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

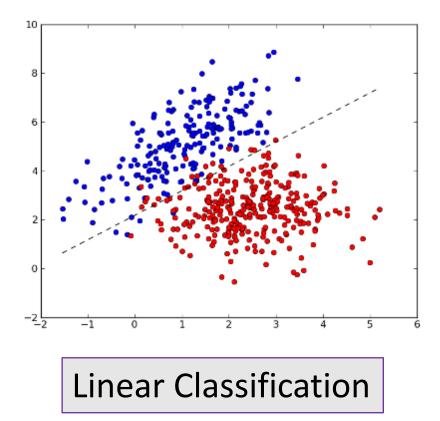
Methods

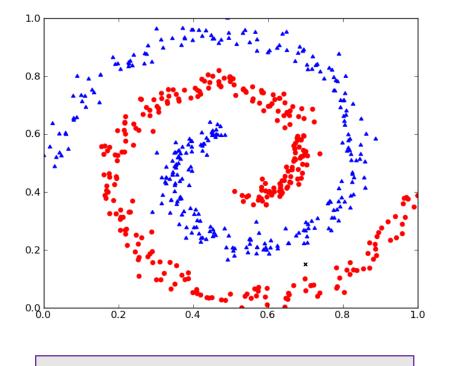
Algorithms

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





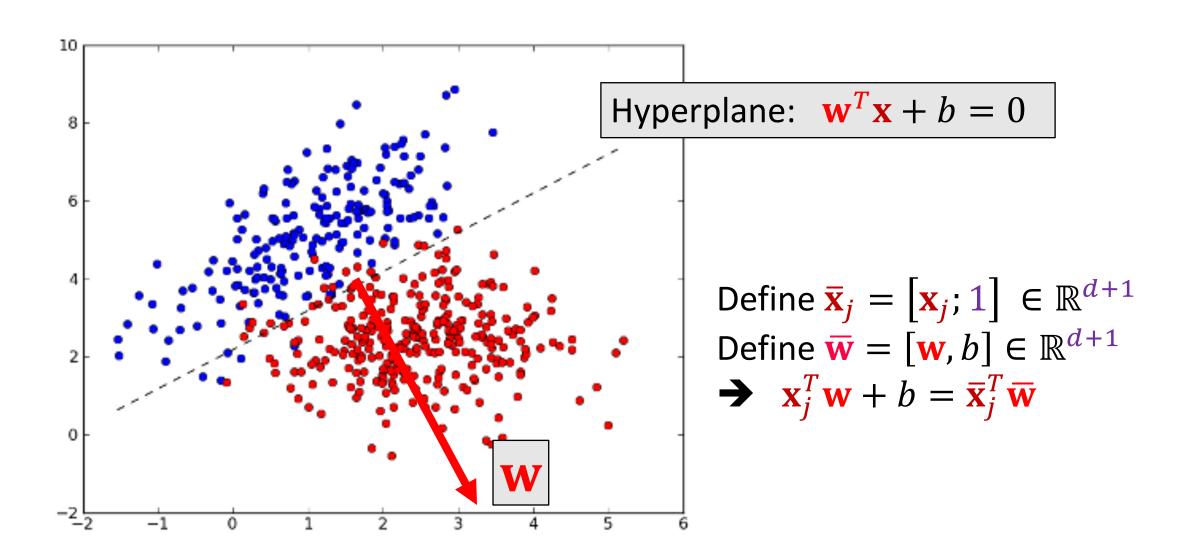
Nonlinear Classification

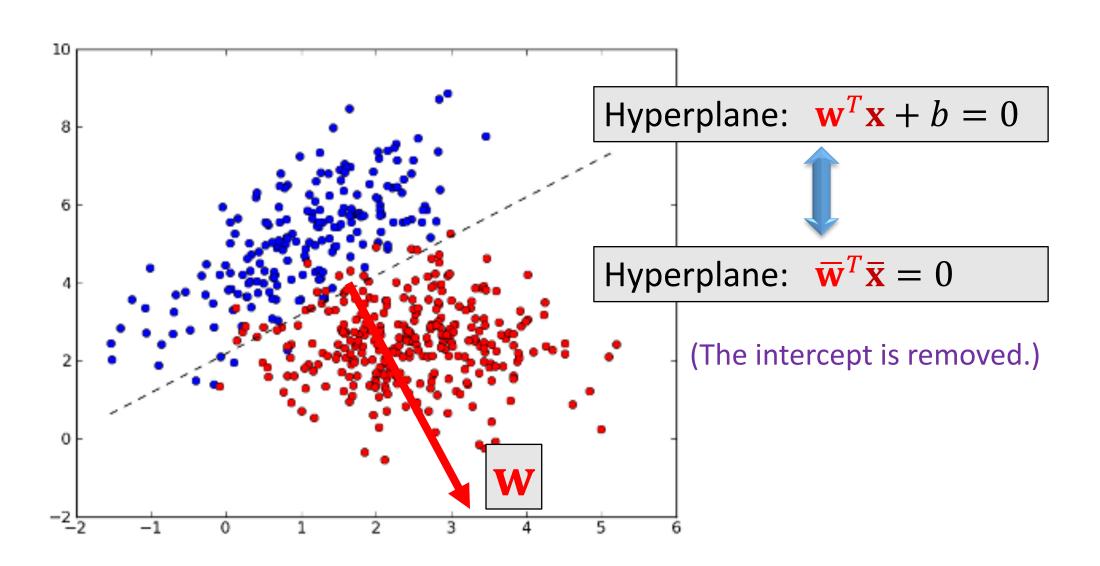
Logistic Regression (Linear Classification)

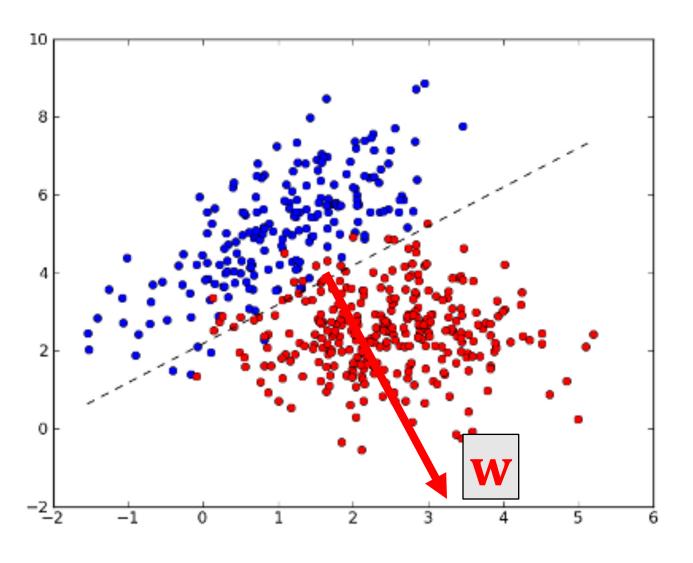
Tasks

Methods

Algorithms

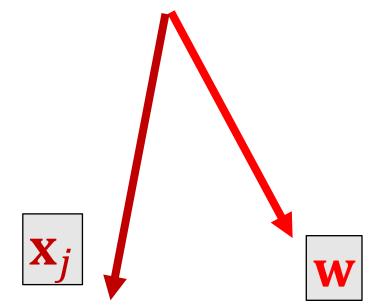


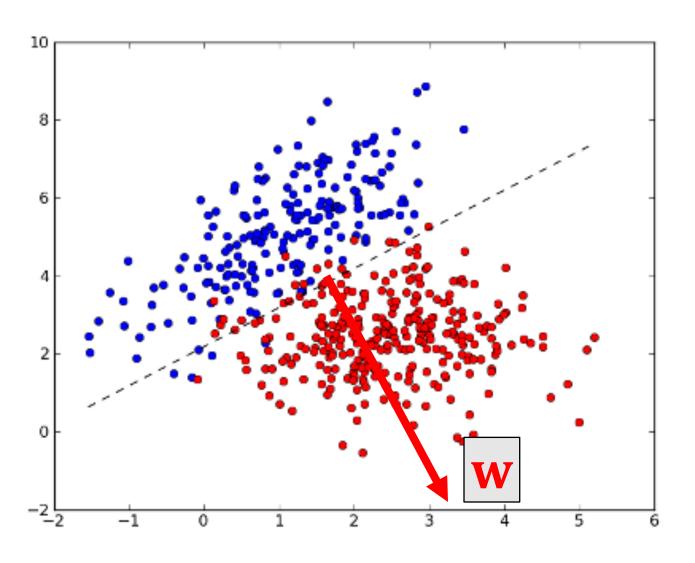




Learn a vector w such that

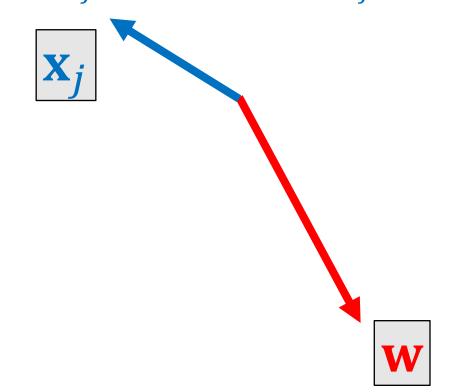
• If $y_j = +1$, then $\mathbf{w}^T \mathbf{x}_j > 0$.

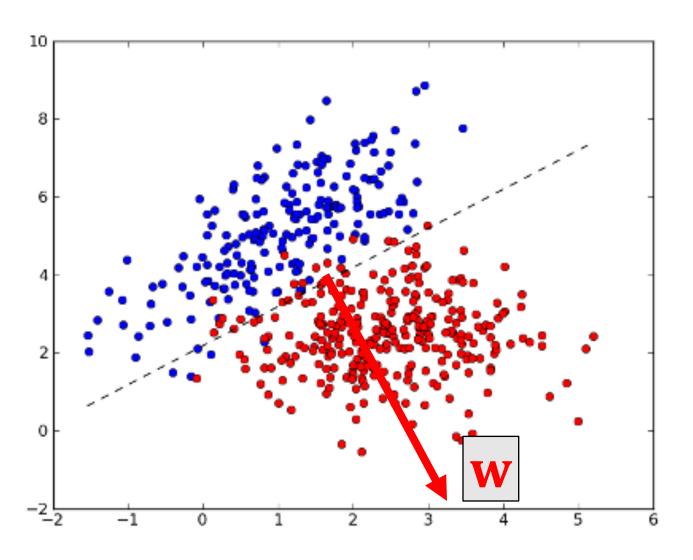




Learn a vector w such that

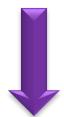
- If $y_i = +1$, then $\mathbf{w}^T \mathbf{x}_i > 0$.
- If $y_j = -1$, then $\mathbf{w}^T \mathbf{x}_j < 0$.





Learn a vector w such that

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

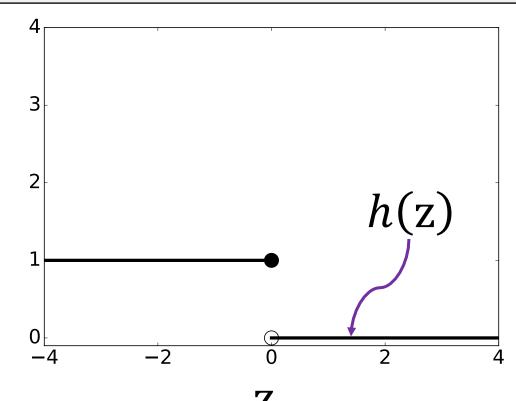


Key Idea:

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

Directly Minimize the Classification Error?

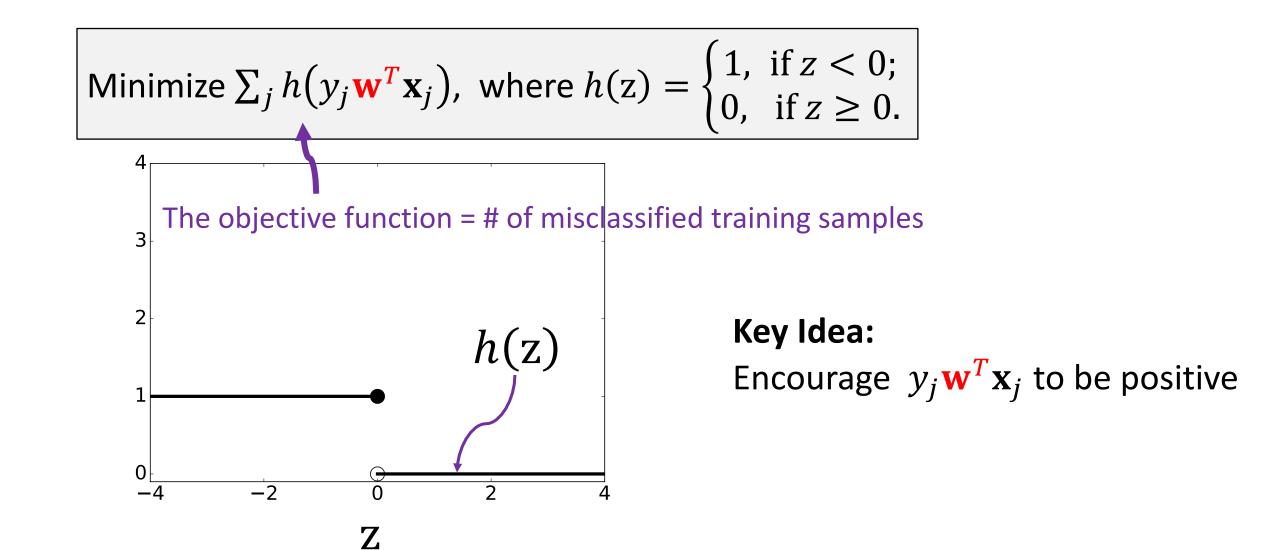
Minimize
$$\sum_{j} h(y_{j} \mathbf{w}^{T} \mathbf{x}_{j})$$
, where $h(z) = \begin{cases} 1, & \text{if } z < 0; \\ 0, & \text{if } z \geq 0. \end{cases}$



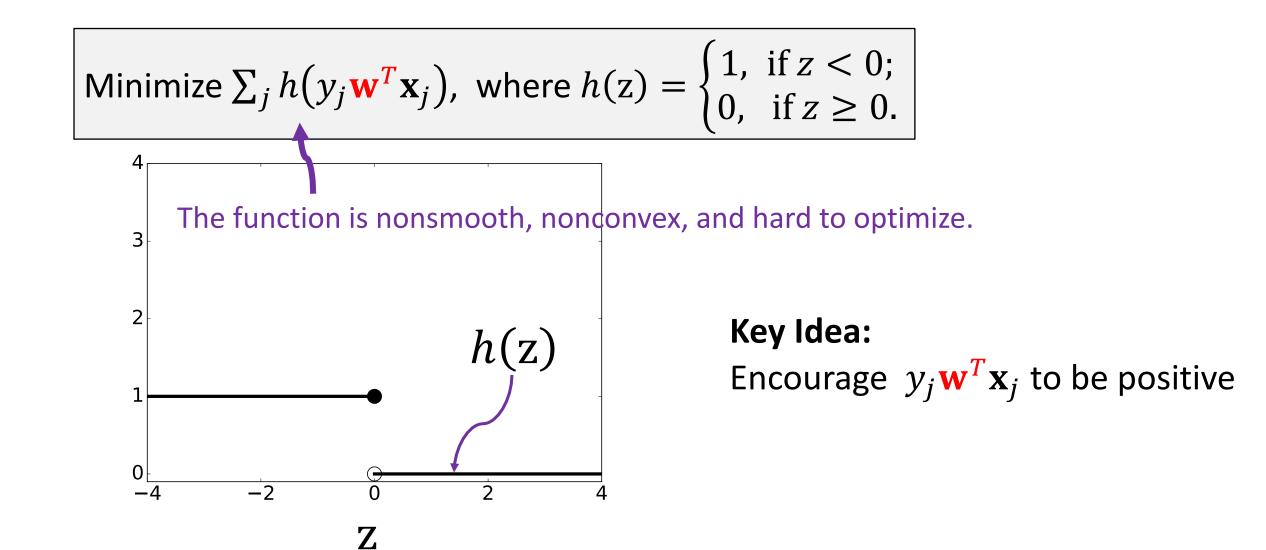
Key Idea:

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

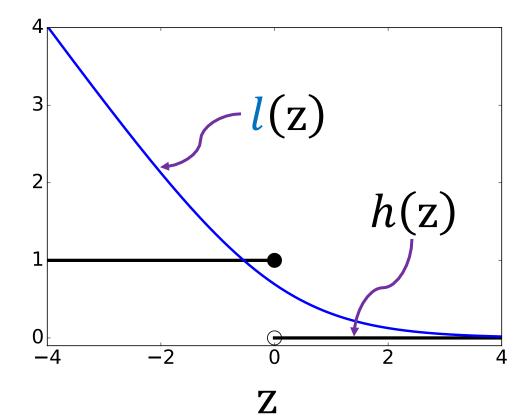
Directly Minimize the Classification Error?



Directly Minimize the Classification Error?



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

Tasks

Methods

Algorithms

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

Tasks

Methods

Algorithms

Binary Classification

SVM

Logistic Regression

Accelerated GD

Multi-Class Classification

Neural Networks

Stochastic GD

Gradient Descent (GD)

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

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

- Chain rule:
 - Define $z_j = y_j \mathbf{w}^T \mathbf{x}_j$

•
$$\frac{\partial l(y_j \mathbf{w}^T \mathbf{x}_j)}{\partial \mathbf{w}} = \frac{\partial z_j}{\partial \mathbf{w}} \cdot \frac{\partial l(z_j)}{\partial z_j} = (y_j \mathbf{x}_j) \left(-\frac{1}{1 + e^{z_j}} \right) = -\frac{y_j \mathbf{x}_j}{1 + \exp(y_j \mathbf{w}_t^T \mathbf{x}_j)}$$

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

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

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

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

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

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

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) α

Algorithms

Gradient Descent (GD)

Accelerated GD

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

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

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 α and β ($0 \le \beta < 1$)

Algorithms

Gradient Descent (GD)

Accelerated GD

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

Per-iteration time complexity is O(nd)

- O(d) time for computing $\mathbf{w}_t^T \mathbf{x}_i$
- O(d) time for computing $\tilde{\mathbf{g}}_{t,j}$
- O(nd) time for computing $\mathbf{g}_t = \frac{1}{n} \sum_j \tilde{\mathbf{g}}_{t,j}$

Algorithms

Gradient Descent (GD)

Accelerated GD

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
$$\mathbf{w}_t$$
: $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \tilde{\mathbf{g}}_{t,j}$, 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

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
$$\mathbf{w}_t$$
: $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \tilde{\mathbf{g}}_{t,j}$, 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 $\tilde{\mathbf{g}}_{t,j}$.
- 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

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
$$\mathbf{w}_t$$
: $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \tilde{\mathbf{g}}_{t,j}$, 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

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
$$\mathbf{w}_t$$
: $\mathbf{g}_t = \frac{1}{n} \sum_{j=1}^n \tilde{\mathbf{g}}_{t,j}$, 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

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.

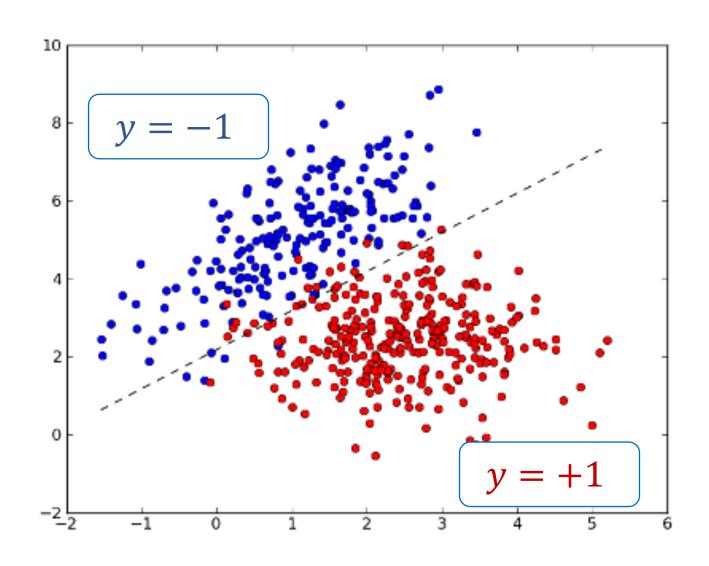
$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{j} l(y_j \mathbf{w}^T \mathbf{x}_j)$$
, where $l(\mathbf{z}) = \log(1 + e^{-z})$.

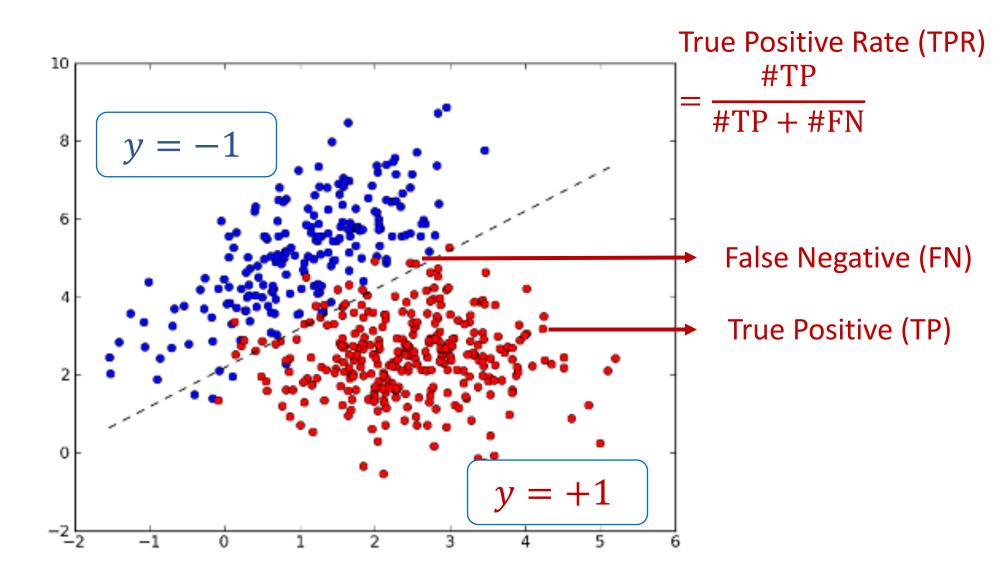
- Compute the gradient using vector derivatives and the chain rule.
- Gradient-based algorithms: GD, AGD, SGD, etc.
- Make prediction using $sign(x'^Tw^*)$.

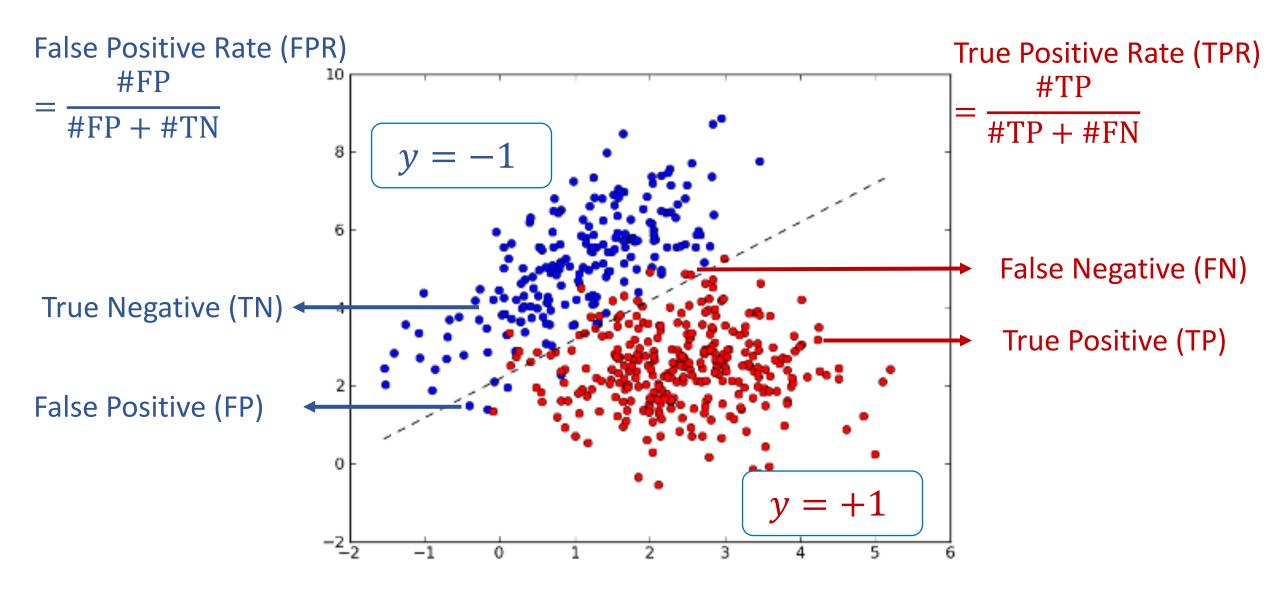
- Error Rate = $\frac{\text{\# Classification Errors}}{\text{\# Samples}}$
- Accuracy = 1 Error Rate

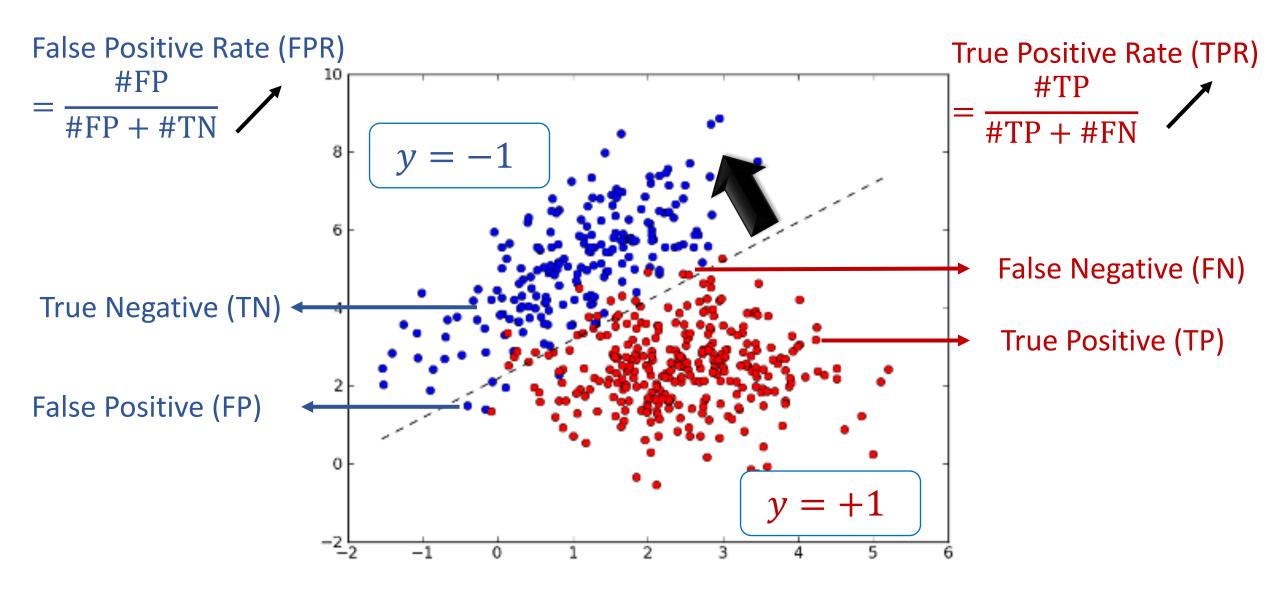
- Error Rate = $\frac{\text{# Classification Errors}}{\text{# Samples}}$
- Accuracy = 1 Error Rate

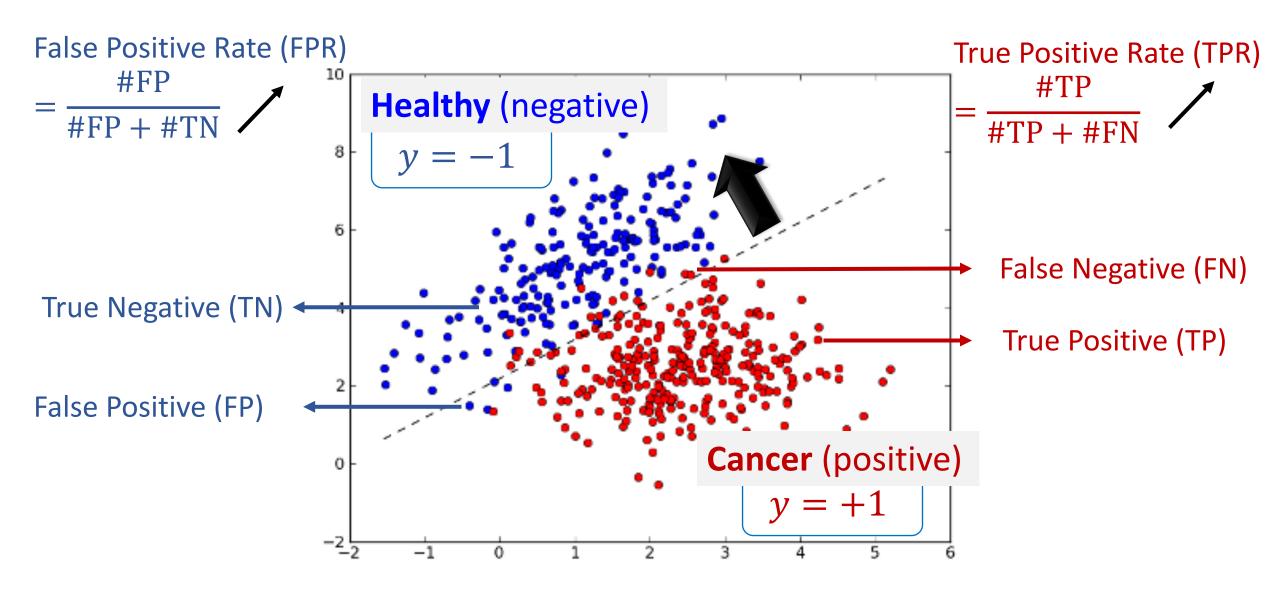
Error rate and Accuracy are not meaningful in class-imbalance problems.

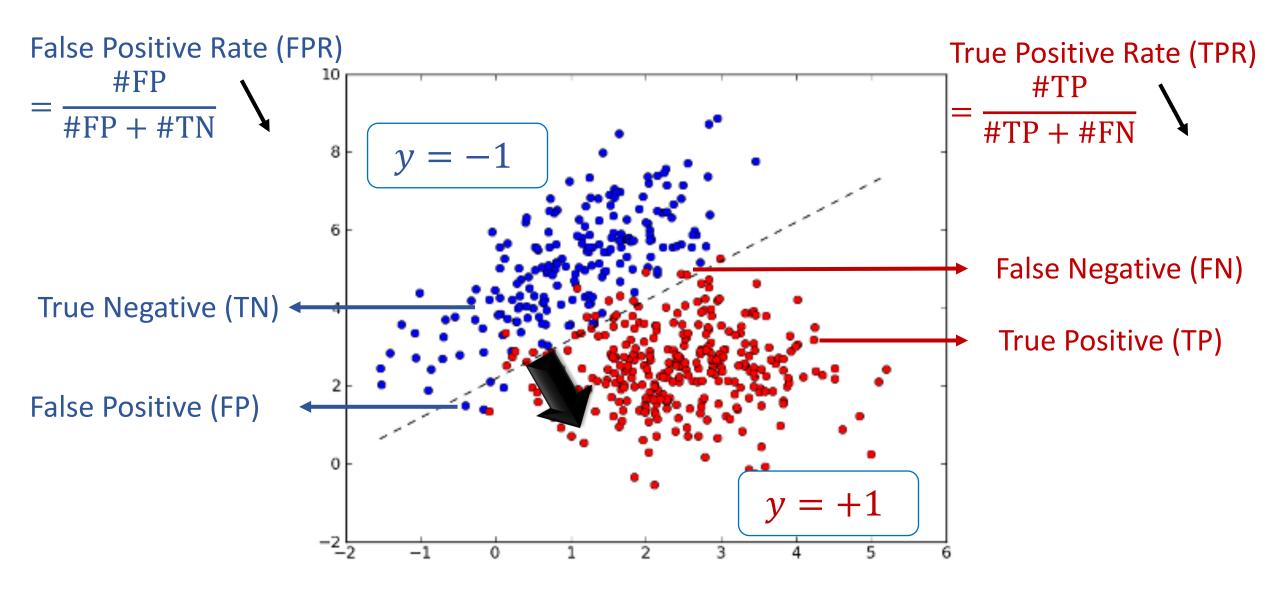


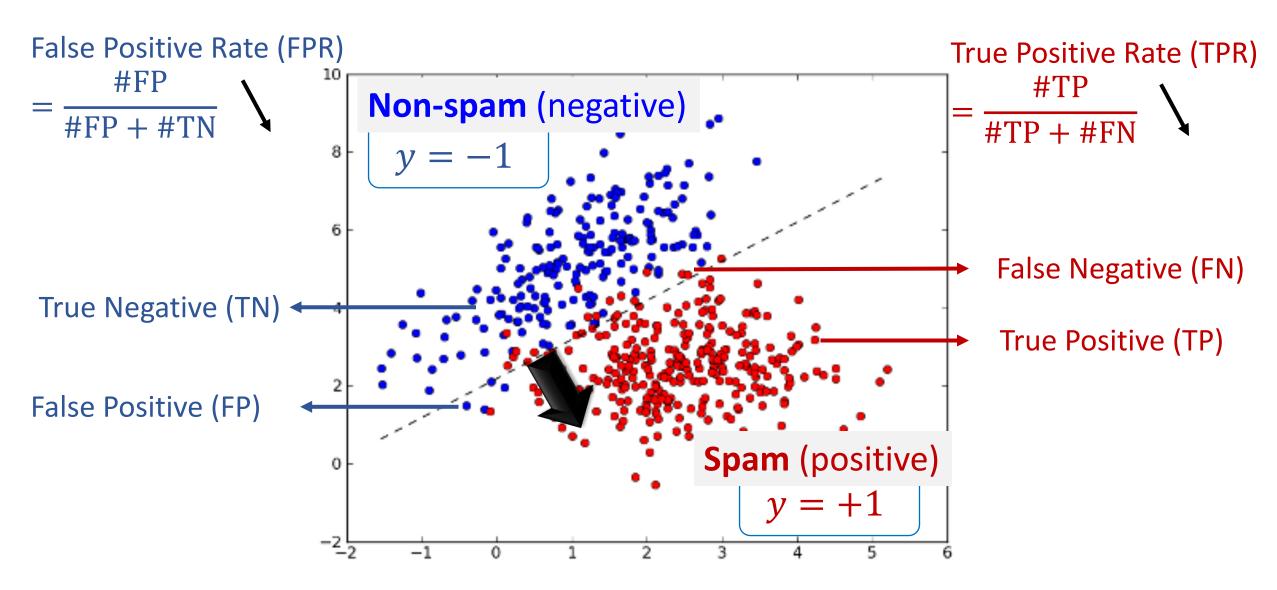


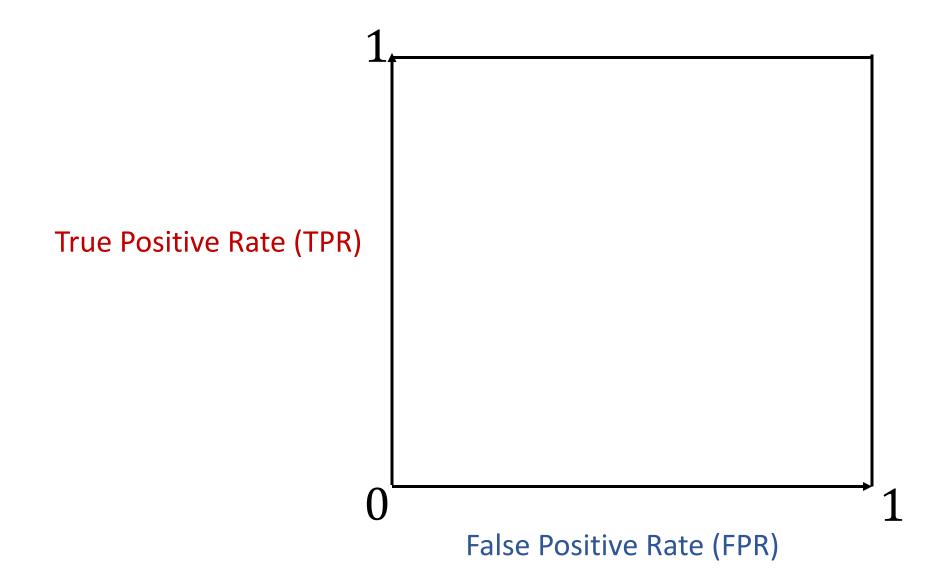


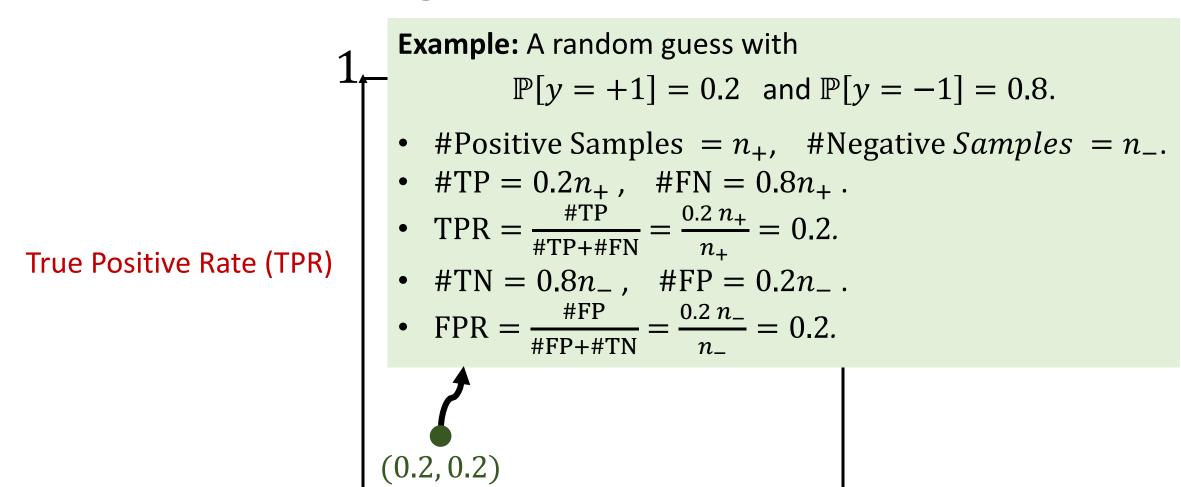












False Positive Rate (FPR)

