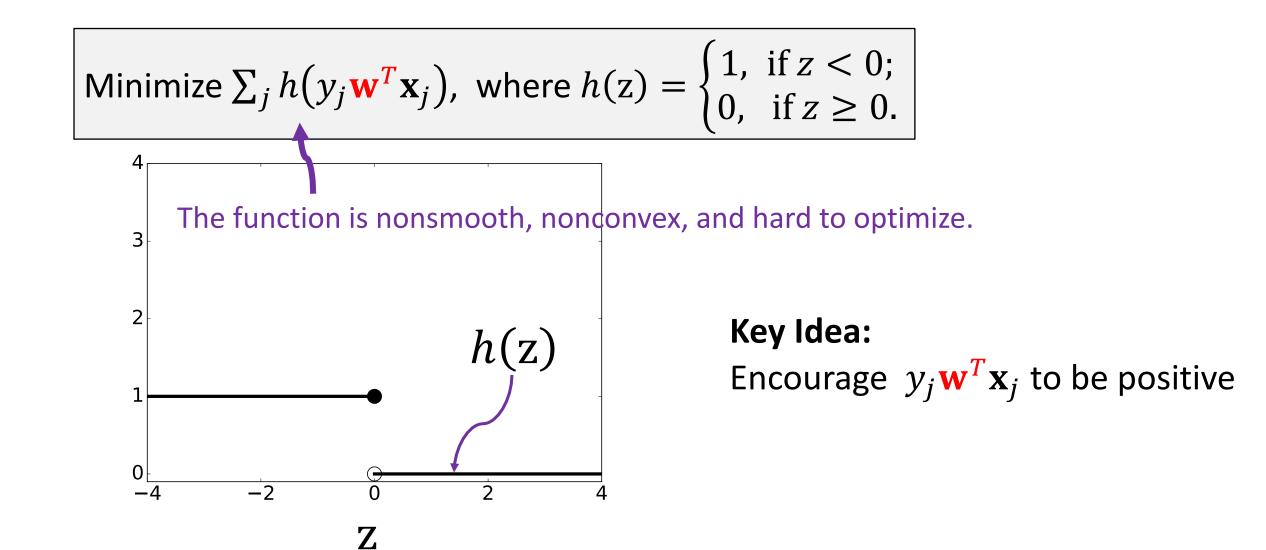
#### **Key Idea:**

Encourage  $y_i \mathbf{w}^T \mathbf{x}_i$  to be positive

# Directly Minimize the Classification Error?

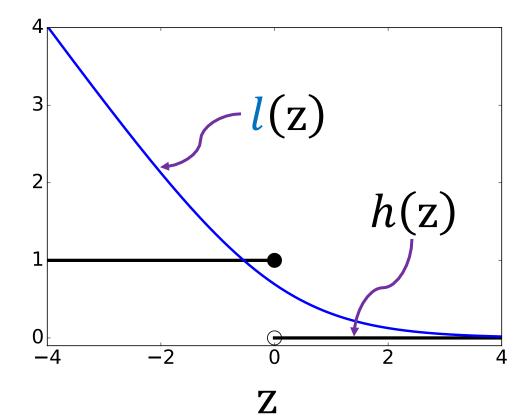


# Directly Minimize the Classification Error?



# Logistic Regression

Minimize  $\sum_{j} l(y_{j} \mathbf{w}^{T} \mathbf{x}_{j})$ , where  $l(\mathbf{z}) = \log(1 + e^{-z})$ .



#### **Key Idea:**

Encourage  $y_j \mathbf{w}^T \mathbf{x}_j$  to be positive

# **Logistic Regression**

Tasks

Methods

**Algorithms** 

# **Logistic Regression**

Logistic regression: 
$$\min_{\mathbf{w}} \frac{1}{n} \sum_{j=1}^{n} l(y_j \mathbf{w}^T \mathbf{x}_j)$$
, where  $l(\mathbf{z}) = \log(1 + e^{-z})$ .

### Tasks

### Methods

**Logistic Regression** 

SVM

## **Algorithms**

**Binary Classification** 

**Accelerated GD** 

**Neural Networks** 

**Gradient Descent (GD)** 

### Gradient

Logistic regression:  $\min_{\mathbf{w}} \frac{1}{n} \sum_{j=1}^{n} l(y_j \mathbf{w}^T \mathbf{x}_j)$ , where  $l(\mathbf{z}) = \log(1 + e^{-z})$ .

$$z = y \mathbf{w}^T \mathbf{x} \qquad l = \log(1 + e^{-z})$$

### Gradient

Logistic regression:  $\min_{\mathbf{w}} \frac{1}{n} \sum_{j=1}^{n} l(y_j \mathbf{w}^T \mathbf{x}_j)$ , where  $l(\mathbf{z}) = \log(1 + e^{-z})$ .

$$z = y \mathbf{w}^T \mathbf{x} \qquad l = \log(1 + e^{-z})$$

• 
$$\frac{\partial z}{\partial \mathbf{w}} = y\mathbf{x}$$
,  $\frac{\partial l(z)}{\partial z} = \frac{-e^{-z}}{1+e^{-z}} = -\frac{1}{1+e^{z}}$ .

• Chain rule: 
$$\frac{\partial l}{\partial \mathbf{w}} = \frac{\partial z}{\partial \mathbf{w}} \cdot \frac{\partial l}{\partial z} = (y\mathbf{x}) \left( -\frac{1}{1+e^z} \right) = -\frac{y\mathbf{x}}{1+\exp(y\mathbf{w}^T\mathbf{x})}.$$

### Gradient

Logistic regression: 
$$\min_{\mathbf{w}} \frac{1}{n} \sum_{j=1}^{n} l(y_j \mathbf{w}^T \mathbf{x}_j)$$
, where  $l(\mathbf{z}) = \log(1 + e^{-z})$ .

Gradient at 
$$\mathbf{w}_t$$
:  $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \frac{-y_j \mathbf{x}_j}{1 + \exp(y_j \mathbf{w}_t^T \mathbf{x}_j)}$ .

- We have shown:  $\frac{\partial l(y\mathbf{w}^T\mathbf{x})}{\partial \mathbf{w}} = \frac{-y\mathbf{x}}{1 + \exp(y\mathbf{w}^T\mathbf{x})}$ .
- Objective function:  $f(\mathbf{w}) = \frac{1}{n} \sum_{j} l(y_j \mathbf{w}^T \mathbf{x}_j)$ .

• 
$$\frac{\partial f(\mathbf{w})}{\partial \mathbf{w}} = \frac{1}{n} \sum_{j} \frac{\partial l(y_{j} \mathbf{w}^{T} \mathbf{x}_{j})}{\partial \mathbf{w}} = \frac{1}{n} \sum_{j} \frac{-y_{j} \mathbf{x}_{j}}{1 + \exp(y_{j} \mathbf{w}^{T} \mathbf{x}_{j})}.$$

# Gradient Descent (GD) Algorithm

Logistic regression: 
$$\min_{\mathbf{w}} \frac{1}{n} \sum_{j=1}^{n} l(y_j \mathbf{w}^T \mathbf{x}_j)$$
, where  $l(\mathbf{z}) = \log(1 + e^{-z})$ .

Gradient at 
$$\mathbf{w}_t$$
:  $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \frac{-y_j \mathbf{x}_j}{1 + \exp(y_j \mathbf{w}_t^T \mathbf{x}_j)}$ .

#### **GD** repeat:

- 1. Compute gradient:  $\mathbf{g}_t$
- 2. Update:  $\mathbf{w}_{t+1} = \mathbf{w}_t \alpha \mathbf{g}_t$



Tune the step size (learning rate)  $\alpha$ 

# **Algorithms**

**Gradient Descent (GD)** 

**Accelerated GD** 

# **AGD Algorithm**

Logistic regression: 
$$\min_{\mathbf{w}} \frac{1}{n} \sum_{j=1}^{n} \mathbf{l}(y_j \mathbf{w}^T \mathbf{x}_j)$$
, where  $\mathbf{l}(\mathbf{z}) = \log(1 + e^{-z})$ .

Gradient at 
$$\mathbf{w}_t$$
:  $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \frac{-y_j \mathbf{x}_j}{1 + \exp(y_j \mathbf{w}_t^T \mathbf{x}_j)}$ .

#### **AGD** repeat:

- 1. Compute gradient:  $\mathbf{g}_t$
- 2. Update momentum:  $\mathbf{v}_{t+1} = \beta \mathbf{v}_t + \mathbf{g}_t$
- 3. Update:  $\mathbf{w}_{t+1} = \mathbf{w}_t \alpha \mathbf{v}_{t+1}$

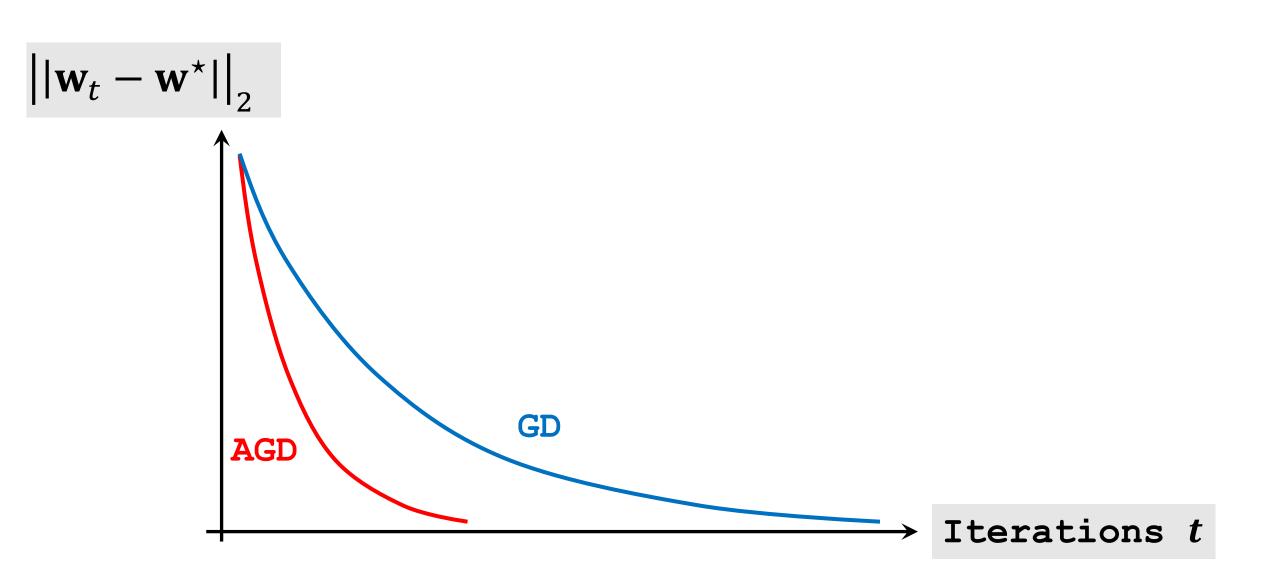
Tune  $\alpha$  and  $\beta$  ( $0 \le \beta < 1$ )

# **Algorithms**

**Gradient Descent (GD)** 

Accelerated GD

### **GD** versus **AGD**



# **Time Complexity**

Gradient at 
$$\mathbf{w}_t$$
:  $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \tilde{\mathbf{g}}_{t,j}$ , where  $\tilde{\mathbf{g}}_{t,j} = \frac{-y_j \mathbf{x}_j}{1 + \exp(y_i \mathbf{w}_t^T \mathbf{x}_j)}$ .

Per-iteration time complexity is O(nd).

- O(d) time for computing  $\mathbf{w}_t^T \mathbf{x}_i$ .
- O(d) time for computing  $\tilde{\mathbf{g}}_{t,i}$ .
- O(nd) time for computing all the  $\tilde{\mathbf{g}}_{t,j}$ .

# **Algorithms**

**Gradient Descent (GD)** 

Accelerated GD

# **SGD** Algorithm

Gradient at 
$$\mathbf{w}_t$$
:  $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \tilde{\mathbf{g}}_{t,j}$ , where  $\tilde{\mathbf{g}}_{t,j} = \frac{-y_j \mathbf{x}_j}{1 + \exp(y_j \mathbf{w}_t^T \mathbf{x}_j)}$ .

The stochastic gradient is close to the full gradient:

$$\mathbf{g}_t = \mathbb{E}_j \big[ \widetilde{\mathbf{g}}_{t,j} \big],$$

where j is randomly sampled from  $\{1, \dots, n\}$ .

# **Algorithms**

**Gradient Descent (GD)** 

Accelerated GD

# **SGD** Algorithm

Gradient at 
$$\mathbf{w}_t$$
:  $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \tilde{\mathbf{g}}_{t,j}$ , where  $\tilde{\mathbf{g}}_{t,j} = \frac{-y_j \mathbf{x}_j}{1 + \exp(y_j \mathbf{w}_t^T \mathbf{x}_j)}$ .

#### **SGD** repeats

- 1. Randomly draw j from  $\{1, 2, \dots, n\}$ .
- 2. Compute the stochastic gradient  $\tilde{\mathbf{g}}_{t,i}$ .
- 3. Update:  $\mathbf{w}_{t+1} = \mathbf{w}_t \alpha \ \tilde{\mathbf{g}}_{t,i}$ .

Per-iteration time complexity is O(d).

# **Algorithms**

**Gradient Descent (GD)** 

Accelerated GD

## Accelerated SGD Algorithm

Gradient at 
$$\mathbf{w}_t$$
:  $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \tilde{\mathbf{g}}_{t,j}$ , where  $\tilde{\mathbf{g}}_{t,j} = \frac{-y_j \mathbf{x}_j}{1 + \exp(y_j \mathbf{w}_t^T \mathbf{x}_j)}$ .

#### **Accelerated SGD repeats**

- 1. Randomly draw j from  $\{1, 2, \dots, n\}$ .
- 2. Compute the stochastic gradient  $\tilde{\mathbf{g}}_{t,j}$ .
- 3. Update momentum:  $\mathbf{v}_{t+1} = \beta \mathbf{v}_t + \tilde{\mathbf{g}}_{t,j}$ .
- 4. Update:  $\mathbf{w}_{t+1} = \mathbf{w}_t \alpha \mathbf{v}_{t+1}$ .

## **Algorithms**

**Gradient Descent (GD)** 

**Accelerated GD** 

Stochastic GD

## **SGD** Algorithm

Gradient at 
$$\mathbf{w}_t$$
:  $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \tilde{\mathbf{g}}_{t,j}$ , where  $\tilde{\mathbf{g}}_{t,j} = \frac{-y_j \mathbf{x}_j}{1 + \exp(y_j \mathbf{w}_t^T \mathbf{x}_j)}$ .

#### **Output of SGD:**

- Option 1: output the last iteration  $\mathbf{w}_{T+1}$
- Option 2: output the average of w produced by the last tens of iteration.

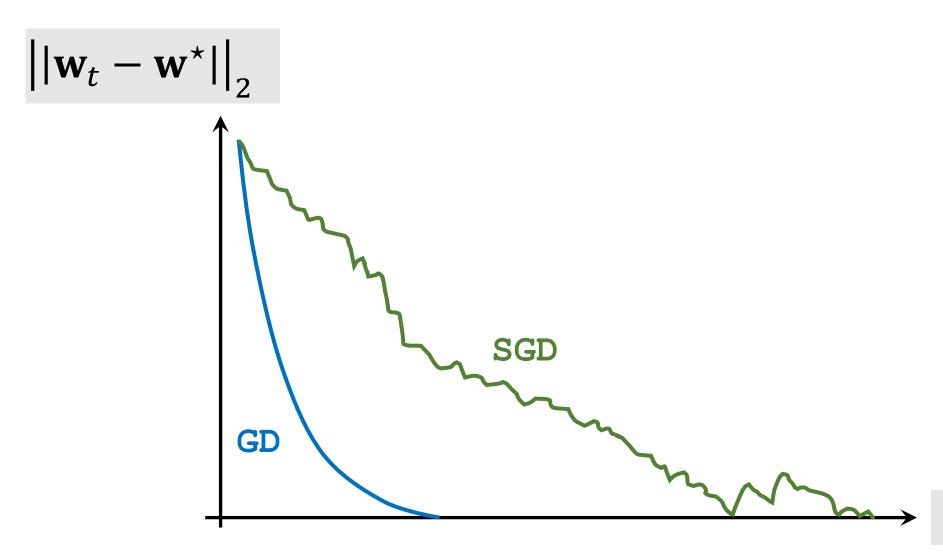
### **Algorithms**

**Gradient Descent (GD)** 

Accelerated GD

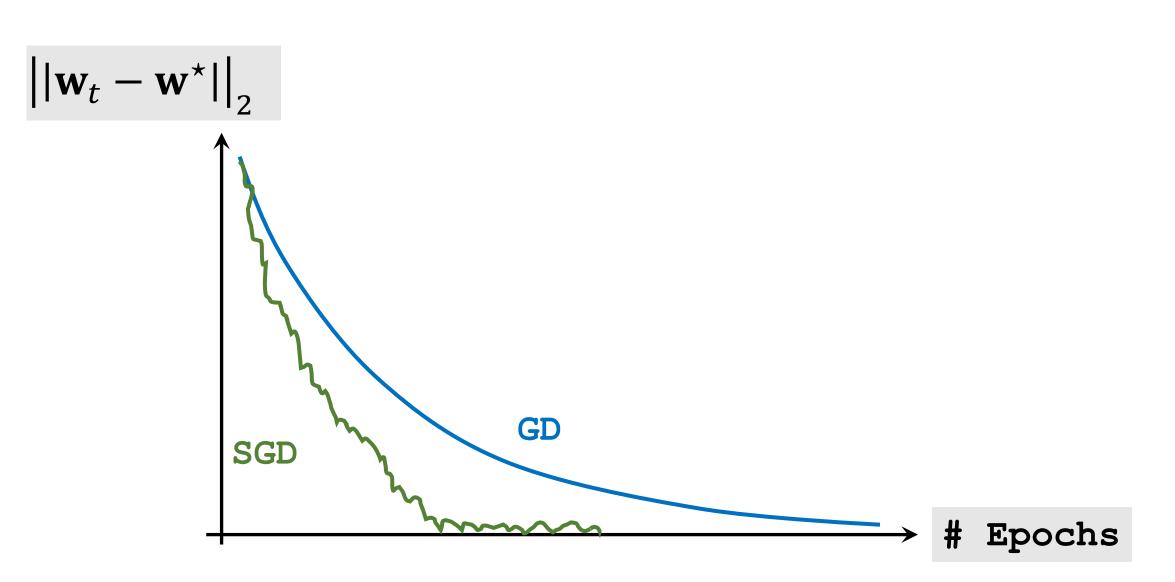
Stochastic GD

### **GD** versus **SGD**



Iterations t

## **GD** versus **SGD**



## **Training and Prediction**

• Training:

$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{j} l(y_j \mathbf{w}^T \mathbf{x}_j)$$
, where  $l(\mathbf{z}) = \log(1 + e^{-z})$ .

• For a test feature vector  $\mathbf{x}' \in \mathbb{R}^d$ , make prediction by  $\mathrm{sign}(\mathbf{x'}^T\mathbf{w}^\star).$ 

## Summary

Logistic regression model for linear binary classification.

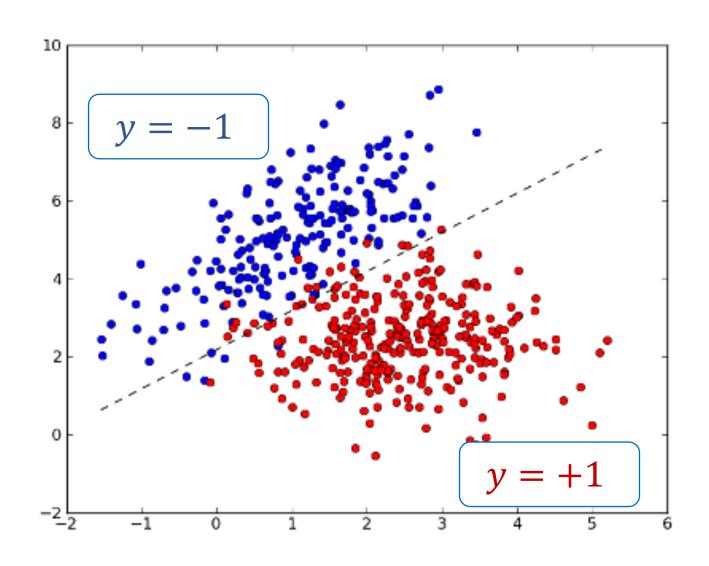
$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{j} l(y_j \mathbf{w}^T \mathbf{x}_j)$$
, where  $l(\mathbf{z}) = \log(1 + e^{-z})$ .

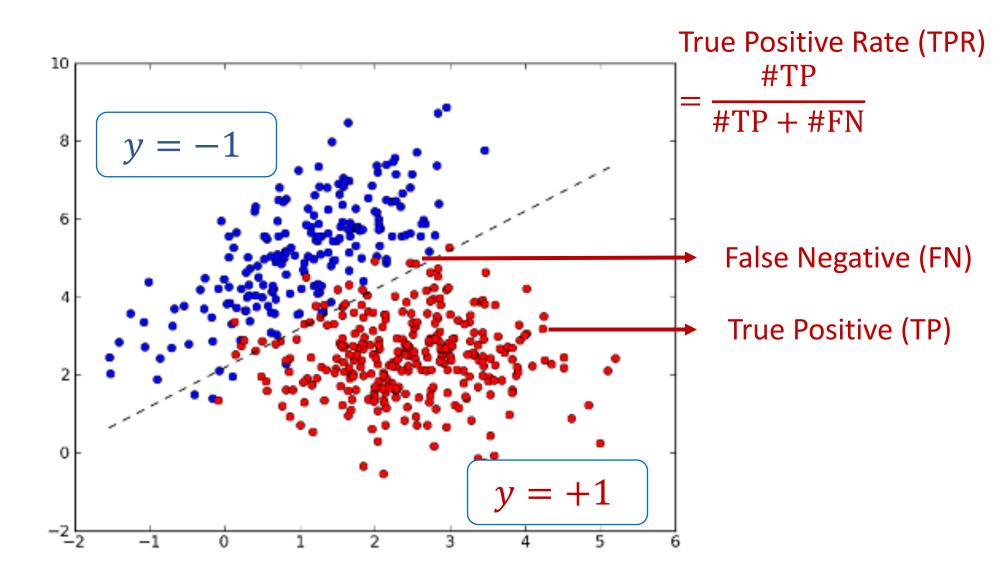
- Compute the gradient using vector derivatives and the chain rule.
- Gradient-based algorithms: GD, AGD, SGD, etc.
- Make prediction using  $sign(x'^Tw^*)$ .

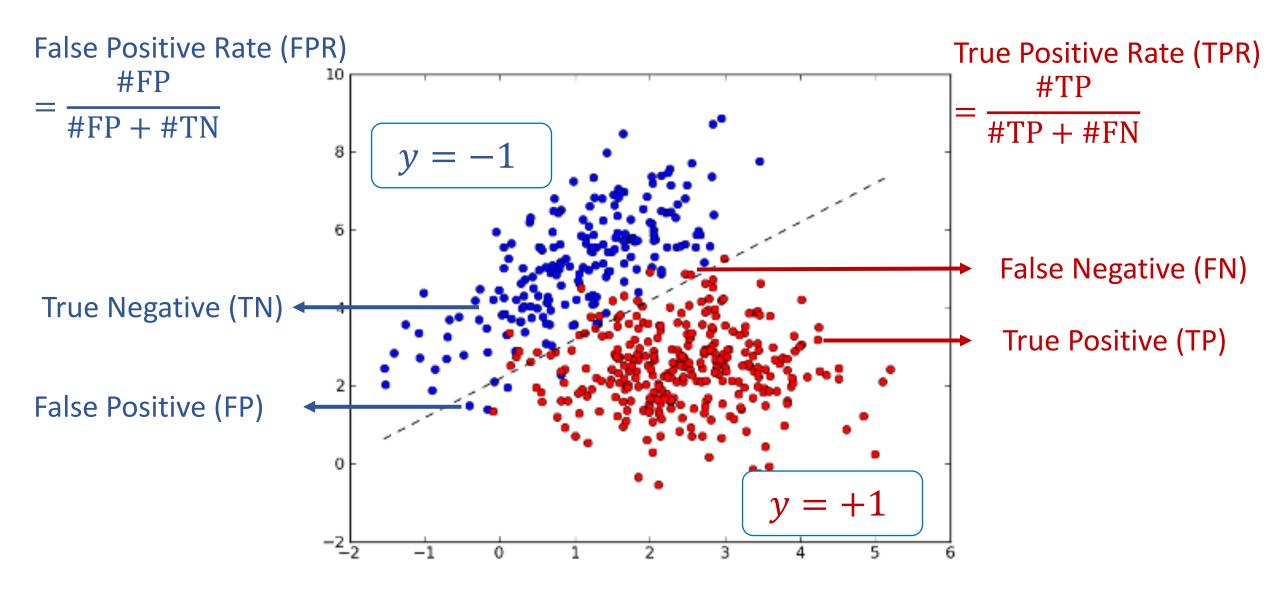
- Error Rate =  $\frac{\text{\# Classification Errors}}{\text{\# Samples}}$
- Accuracy = 1 Error Rate

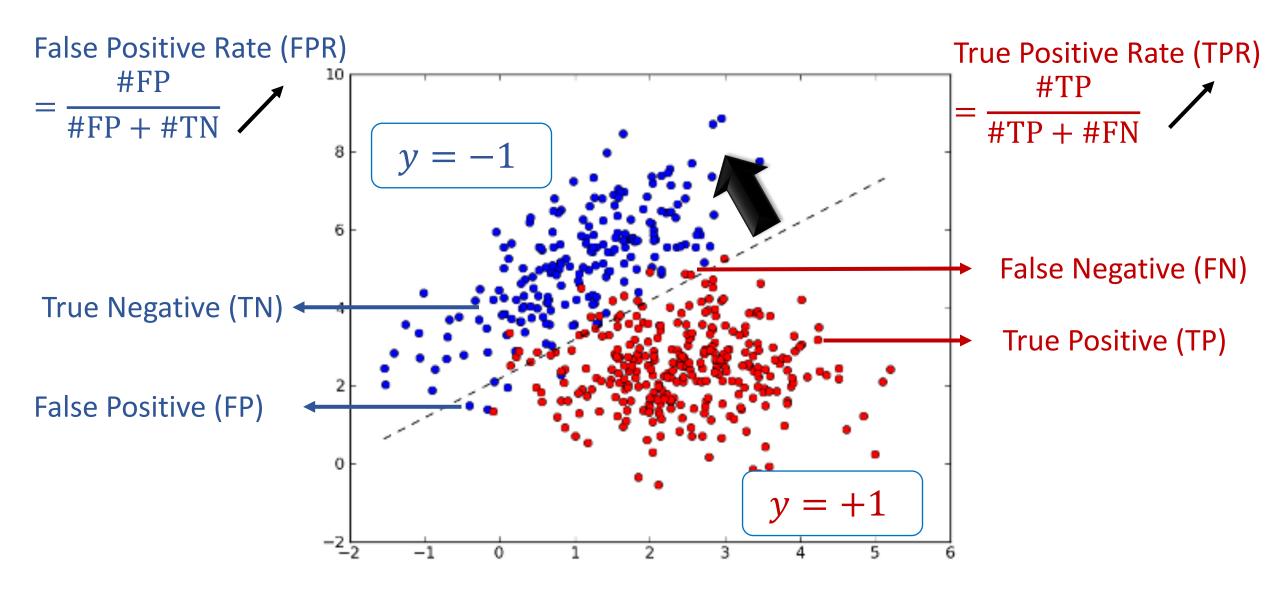
- Error Rate =  $\frac{\text{# Classification Errors}}{\text{# Samples}}$
- Accuracy = 1 Error Rate

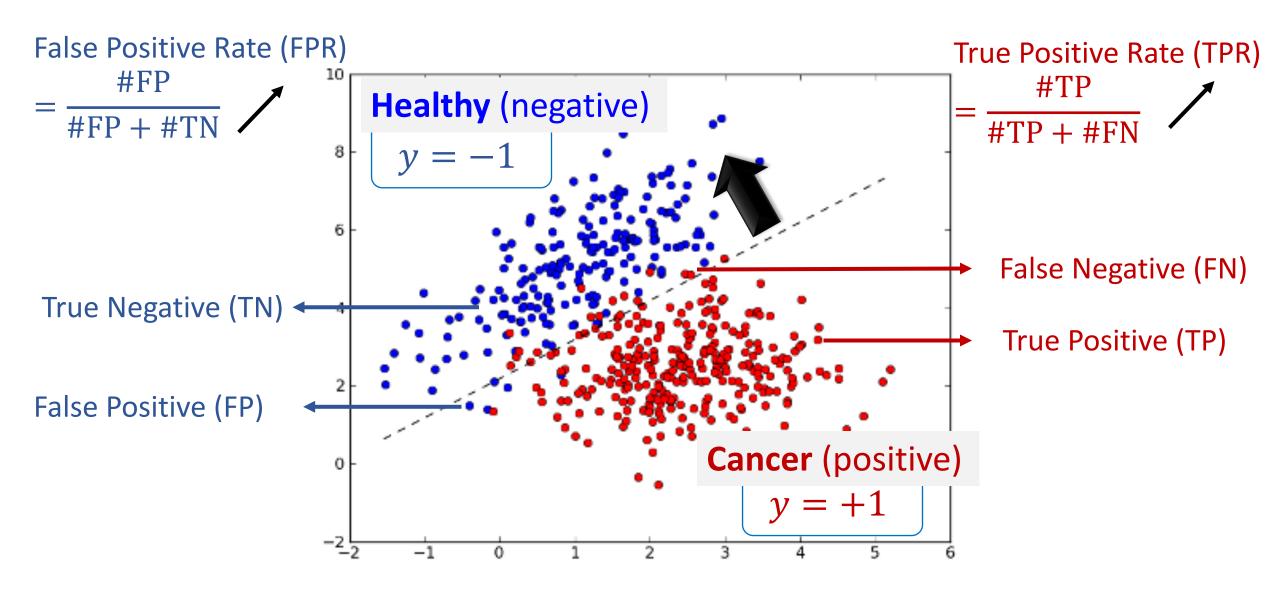
Error rate and Accuracy are not meaningful in class-imbalanced problems.

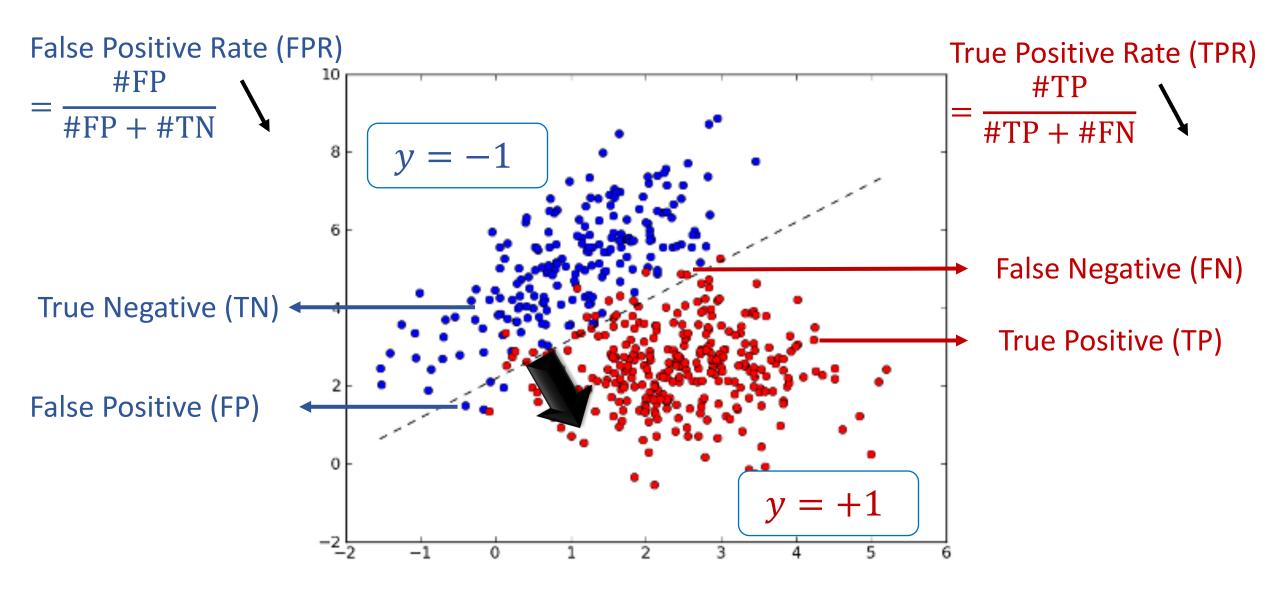


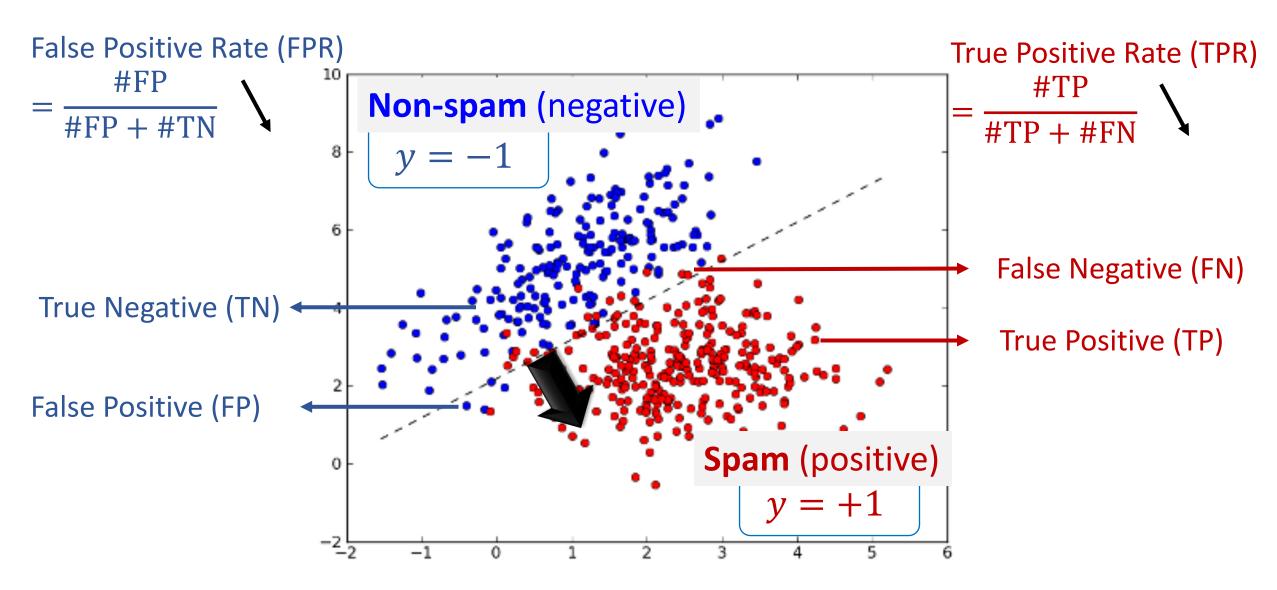


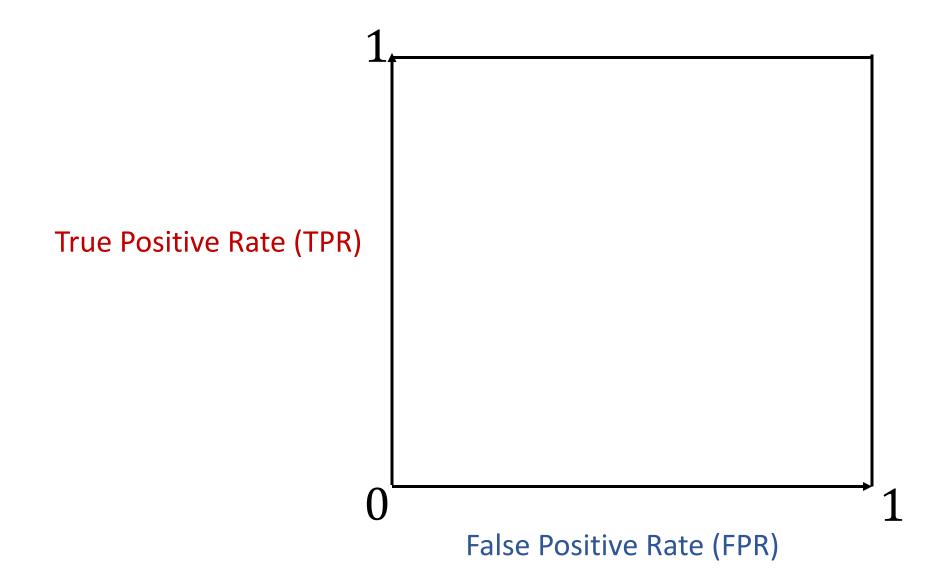


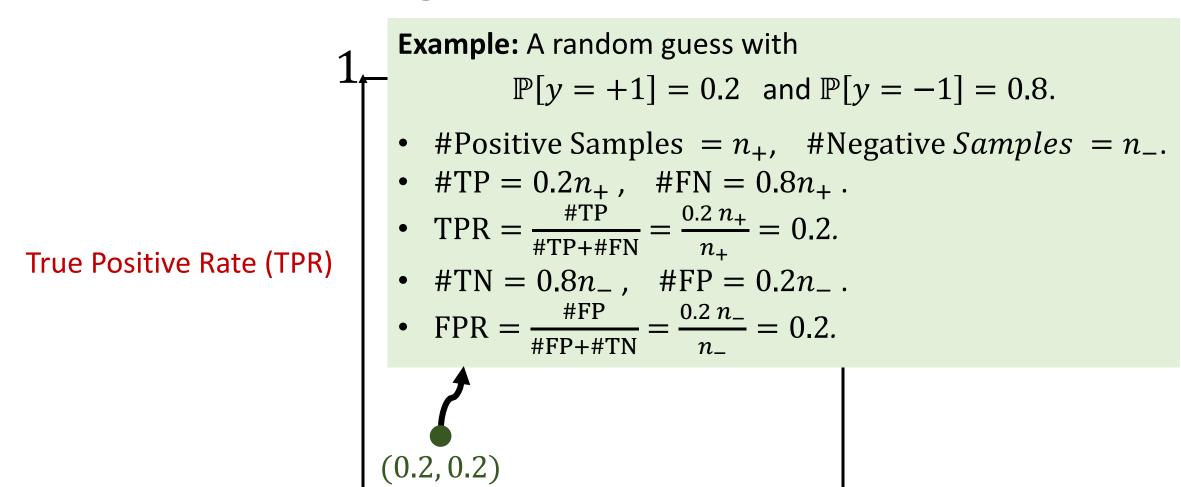




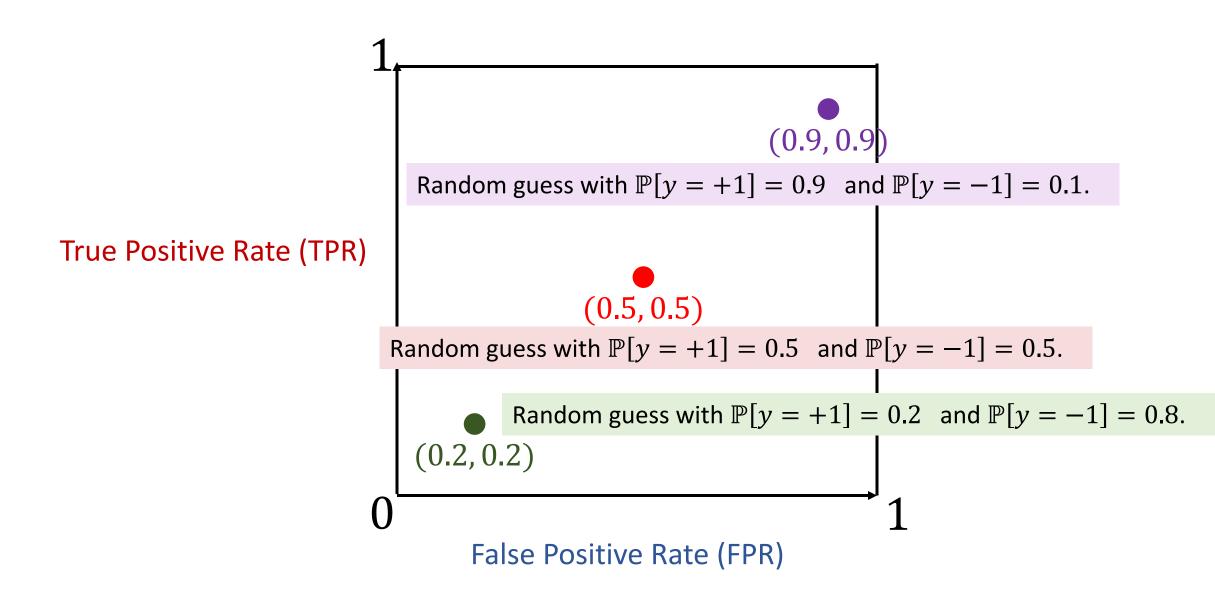


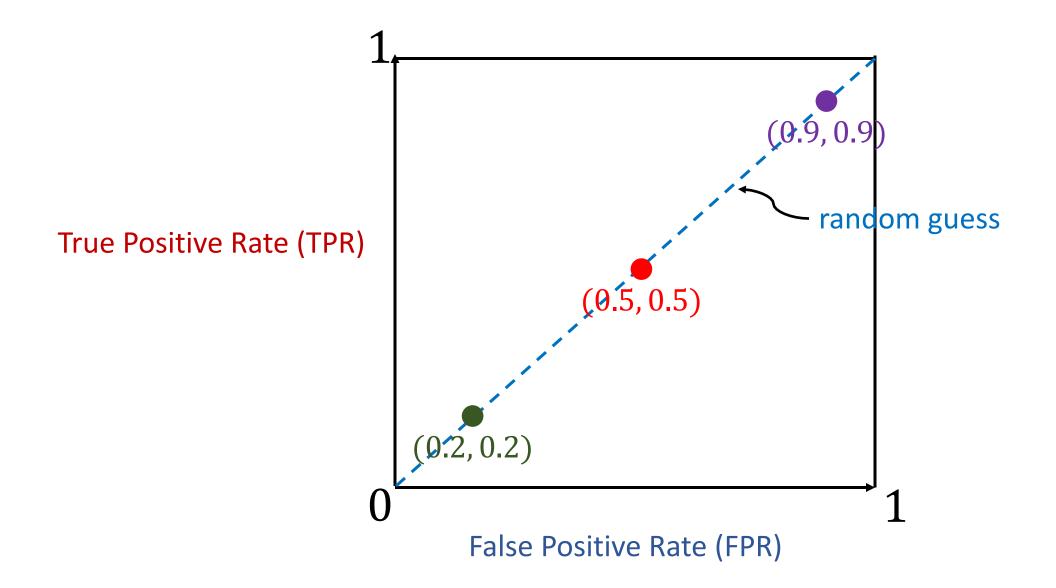


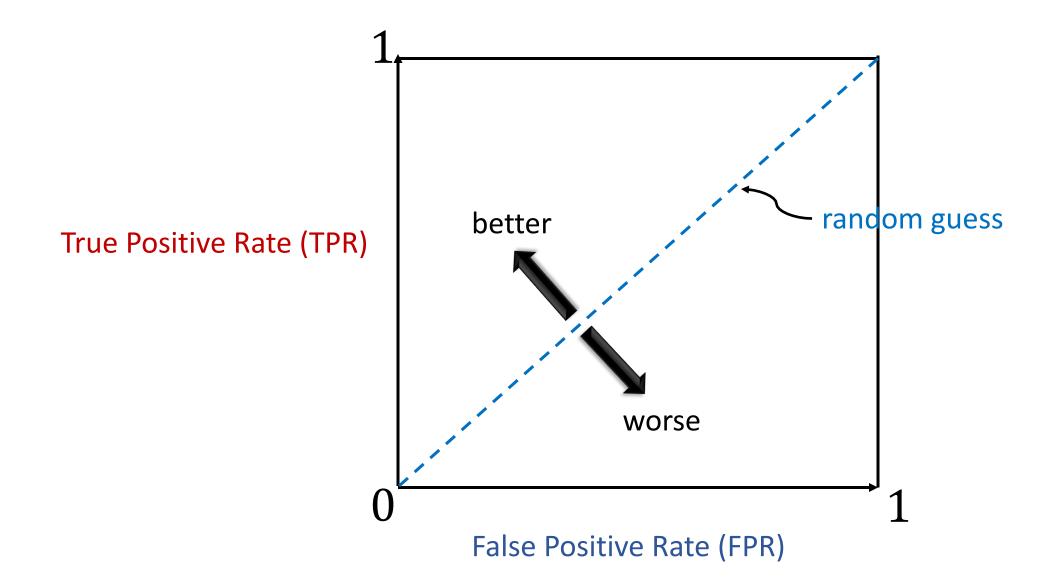


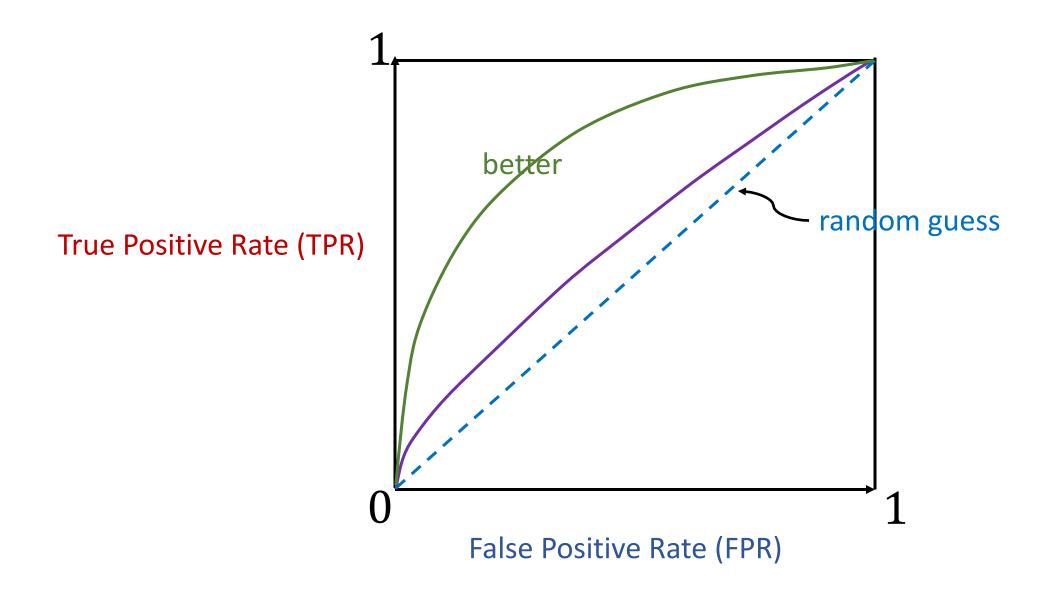


False Positive Rate (FPR)









# Thank you!