

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:

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

Derivative of Scalar w.r.t. Vector

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

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

- Example 1:

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

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:

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

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:

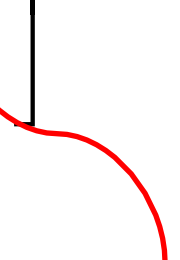
$$y = \sum_{i=1}^m \log(1 + e^{-x_i}), \quad \frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial \log(1+e^{-x_1})}{\partial x_1} \\ \vdots \\ \frac{\partial \log(1+e^{-x_m})}{\partial x_m} \end{bmatrix} = \begin{bmatrix} -\frac{1}{1+e^{x_1}} \\ \vdots \\ -\frac{1}{1+e^{x_m}} \end{bmatrix}$$

Derivative of Vector w.r.t. Vector

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

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

$m \times n$ matrix



- Example 1:

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

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 $\mathbf{x} \in \mathbb{R}^m$:

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_m} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_2}{\partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \frac{\partial y_n}{\partial x_2} & \cdots & \frac{\partial y_n}{\partial x_m} \end{bmatrix} \quad m \times n \text{ matrix}$$

- Example 2:

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

Derivative of Vector w.r.t. Vector

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

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_m} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_2}{\partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \frac{\partial y_n}{\partial x_2} & \cdots & \frac{\partial y_n}{\partial x_m} \end{bmatrix} \quad m \times n \text{ matrix}$$

- Example 3:

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

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 $\mathbf{x} \in \mathbb{R}^{n_x}$.

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

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 $\frac{\partial y}{\partial \mathbf{x}} \in \mathbb{R}^{pq \times 1}$.
 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

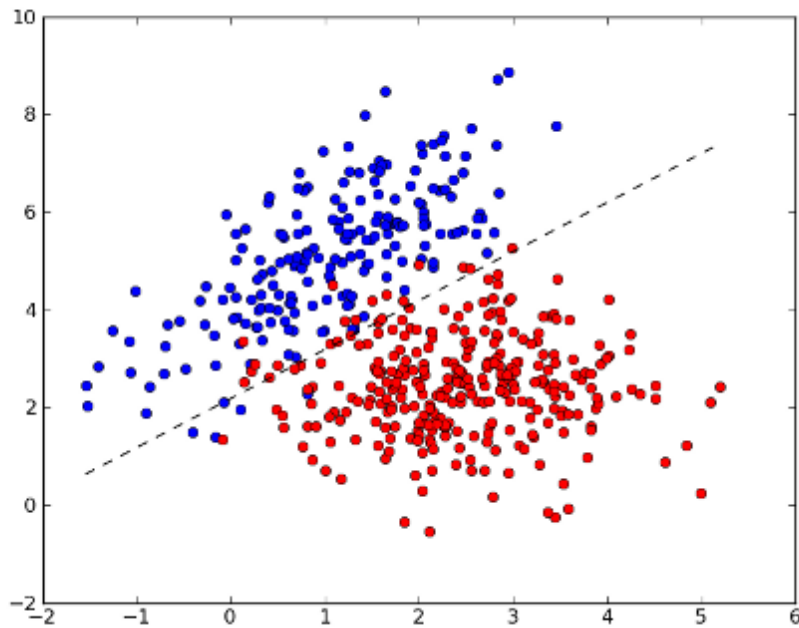
Methods

Algorithms

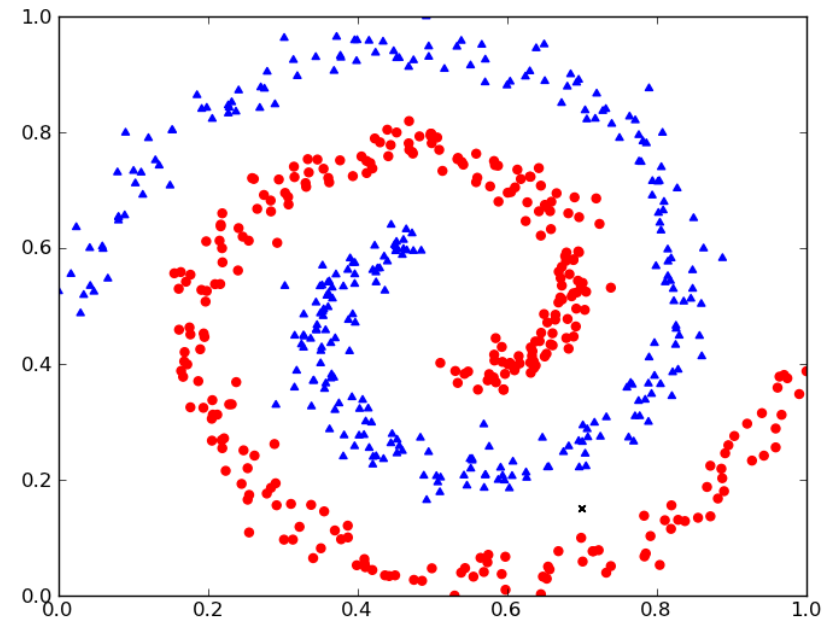
Binary Classification

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



Linear Classification



Nonlinear Classification

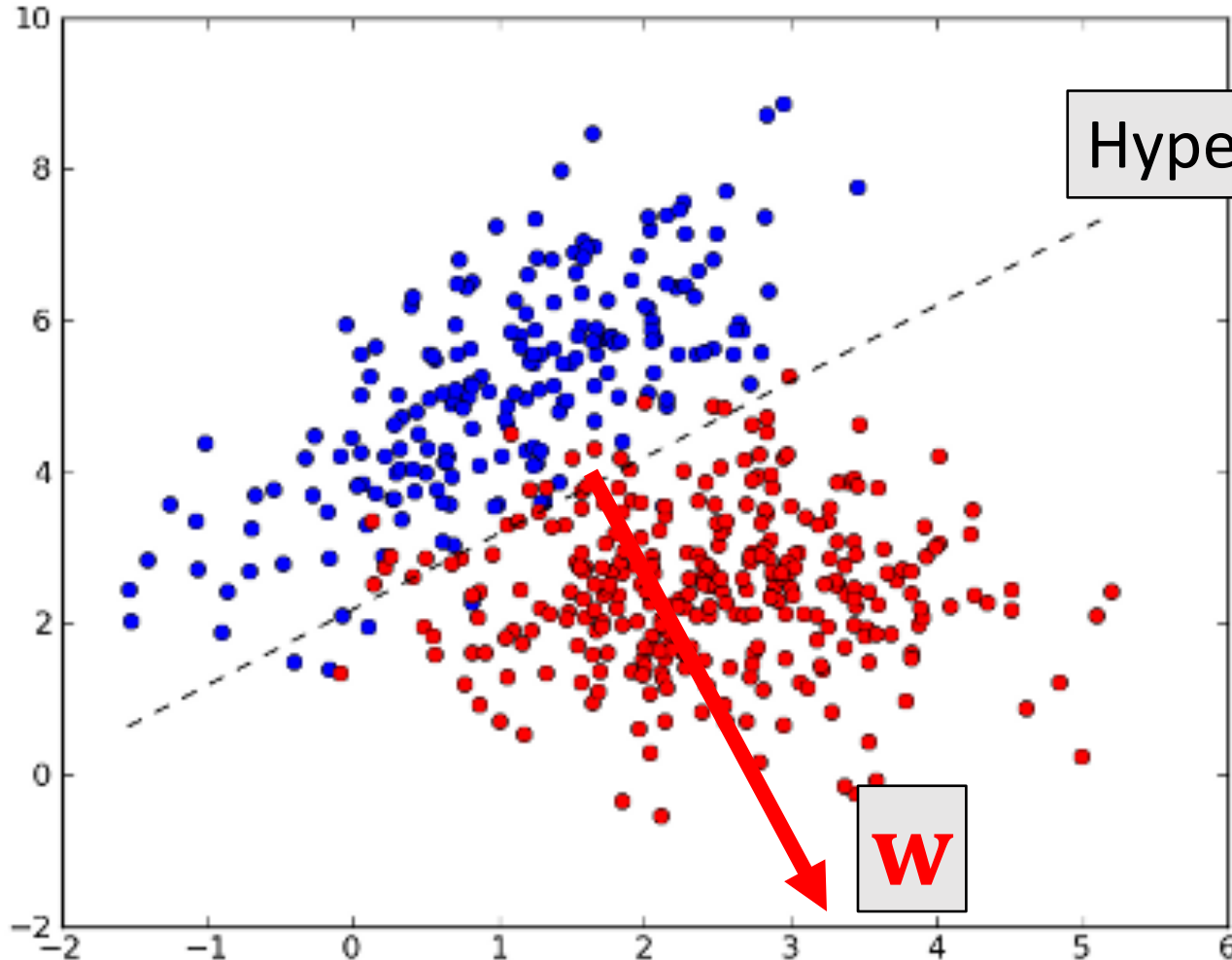
Logistic Regression (Linear Classification)

Tasks

Methods

Algorithms

Linear Classifier



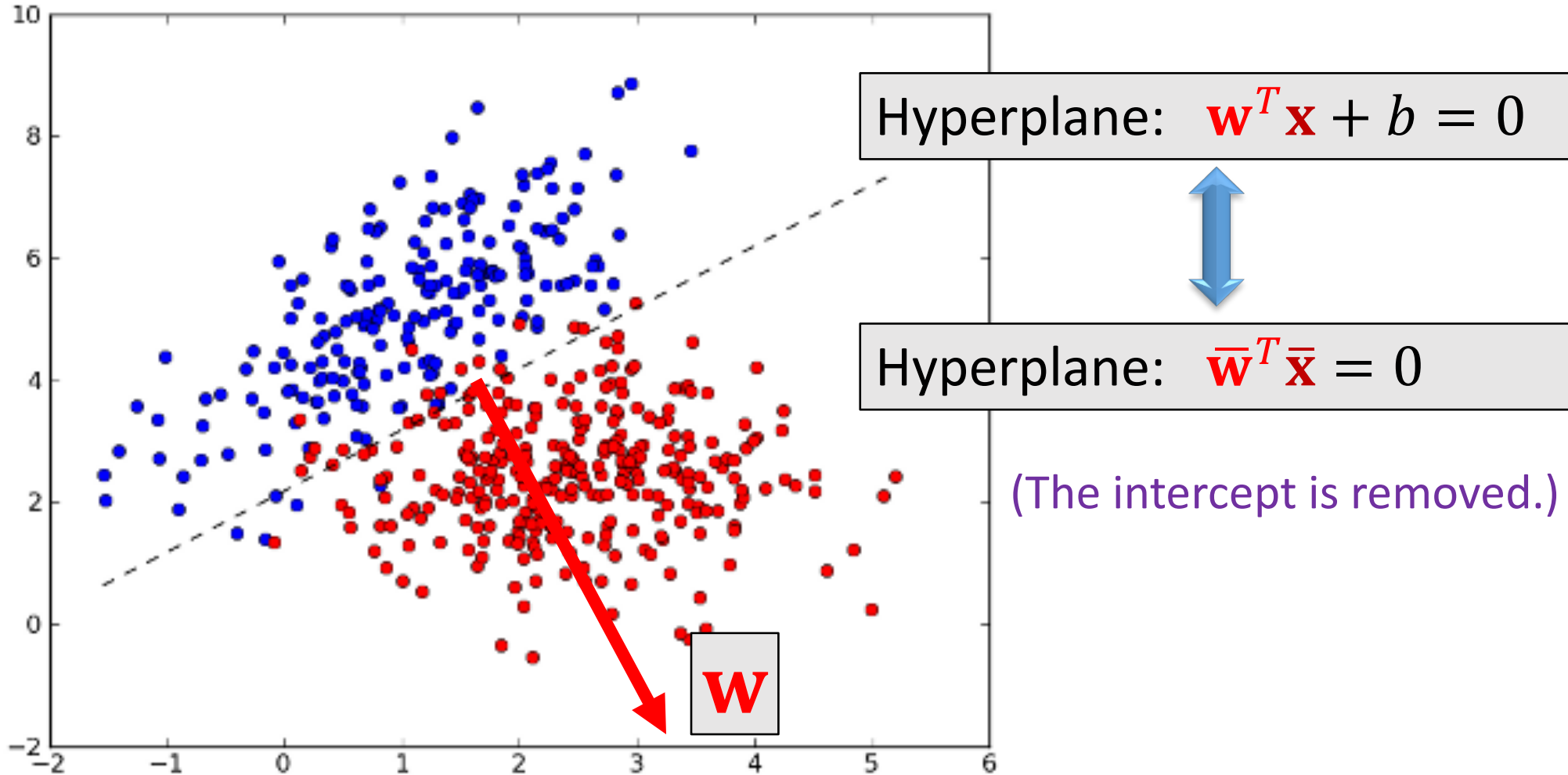
$$\text{Hyperplane: } \mathbf{w}^T \mathbf{x} + b = 0$$

Define $\bar{\mathbf{x}}_j = [\mathbf{x}_j; 1] \in \mathbb{R}^{d+1}$

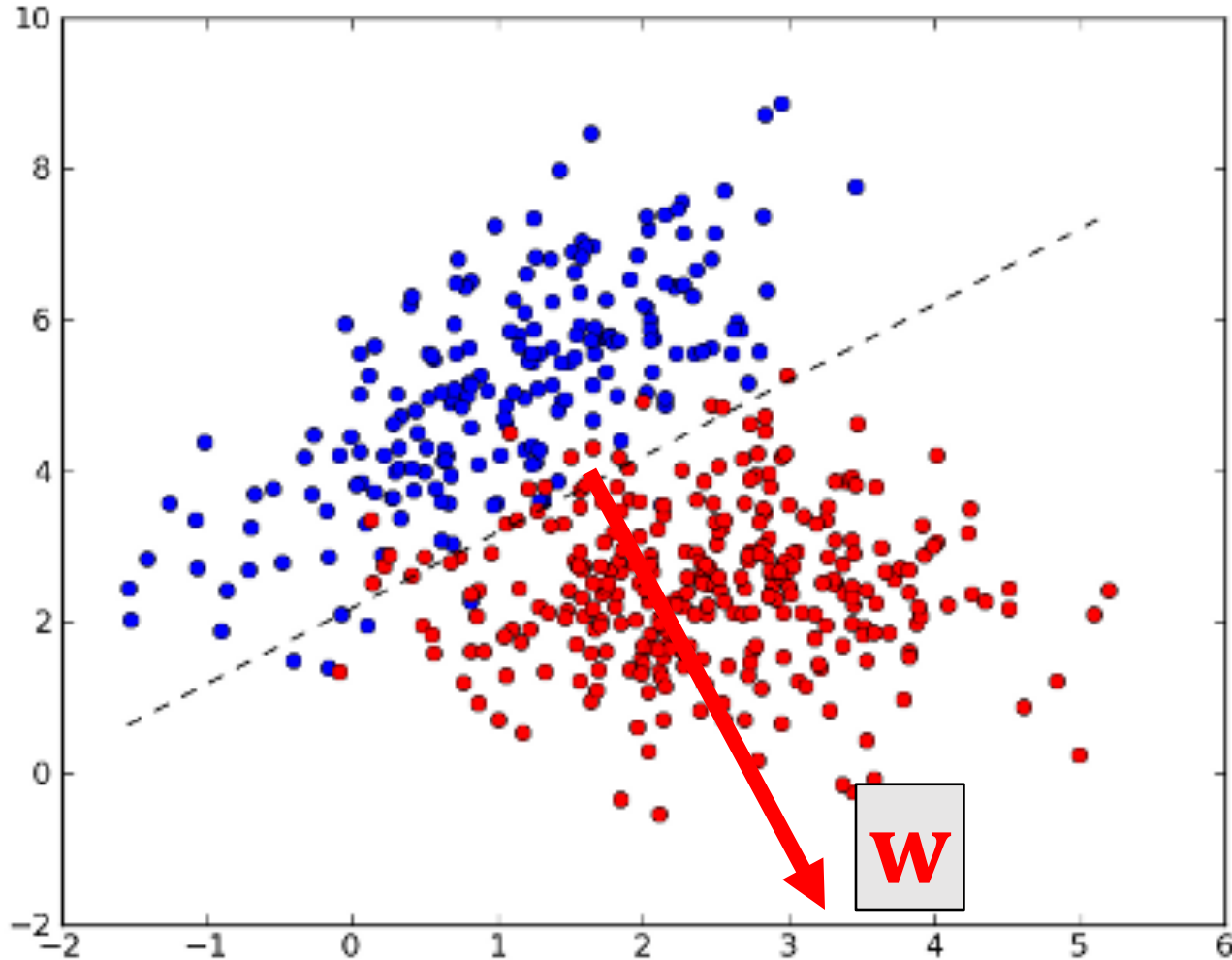
Define $\bar{\mathbf{w}} = [\mathbf{w}, b] \in \mathbb{R}^{d+1}$

$$\Rightarrow \mathbf{x}_j^T \mathbf{w} + b = \bar{\mathbf{x}}_j^T \bar{\mathbf{w}}$$

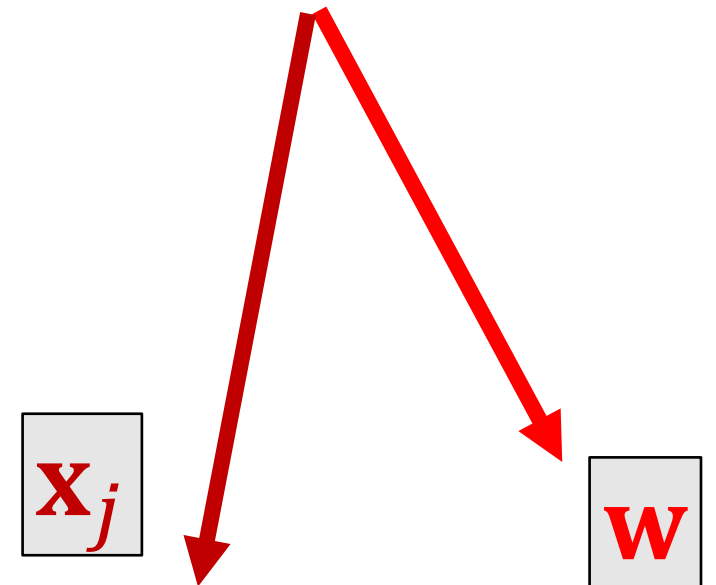
Linear Classifier



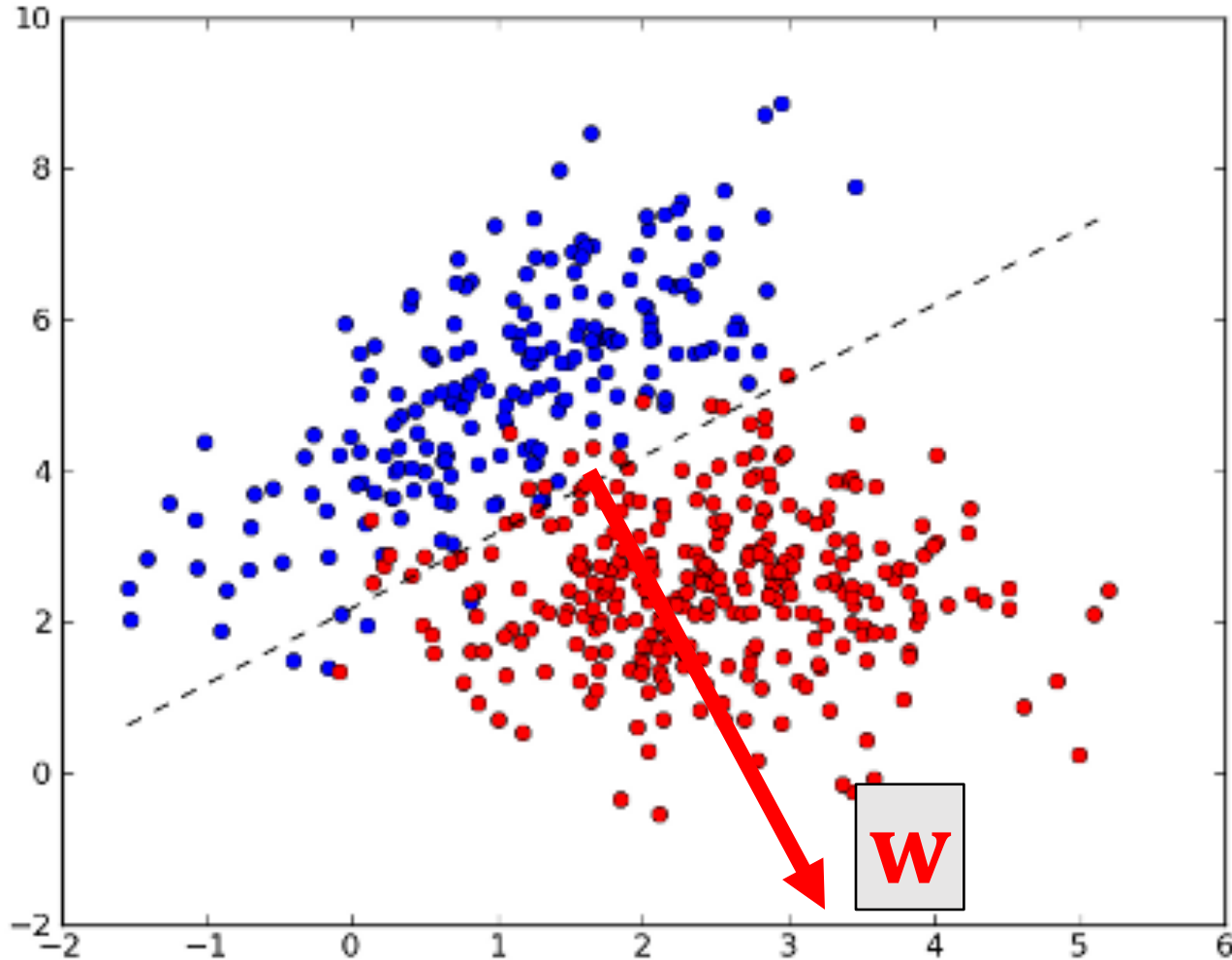
Linear Classifier



- Learn a vector \mathbf{w} such that
- If $y_j = +1$, then $\mathbf{w}^T \mathbf{x}_j > 0$.



Linear Classifier



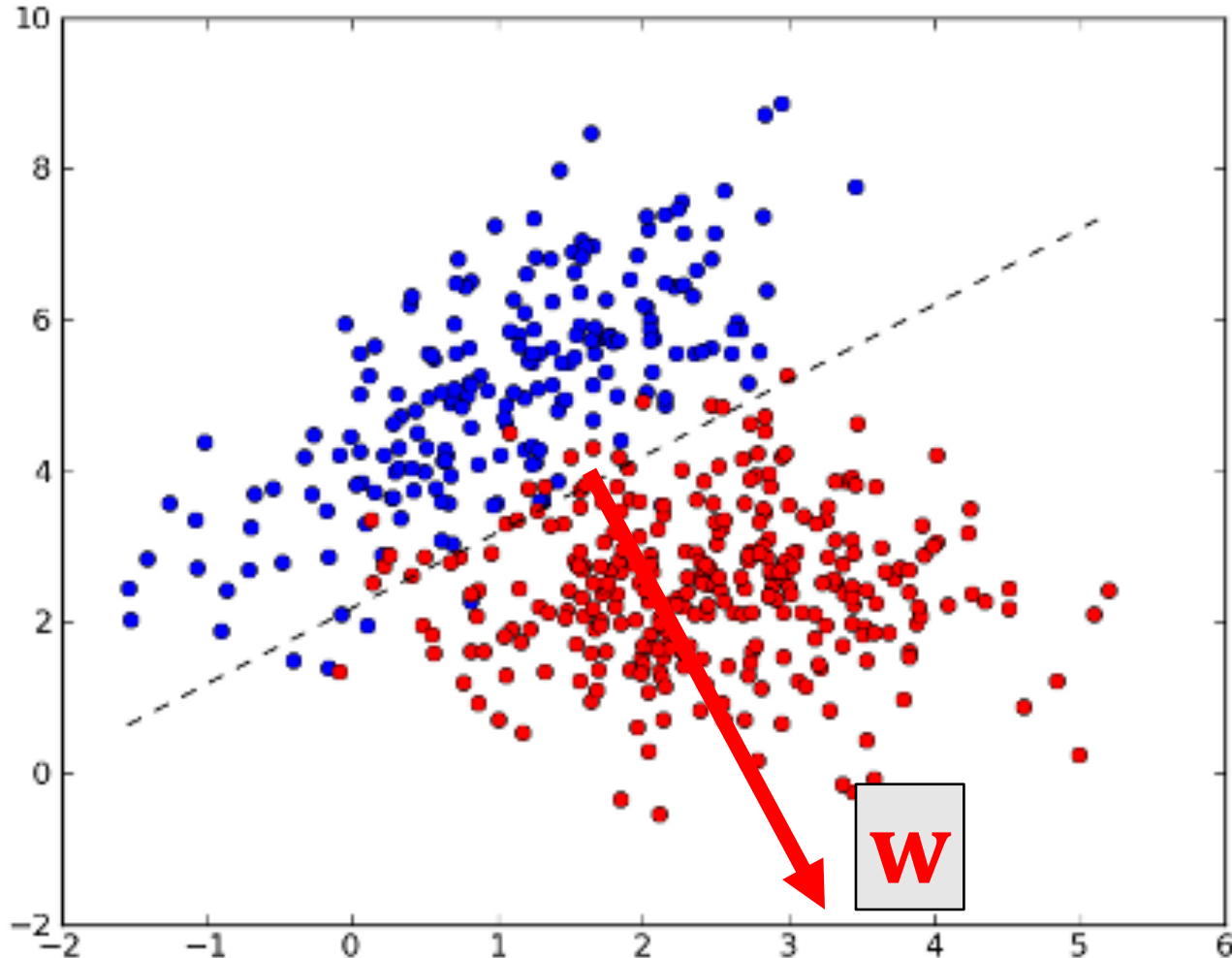
Learn a vector w such that

- If $y_j = +1$, then $w^T x_j > 0$.
- If $y_j = -1$, then $w^T x_j < 0$.

x_j

w

Linear Classifier



Learn a vector \mathbf{w} such that

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

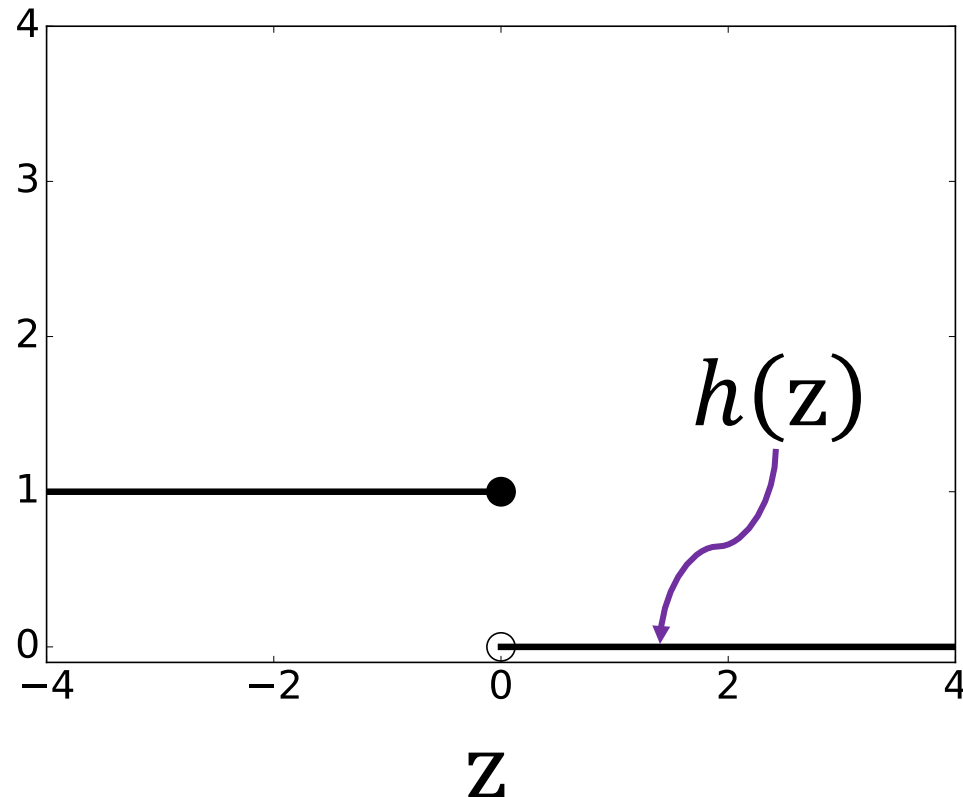


Key Idea:

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

Directly Minimize the Classification Error?

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

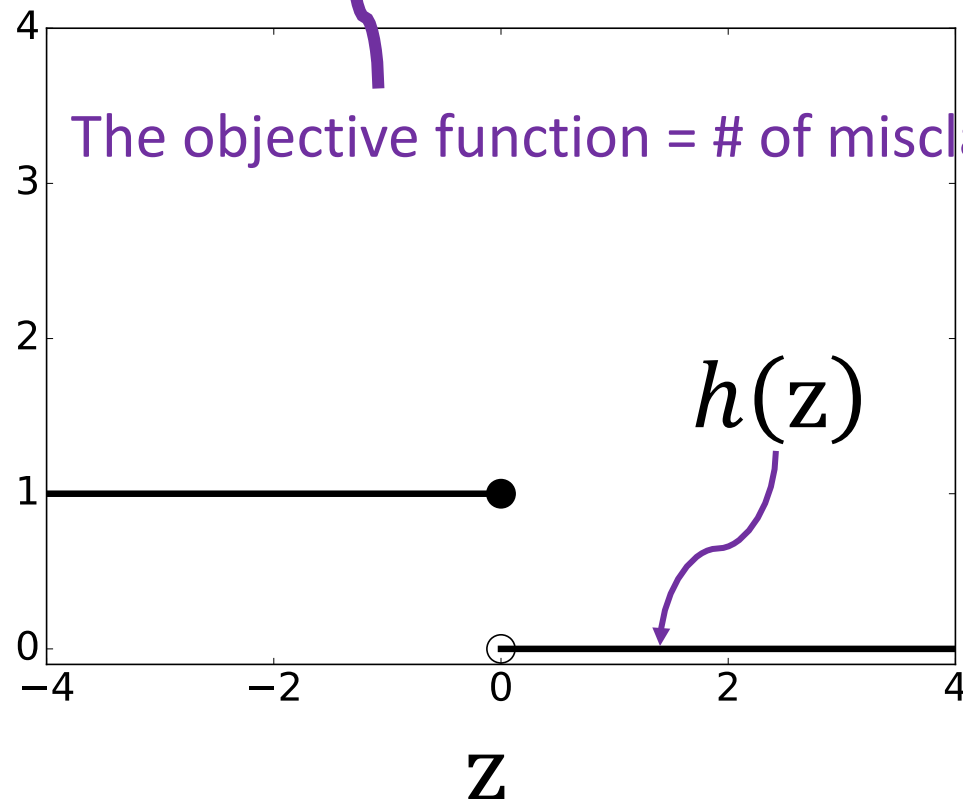


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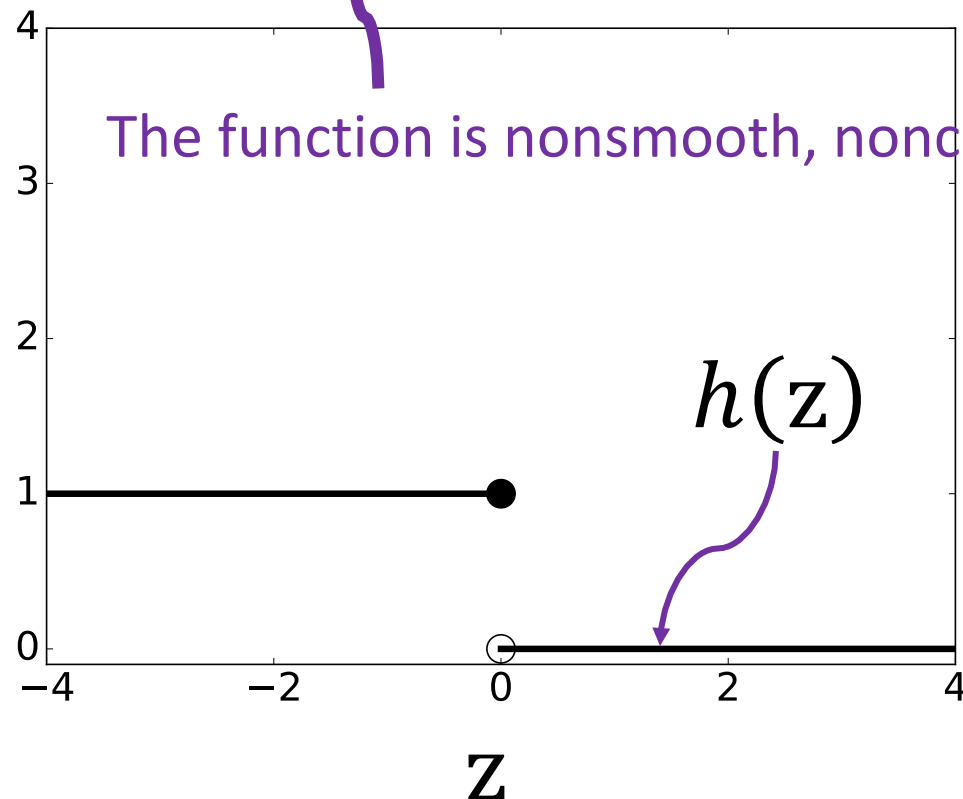
The objective function = # of misclassified training samples

Key Idea:

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

Directly Minimize the Classification Error?

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



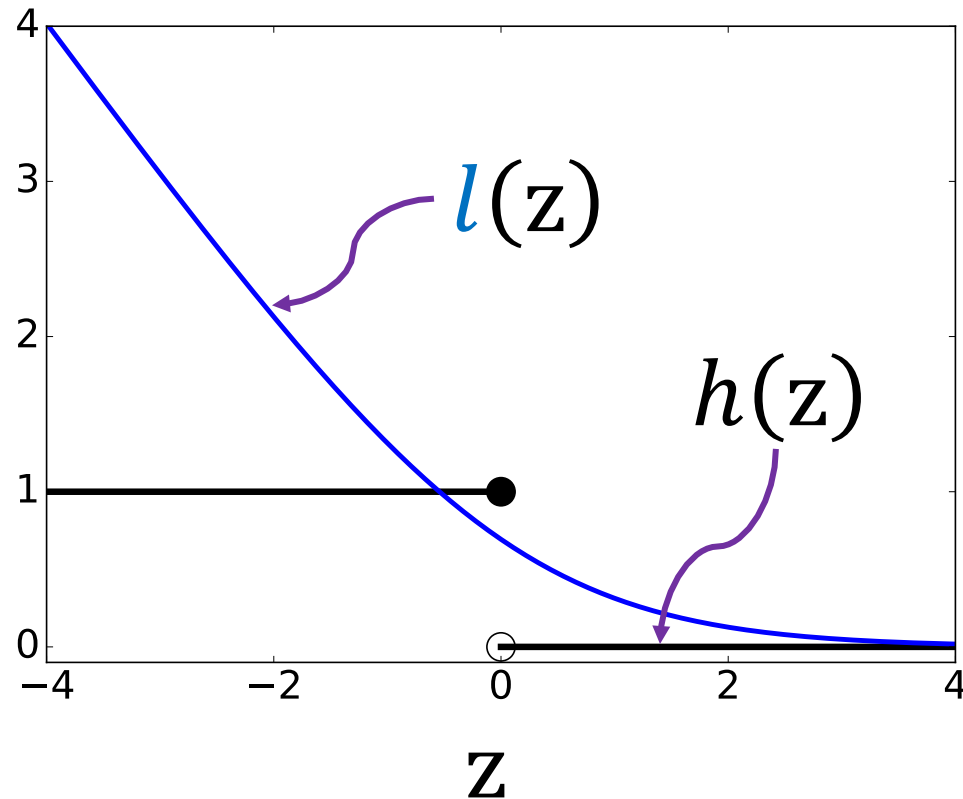
The function is nonsmooth, nonconvex, and hard to optimize.

Key Idea:

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

Logistic Regression

Minimize $\sum_j l(y_j \mathbf{w}^T \mathbf{x}_j)$, where $l(z) = \log(1 + e^{-z})$.



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 $l(z) = \log(1 + e^{-z})$.

Tasks

Binary Classification

Multi-Class Classification

Methods

Logistic Regression

SVM

Neural Networks

Algorithms

Gradient Descent (GD)

Accelerated GD

Stochastic GD

Logistic Regression

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

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

- $\frac{\partial l(z)}{\partial z} = \frac{-e^{-z}}{1+e^{-z}} = -\frac{1}{1+e^z}.$
- 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

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

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

- We have shown: $\frac{\partial l(y_j \mathbf{w}^T \mathbf{x}_j)}{\partial \mathbf{w}} = - \frac{y_j \mathbf{x}_j}{1 + \exp(-y_j \mathbf{w}^T \mathbf{x}_j)}$
- 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

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

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

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

Stochastic GD

Logistic Regression

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

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

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 ($0 \leq \beta < 1$)

Algorithms

Gradient Descent (GD)

Accelerated GD

Stochastic GD

Logistic Regression

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

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 $\mathbf{w}_t^T \mathbf{x}_j$
- $O(d)$ 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

Stochastic GD

Logistic Regression

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

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:

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

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

Algorithms

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

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: $\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \tilde{\mathbf{g}}_{t,j}$.

Per-iteration time complexity is $O(d)$.

Algorithms

Gradient Descent (GD)

Accelerated GD

Stochastic GD

Logistic Regression

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

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

Stochastic GD

Logistic Regression

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

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 \mathbf{w} produced by the last tens of iteration.

Algorithms

Gradient Descent (GD)

Accelerated GD

Stochastic GD

Training and Prediction

- Training:

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

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

Summary

- Logistic regression model for *linear binary* classification.

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

- Compute the gradient using vector derivatives and the chain rule.
- Gradient-based algorithms: GD, AGD, SGD, etc.
- Make prediction using $\operatorname{sign}(\mathbf{x}'^T \mathbf{w}^*)$.

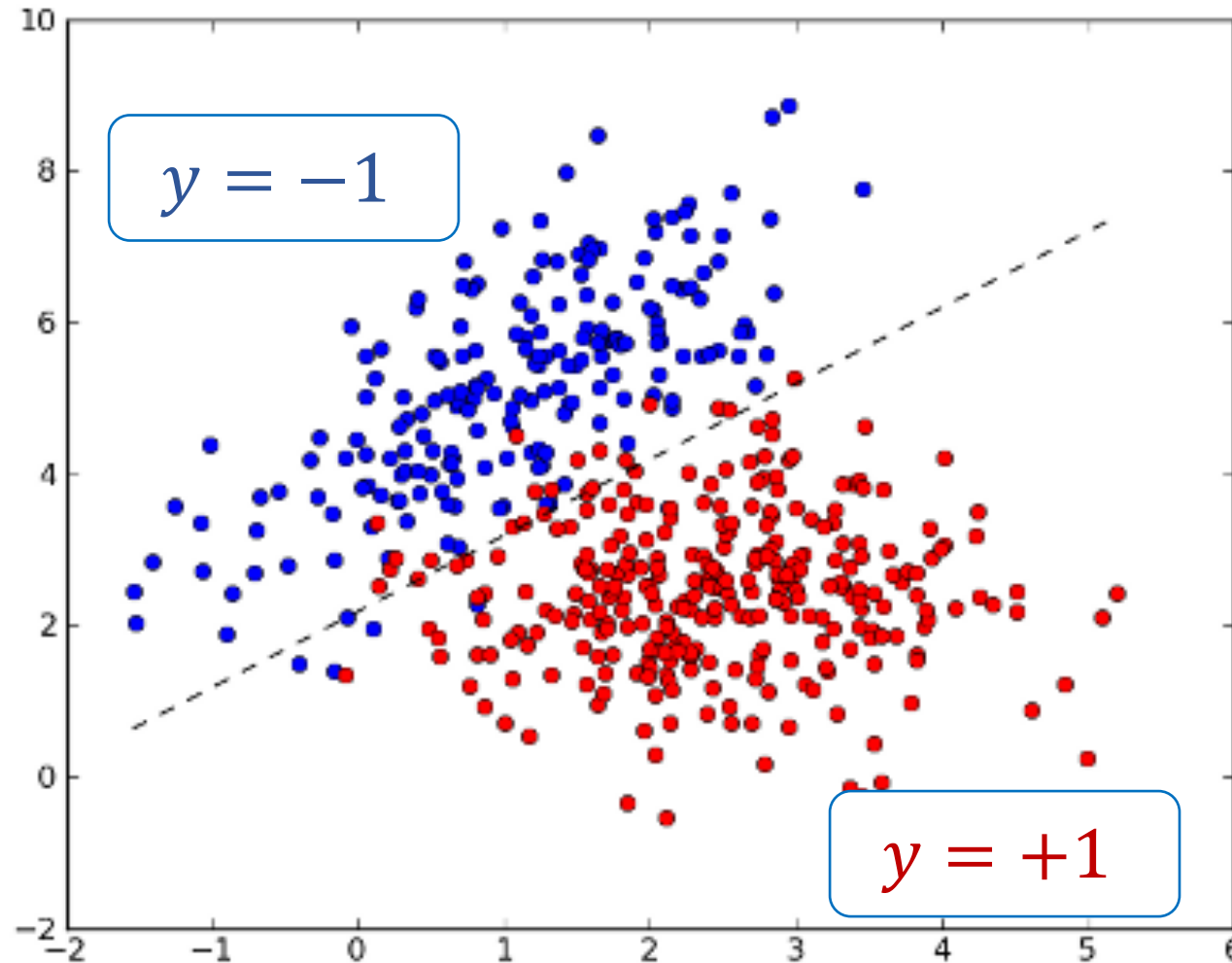
Evaluate Binary Classification

Evaluate Binary Classification

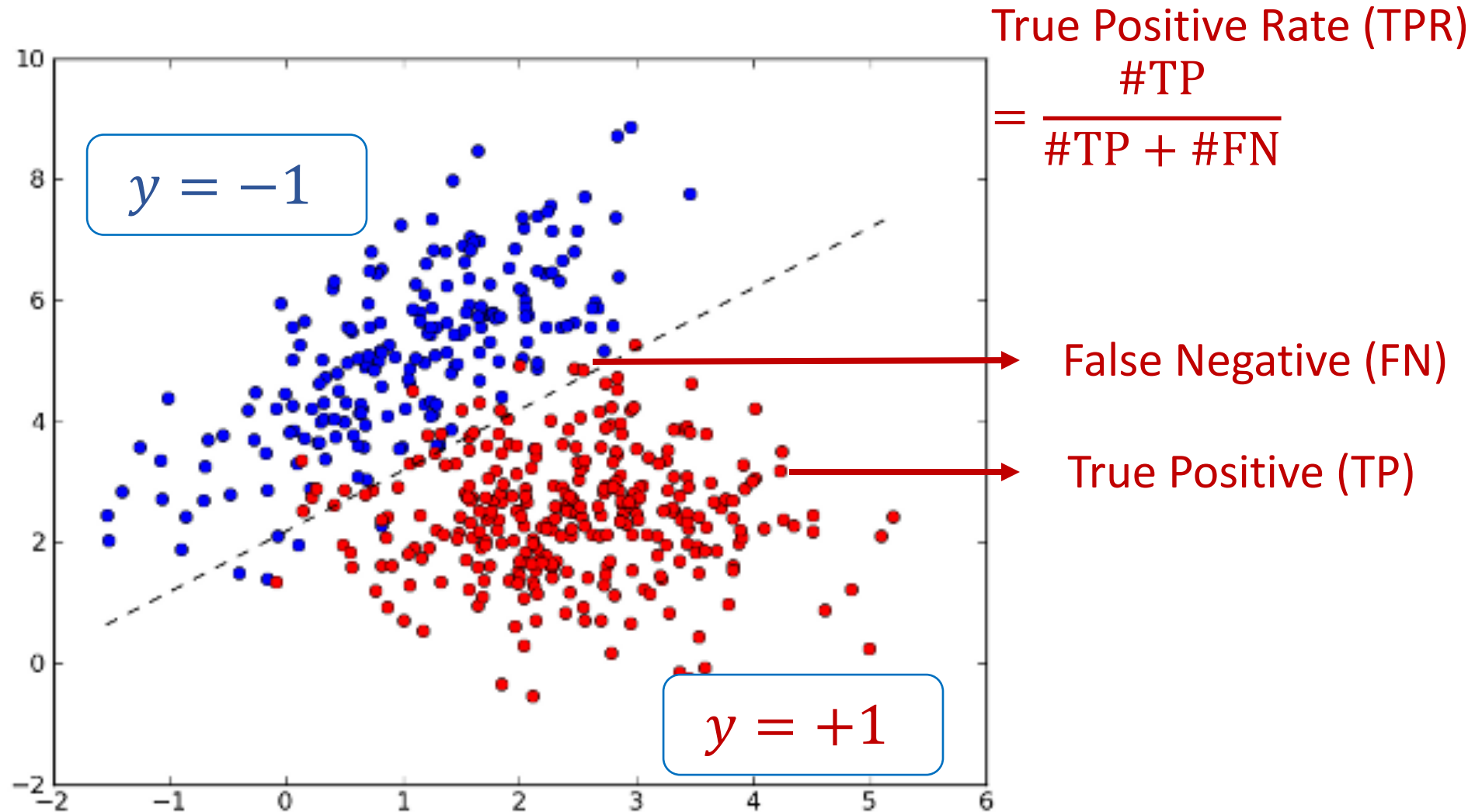
- Error Rate = $\frac{\text{\# Classification Errors}}{\text{\# Samples}}$
- Accuracy = 1 - Error Rate

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

Evaluate Binary Classification



Evaluate Binary Classification



Evaluate Binary Classification

False Positive Rate (FPR)

$$= \frac{\#FP}{\#FP + \#TN}$$

True Positive Rate (TPR)

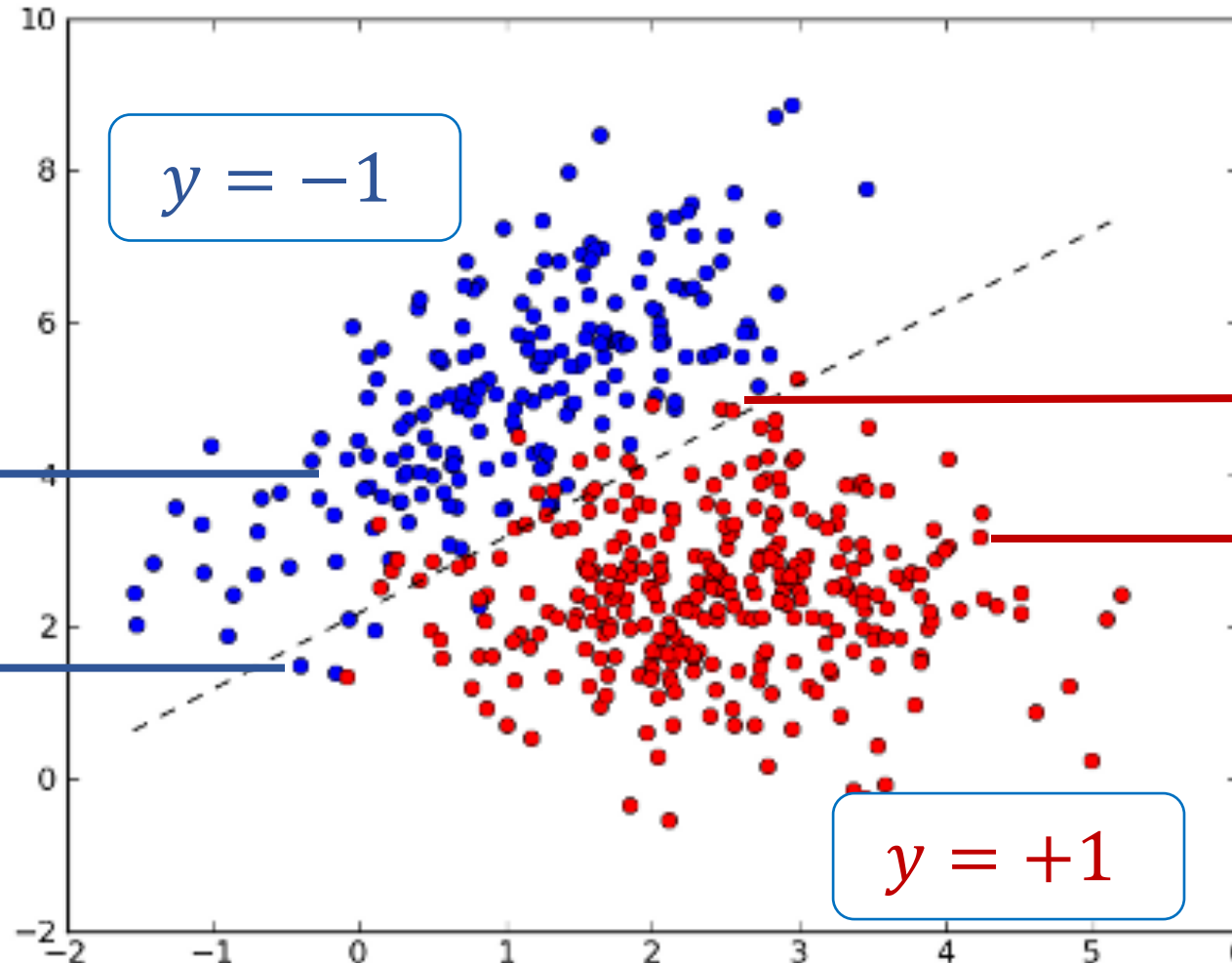
$$= \frac{\#TP}{\#TP + \#FN}$$

True Negative (TN)

False Positive (FP)

False Negative (FN)

True Positive (TP)



Evaluate Binary Classification

False Positive Rate (FPR)

$$= \frac{\#FP}{\#FP + \#TN}$$

True Negative (TN)

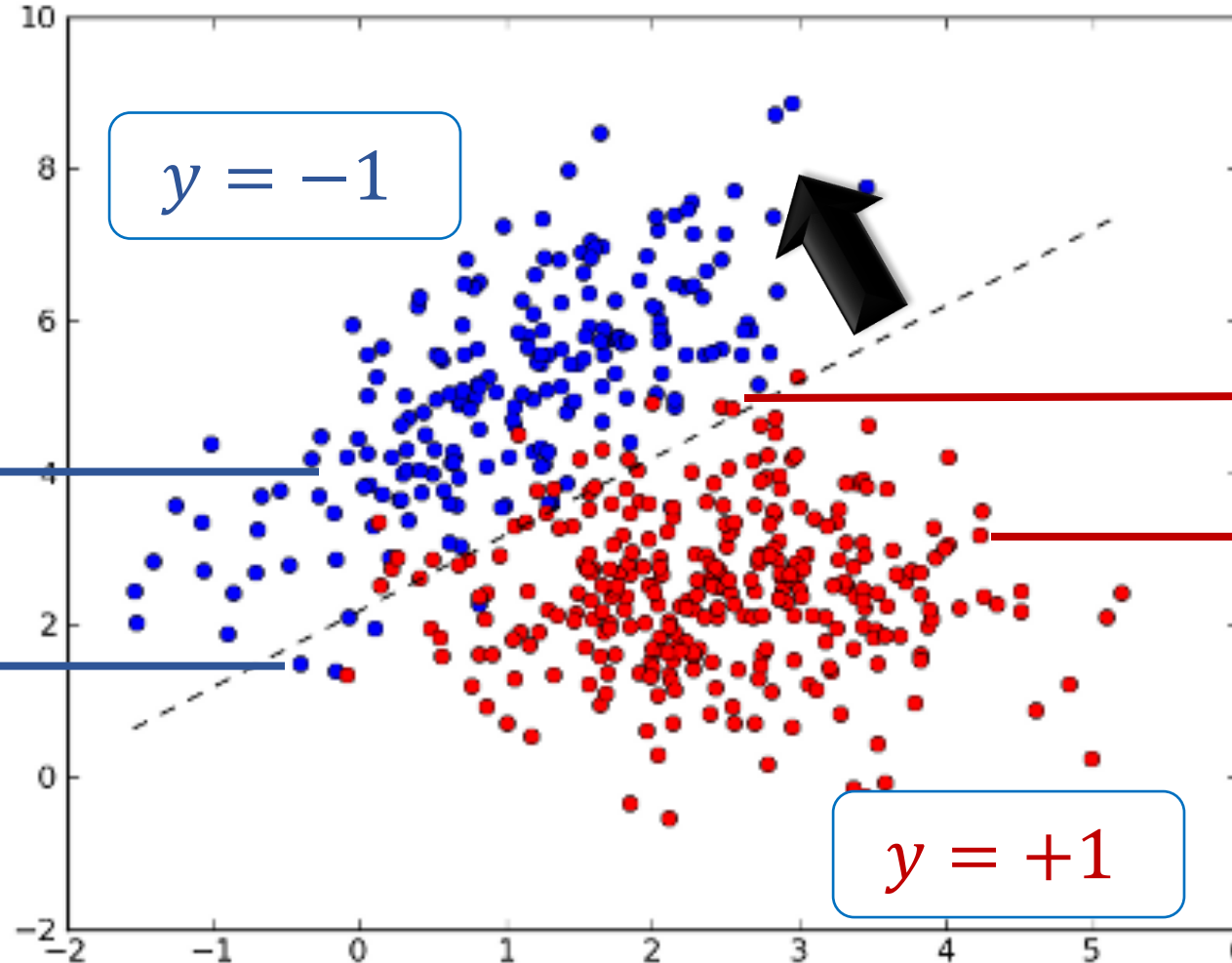
False Positive (FP)

True Positive Rate (TPR)

$$= \frac{\#TP}{\#TP + \#FN}$$

False Negative (FN)

True Positive (TP)



Evaluate Binary Classification

False Positive Rate (FPR)

$$= \frac{\#FP}{\#FP + \#TN}$$

True Positive Rate (TPR)

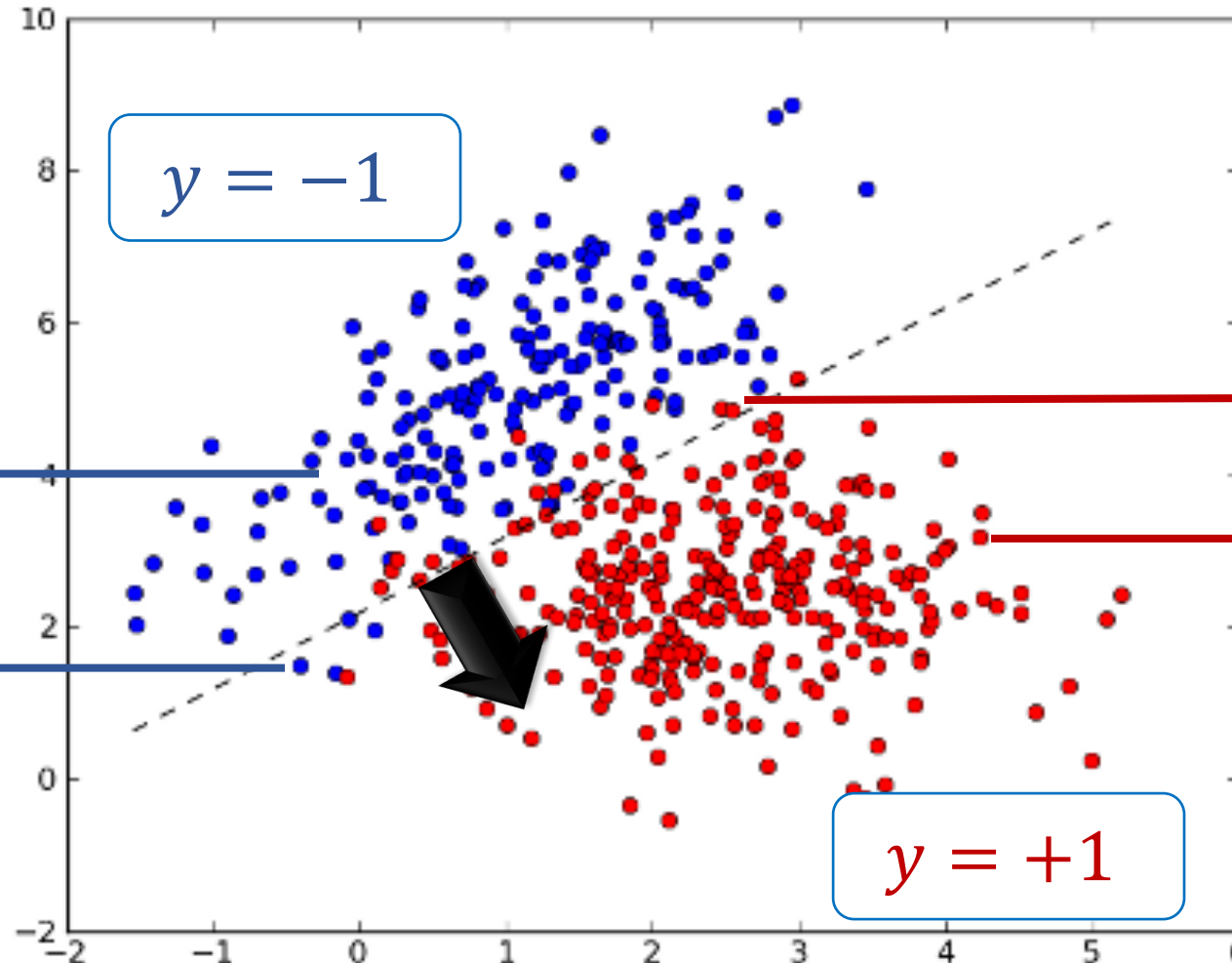
$$= \frac{\#TP}{\#TP + \#FN}$$

True Negative (TN)

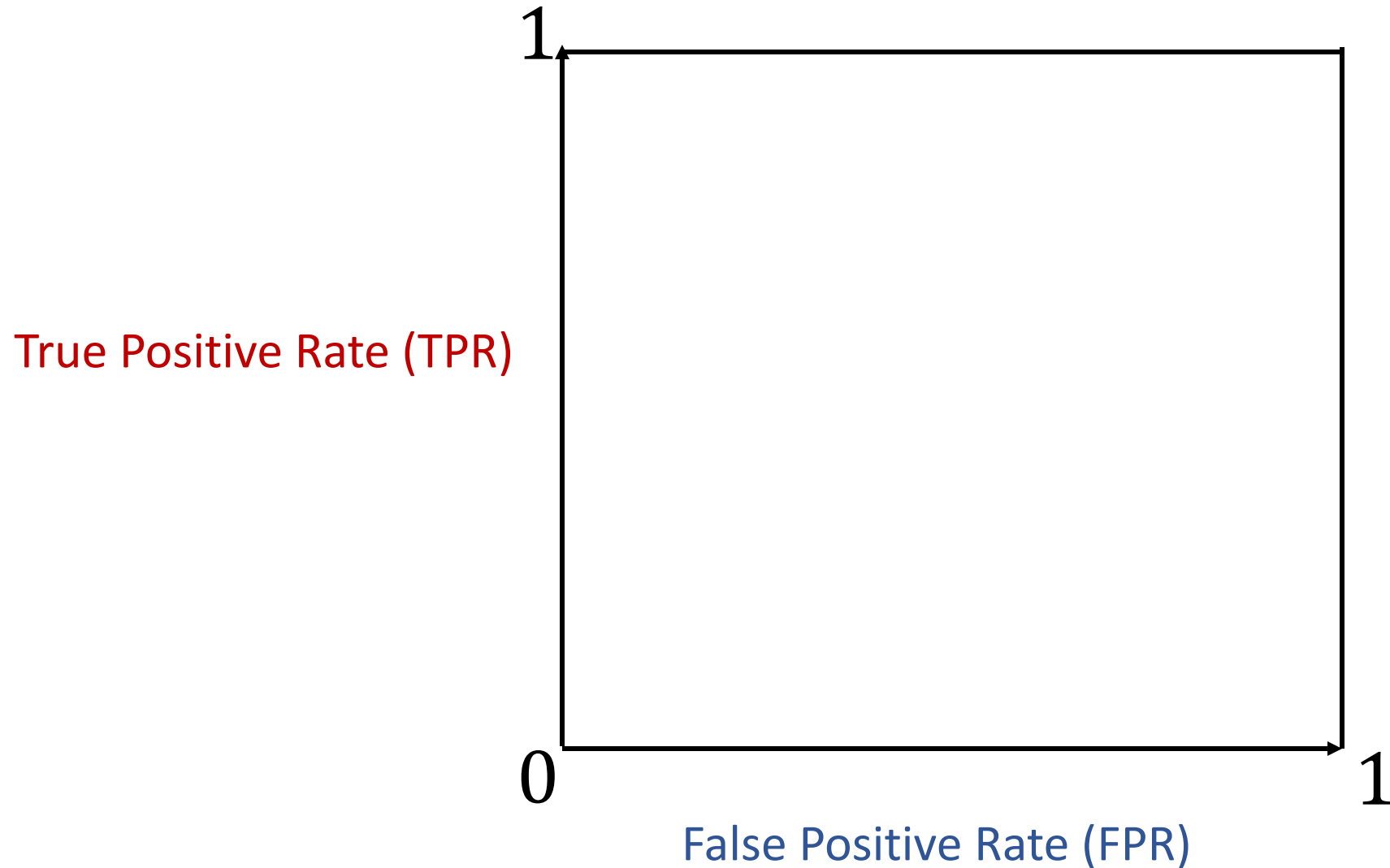
False Positive (FP)

False Negative (FN)

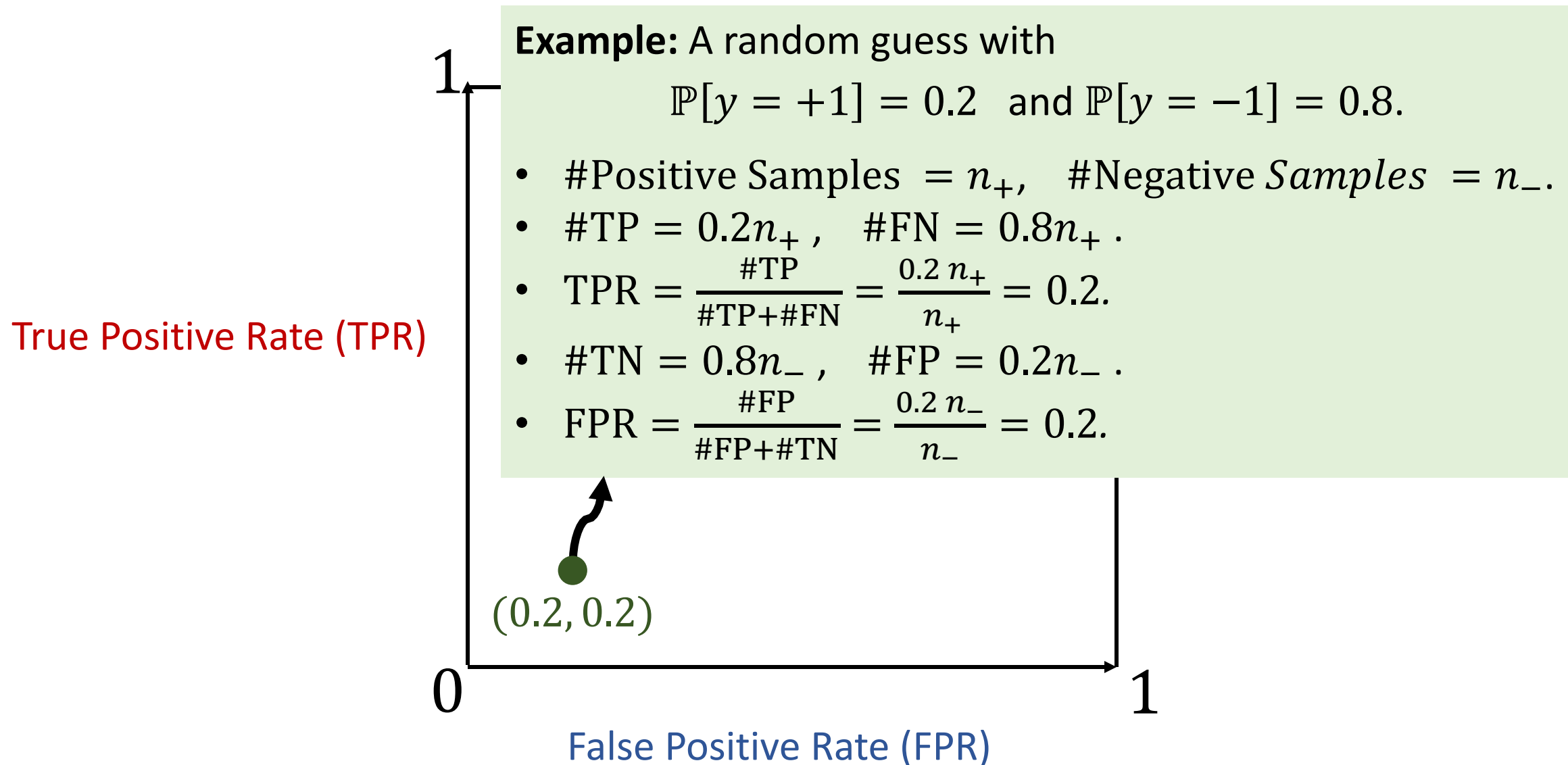
True Positive (TP)



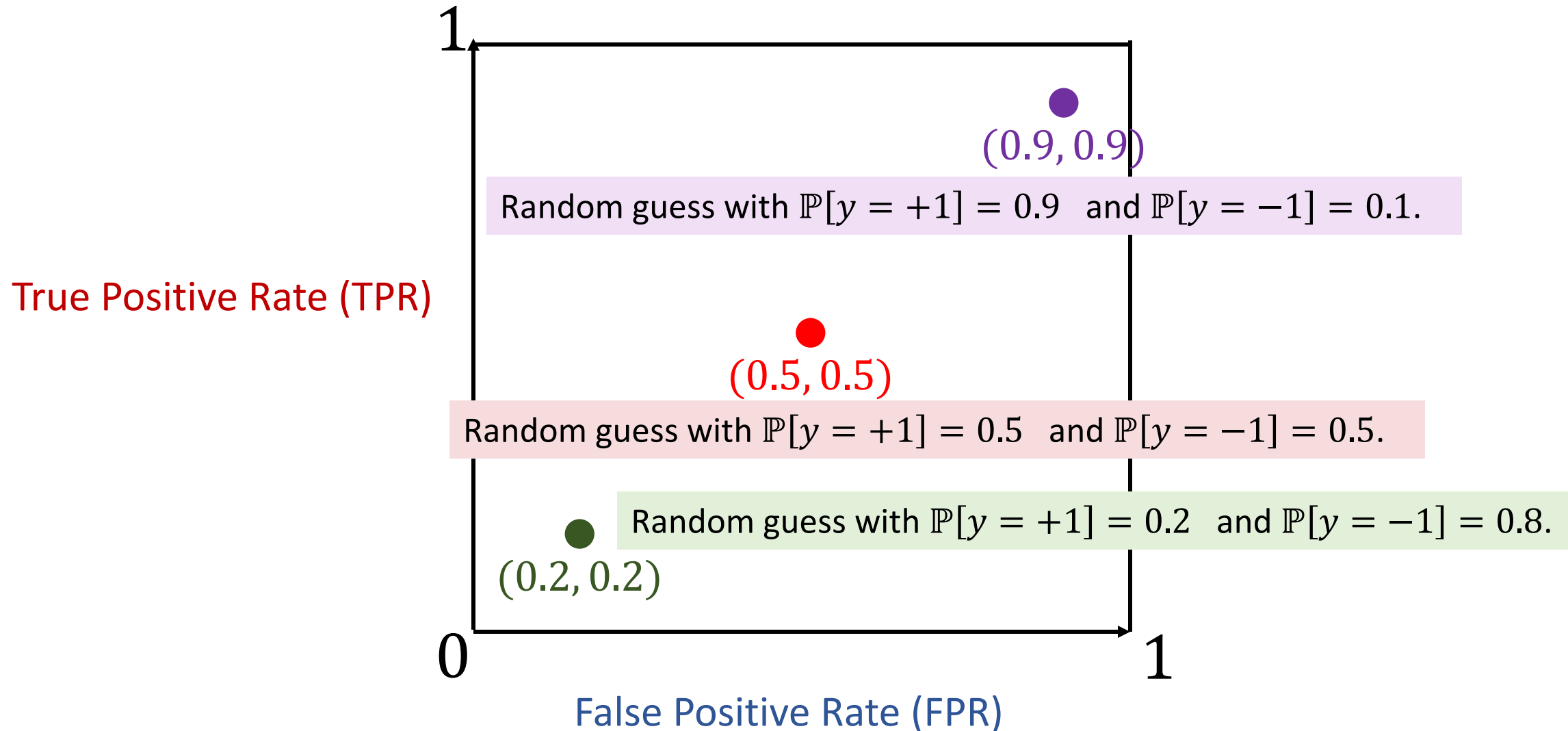
Receiver Operating Characteristic (ROC) Curve



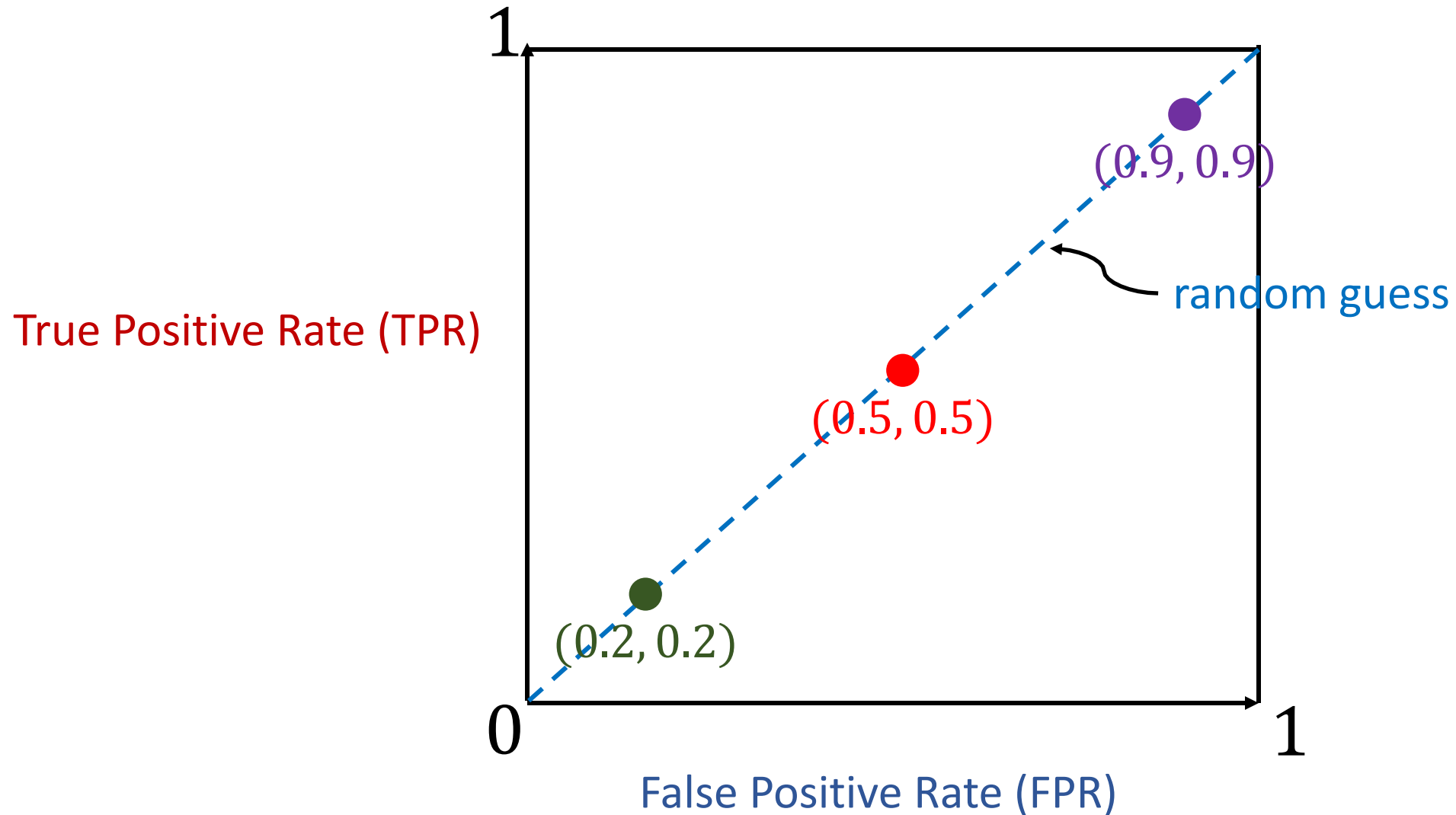
Receiver Operating Characteristic (ROC) Curve



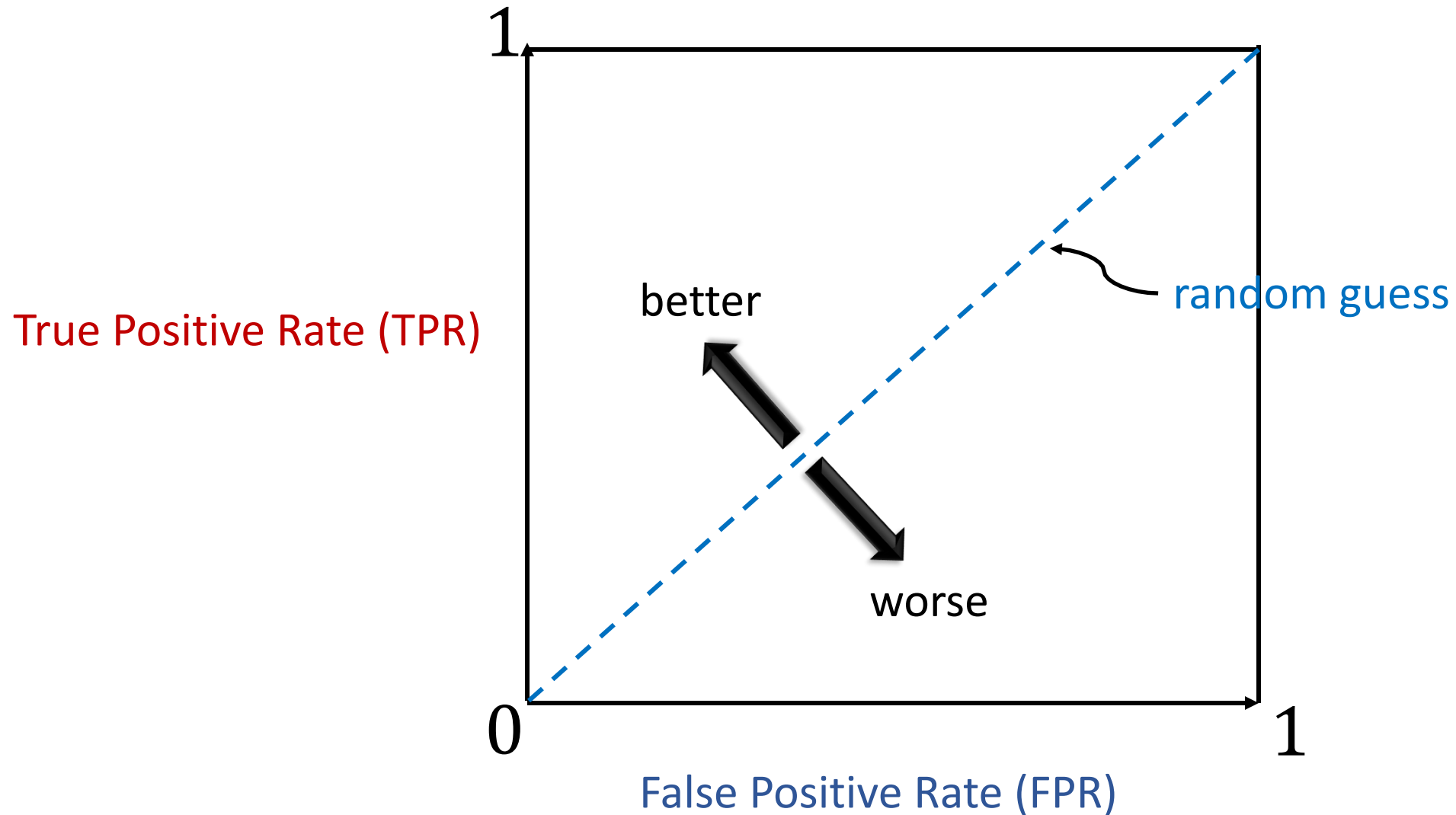
Receiver Operating Characteristic (ROC) Curve



Receiver Operating Characteristic (ROC) Curve



Receiver Operating Characteristic (ROC) Curve



Receiver Operating Characteristic (ROC) Curve

