

COMP5211: Machine Learning

Lecture 2

Minhao Cheng

Last lecture

Matrix Derivates

- Before we have $df = f'(x)dx$
- In the vector view:

- Scalar to vector: $df = \sum_{i=1}^n \frac{\partial f}{\partial x_i} dx_i = \frac{\partial f^T}{\partial x} dx$ where $\frac{\partial f}{\partial x}$ and dx are $n \times 1$ vector

- Similarly, scalar to matrix: $df = \sum_{i=1}^m \sum_{j=1}^n \frac{\partial f}{\partial X_{ij}} dX_{ij} = \text{tr}\left(\frac{\partial f^T}{\partial X} dX\right)$

- For the derivate, we also have $d(X \pm Y) = dX \pm dY$, $d(XY) = (dX)Y + XdY$, $d(X^T) = (dX)^T$, $d\text{tr}(X) = \text{tr}(dX)$, $dX^{-1} = -X^{-1}dXX^{-1}$

- For the trace operation, we also have $a = \text{tr}(a)$, $\text{tr}(A \pm B) = \text{tr}(A) \pm \text{tr}(B)$, $\text{tr}(AB) = \text{tr}(BA)$, $\text{tr}(A^T(B \odot C)) = \text{tr}((A \odot B)^T C)$

Last lecture

Matrix Derivates

- Chain rule: f is a function of Y , let $Y=AXB$, to get $\frac{\partial f}{\partial X}$
- $df = tr\left(\frac{\partial f^T}{\partial Y} dY\right) = tr\left(\frac{\partial f^T}{\partial Y} AdXB\right) = tr\left(B\frac{\partial f^T}{\partial Y} AdX\right) = tr\left(\left(A^T\frac{\partial f}{\partial Y}B^T\right)^T dX\right)$
- Since $dY = (dA)XB + A(dX)B + AX(dB) = A(dX)B$ as $dA = 0, dB = 0$
- So we get $\frac{\partial f}{\partial X} = A^T\frac{\partial f}{\partial Y}B^T$

Last lecture

Matrix calculus

- $f = \|Xw - y\|^2$, solve $\frac{\partial f}{\partial w}$, where y is $m \times 1$ vector, X is $m \times n$ matrix, w is $n \times 1$ vector

- $$df = d(\|Xw - y\|^2) = d((Xw - y)^T(Xw - y)) = d((Xw - y)^T)(Xw - y) + (Xw - y)^T d(Xw - y)$$
$$= (Xdw)^T(Xw - y) + (Xw - y)^T(Xdw) = 2(Xw - y)^T Xdw$$

- So $\frac{\partial f}{\partial w} = 2X^T(Xw - y)$

Regression

Example

- Classification:
 - Customer record \longrightarrow Yes/No
- Regression: predicting credit limit
 - Customer record \longrightarrow dollar amount

Regression

Linear regression

- Classification:
 - Customer record \longrightarrow Yes/No
- Regression: predicting credit limit
 - Customer record \longrightarrow dollar amount
- Linear Regression:

$$\bullet \quad h(x) = \sum_{i=0}^d w_i x_i = w^T x$$

Linear Regression

The data set

- Training data:
 - $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$
 - $x_n \in \mathbb{R}^d$: feature vector for a sample
 - $y_n \in \mathbb{R}$: observed output (real number)

Linear Regression

The data set

- Training data:
 - $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$
 - $x_n \in \mathbb{R}^d$: feature vector for a sample
 - $y_n \in \mathbb{R}$: observed output (real number)
- Linear regression: find a function $h(x) = w^T x$ to approximate y

Linear Regression

The data set

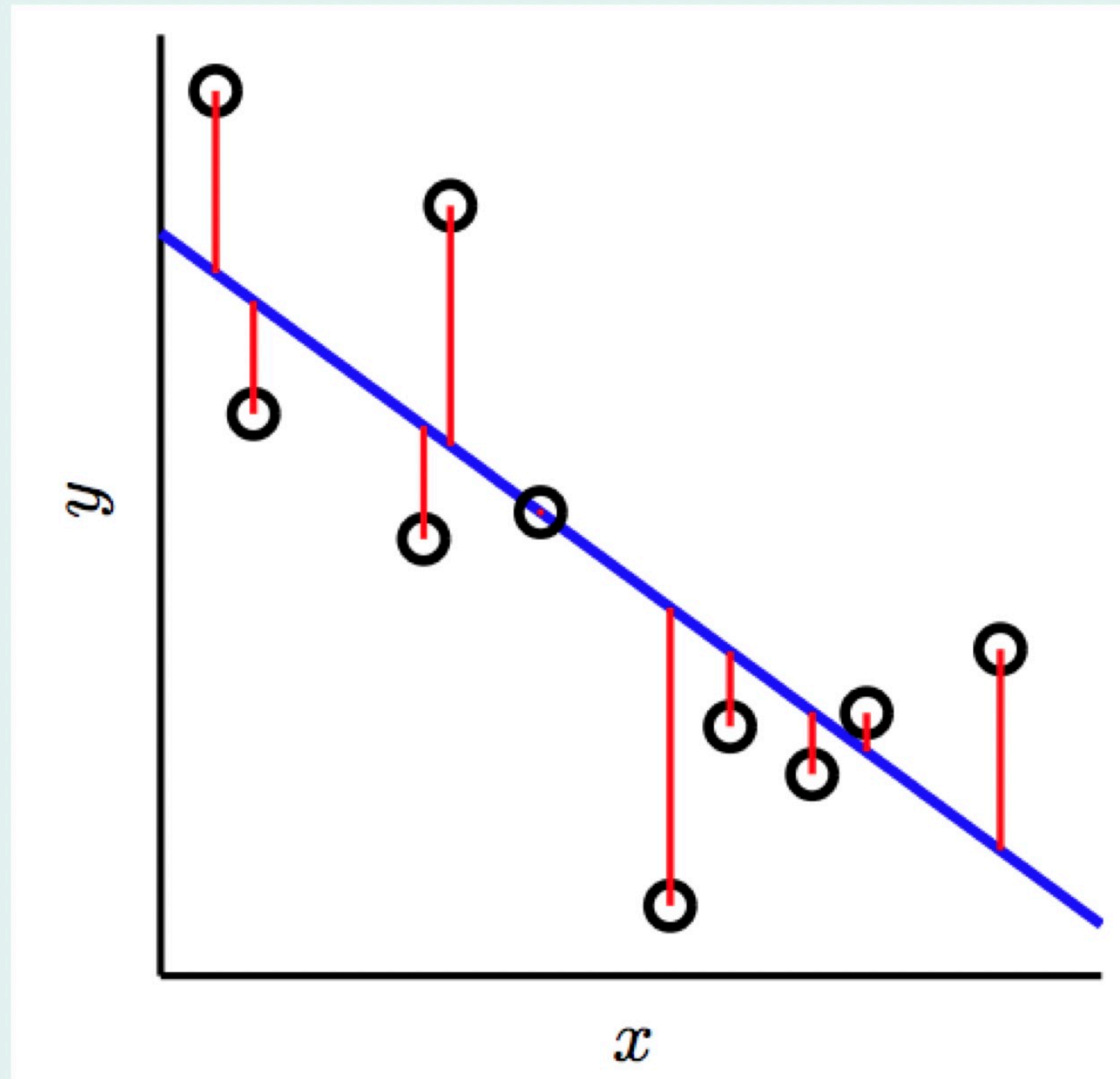
- Training data:
 - $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$
 - $x_n \in \mathbb{R}^d$: feature vector for a sample
 - $y_n \in \mathbb{R}$: observed output (real number)
- Linear regression: find a function $h(x) = w^T x$ to approximate y
- Measure the error by $(h(x) - y)^2$ (square error)

- Training error: $E_{\text{train}}(h) = \frac{1}{N} \sum_{n=1}^N (h(x_n) - y_n)^2$

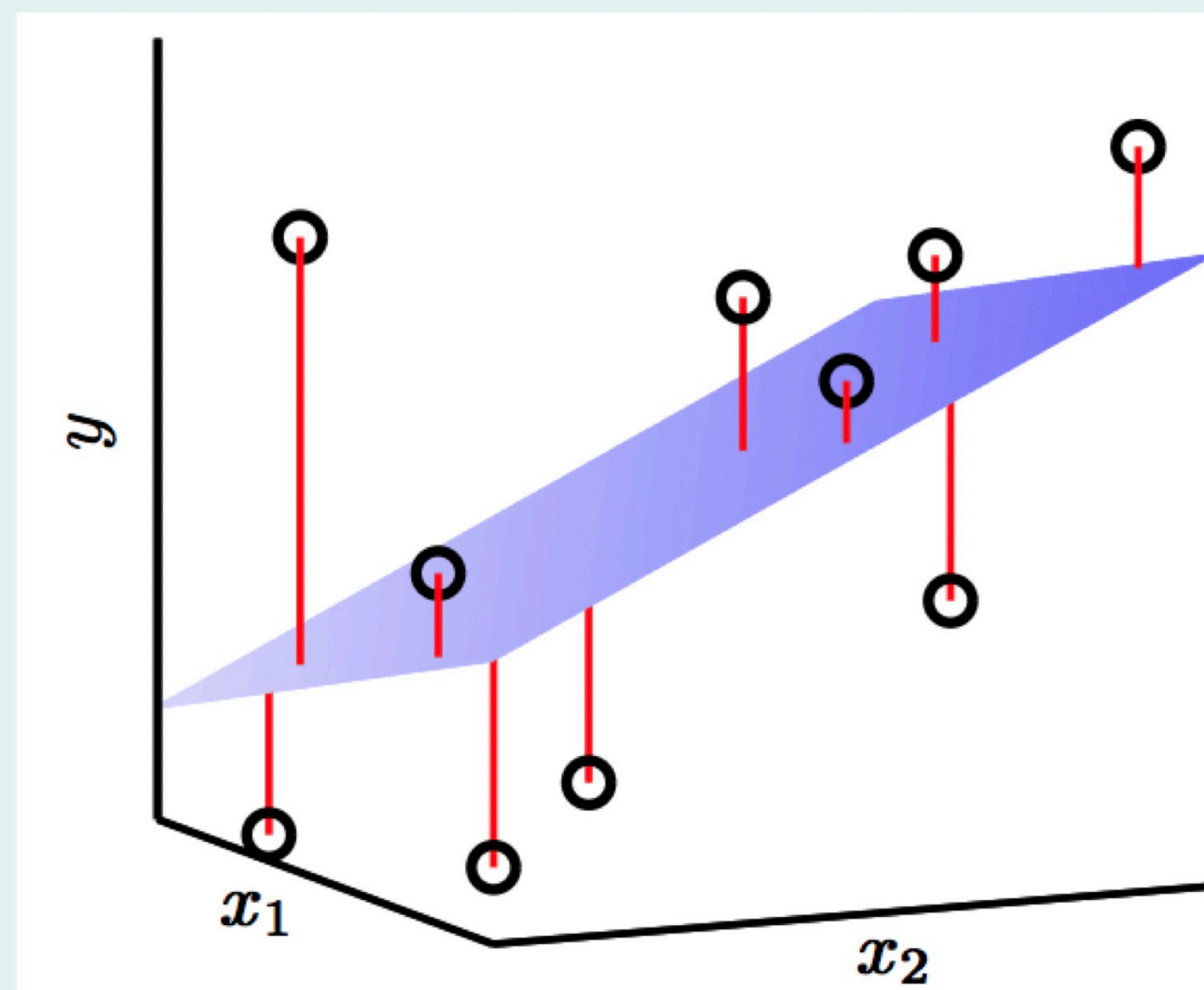
Linear Regression

Illustration

$$\mathbf{x} = (x) \in \mathbb{R}$$



$$\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$$



Linear Regression

Matrix form

$$E_{\text{train}}(w) = \frac{1}{N} \sum_{n=1}^N (x_n^T w - y_n)^2 = \frac{1}{N} \left\| \begin{bmatrix} x_1^T w - y_1 \\ x_2^T w - y_2 \\ \vdots \\ x_N^T w - y_N \end{bmatrix} \right\|^2$$

$$= \frac{1}{N} \left\| \begin{bmatrix} -x_1^T \\ -x_2^T \\ \vdots \\ -x_N^T \end{bmatrix} w - \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \right\|^2$$

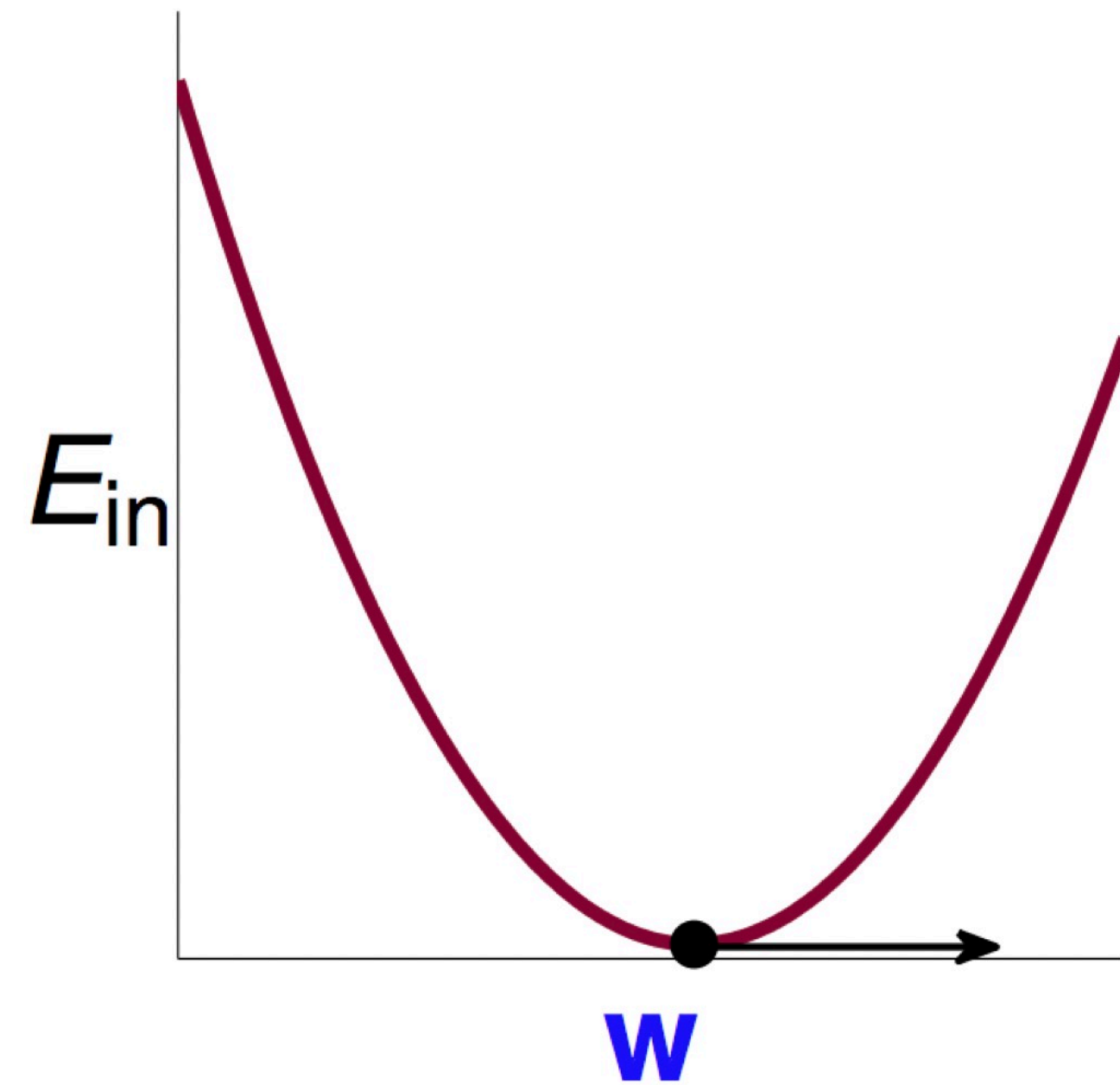
$$= \frac{1}{N} \left\| \underbrace{X}_{N \times d} w - \underbrace{y}_{N \times 1} \right\|^2$$

Linear Regression

Minimize E_{train}

- $\min_w f(w) = \|Xw - y\|^2$
 - E_{train} : continuous, differentiable, **convex**
 - Necessary condition of optimal w :

- $$\nabla f(w^*) = \begin{bmatrix} \frac{\partial f}{\partial w_0}(w^*) \\ \vdots \\ \frac{\partial f}{\partial w_d}(w^*) \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$$



Linear Regression

Minimizing f

$$f(w) = \|Xw - y\|^2 = w^T X^T X w - 2w^T X^T y + y^T y$$

$$\nabla f(w) = 2(X^T X w - X^T y)$$

- $\nabla f(w^*) = 0 \Rightarrow \underbrace{X^T X w^*}_{\text{normal equation}} = X^T y$

Linear Regression

Minimizing f

$$f(w) = \|Xw - y\|^2 = w^T X^T X w - 2w^T X^T y + y^T y$$

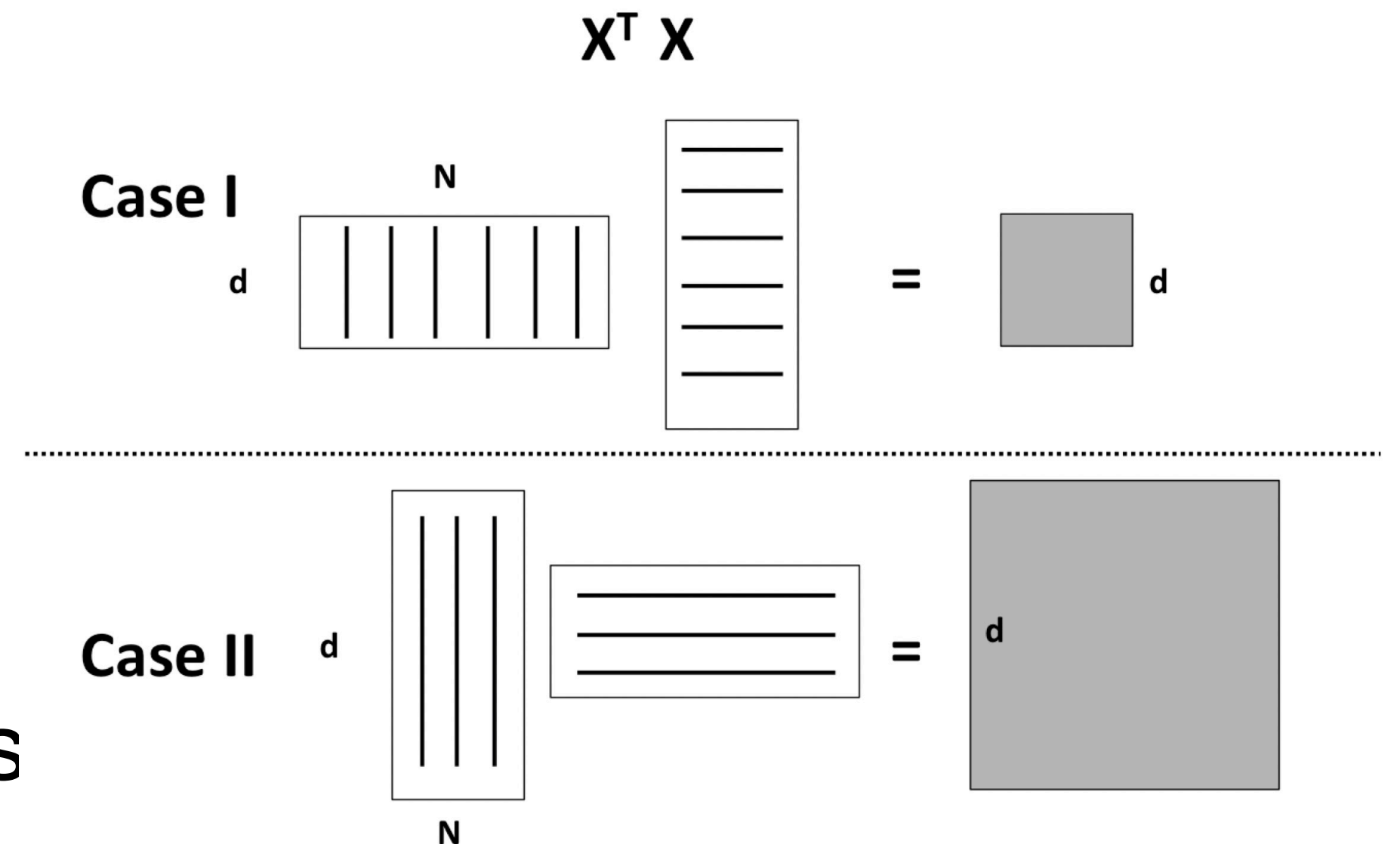
$$\nabla f(w) = 2(X^T X w - X^T y)$$

- $\nabla f(w^*) = 0 \Rightarrow \underbrace{X^T X w^* = X^T y}_{\text{normal equation}}$

- $\Rightarrow w^* = (X^T X)^{-1} X^T y$ **How?**

Linear Regression Solutions

- Case I: $X^T X$ is invertible \Rightarrow Unique solution
 - Often when $N > d$
 - Yes, $w^* = (X^T X)^{-1} X^T y$
- Case II: $X^T X$ is non-invertible \Rightarrow Many solutions
 - Often when $d > N$



Linear Regression

Linear System Solver

- A “linear system”:
 - Find the **minimum 2-norm solution** of $\min_w \|Xw - y\|$

Linear Regression

Linear System Solver

- A “linear system”:
 - Find the **minimum 2-norm solution** of $\min_w \|Xw - y\|$
- Let $X = U\Sigma V^T$ be the SVD of X :
 - $U^T U = I$
 - $V^T V = I$
 - $\Sigma = \text{diag}[\sigma_1, \sigma_2, \dots, \sigma_r, 0, \dots, 0]$, ($\sigma_1, \dots, \sigma_r > 0$)
 - Solution: $w^+ = X^+ y$
 - where $X^+ = V\Sigma^+ U^T$, $\Sigma^+ = \text{diag}[1/\sigma_1, 1/\sigma_2, \dots, 1/\sigma_r, 0, \dots, 0]$

Linear Regression

Linear System Solver

- A “linear system”:
 - Find the **minimum 2-norm solution** of $\min_w \|Xw - y\|$
- Let $X = U\Sigma V^T$ be the SVD of X :
 - $U^T U = I$
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 - $\Sigma = \text{diag}[\sigma_1, \sigma_2, \dots, \sigma_r, 0, \dots, 0]$, ($\sigma_1, \dots, \sigma_r > 0$)
 - Solution: $w^+ = X^+ y$
 - where $X^+ = V\Sigma^+ U^T$, $\Sigma^+ = \text{diag}[1/\sigma_1, 1/\sigma_2, \dots, 1/\sigma_r, 0, \dots, 0]$
 - X^+ : pseudo-inverse of X
 - Why?

Linear Regression

Linear System Solver (Cont*)

- $\|Xw - y\|^2 = \|U\Sigma V^T w - y\|^2 = \|\Sigma V^T w - U^T y\|^2$ since ?
- Let $z = V^T w$,
 - The solution of $\min_w \|\Sigma V^T w - U^T y\|^2$ is equivalent to find the solution of
 - $\min_z \|\Sigma z - U^T y\|^2$
 - Since Σ is diagonal, so the solution is $z^+ = \Sigma^+ U^T y$
 - So $w^+ = Vz^+ = V\Sigma^+ U^T y$

Computation complexity

Dense vector and sparse vector

- If $x, y \in \mathbb{R}^m$ are dense:
 - $x + y, x - y, x^T y : O(m)$ operations
- If $x, y \in \mathbb{R}^m$, x is dense and y is sparse:
 - $x + y, x - y, x^T y : O(\text{nnz}(y))$ operations
- If $x, y \in \mathbb{R}^m$ and both of them are sparse:
 - $x + y, x - y, x^T y : O(\text{nnz}(y) + \text{nnz}(x))$ operations

Dense Array		1.1	2.1	1.8	4.3	7.6	5.2	4.3	1.8
Sparse Array	values	1.1	7.6	1.8					
	idx	1	5	8					

Computation complexity

Dense matrix

- Let $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{m \times n}$, $s \in \mathbb{R}$:
 - $A + B, sA, A^T$: $O(mn)$ operations
- If $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^{n \times 1}$
 - Ab : $O(mn)$ operations
- If $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times n}$,
 - AB : $O(n^3)$ operations; theoretical best: $O(n^{2.xxx})$
- $A \in \mathbb{R}^{m \times k}$, $B \in \mathbb{R}^{k \times n}$,
 - AB : $O(mnk)$ operations;

Matrix

1	5	9
2	6	10
3	7	11
4	8	12



Array (in Memory Space)

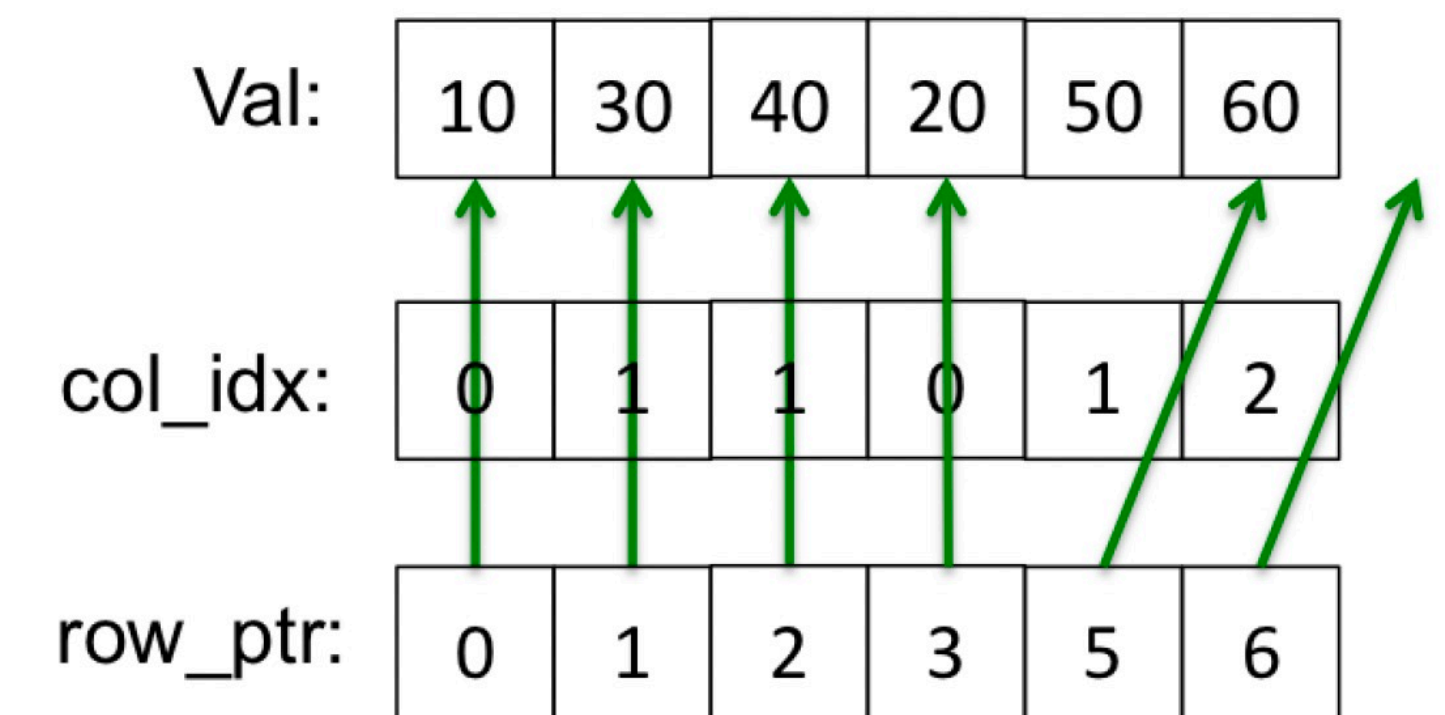
1	2	3	4	5	6	7	8	9	10	11	12
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Computation complexity

Sparse matrix format

- Widely-used format: Compressed Sparse Column (CSC), Compressed Sparse Row (CSR), ...
- CSR: three arrays for storing an $m \times n$ matrix with nnz nonzero
 - *val* (nnz real numbers): the values of each nonzero elements
 - *row_ind* (nnz integers): the column indices corresponding to the values
 - *col_ptr* ($m + 1$ integers): the list of value indexes where each column starts

10	0	0
0	30	0
0	40	0
20	50	0
0	0	60



Computation complexity

Sparse matrix operations

- Let $A \in \mathbb{R}^{m \times n}$ (sparse), $B \in \mathbb{R}^{m \times n}$ (sparse or dense), $s \in \mathbb{R}$:
 - $A + B, sA, A^T : O(nnz)$ operations
- If $A \in \mathbb{R}^{m \times n}$ (sparse), $b \in \mathbb{R}^{n \times 1}$
 - $Ab : O(nnz)$ operations
- If $A \in \mathbb{R}^{n \times k}$ (sparse), $B \in \mathbb{R}^{k \times n}$ (dense),
 - $AB : O(nnz(A)n)$ operations (use sparse BLAS)
- $A \in \mathbb{R}^{n \times k}$ (sparse), $B \in \mathbb{R}^{k \times n}$ (sparse),
 - $AB : O(nnz(A)nnz(B)/k)$ in average
 - $AB : O(nnz(A)n)$ worst case
 - The resulting matrix will be much denser

Linear Regression

Computational complexity

- Computational cost for computing $(X^T X)^{-1} X^T y$:
 - Computing $X^T X$: $O(d^2 N)$ time
 - Computing matrix inversion: $O(d^3)$ time
 - Overall complexity: $O(d^2 N + d^3)$
- What if $d, N \approx$ millions?
 - (Use iterative algorithms, next class)

Logistic Regression

Binary Classification

- Input: training data $x_1, x_2, \dots, x_n \in \mathbb{R}^d$ and corresponding outputs $y_1, y_2, \dots, y_n \in \{+1, -1\}$
- Training: compute a function f such that $\text{sign}(f(x_i)) \approx y_i$ for all i
- Prediction: given a testing sample \tilde{x} , predict the output as $\text{sign}(f(x_i))$

Logistic Regression

Binary Classification

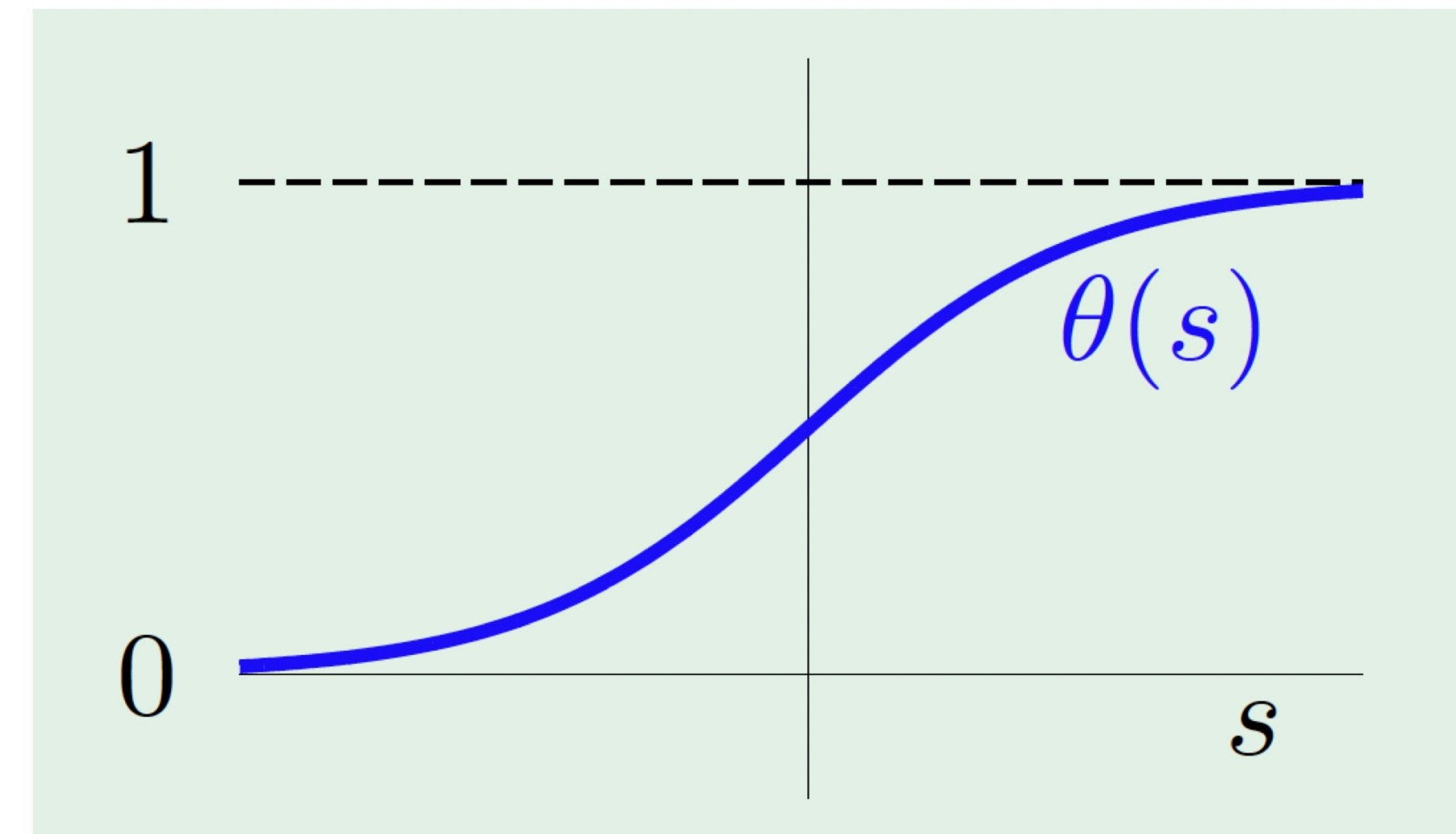
- Assume **linear** scoring function: $s = f(x) = w^T x$

- **Logistic hypothesis:**

- $P(y = 1 | x) = \theta(w^T x),$

- Where $\theta(s) = \frac{e^s}{1 + e^s} = \frac{1}{1 + e^{-s}}$

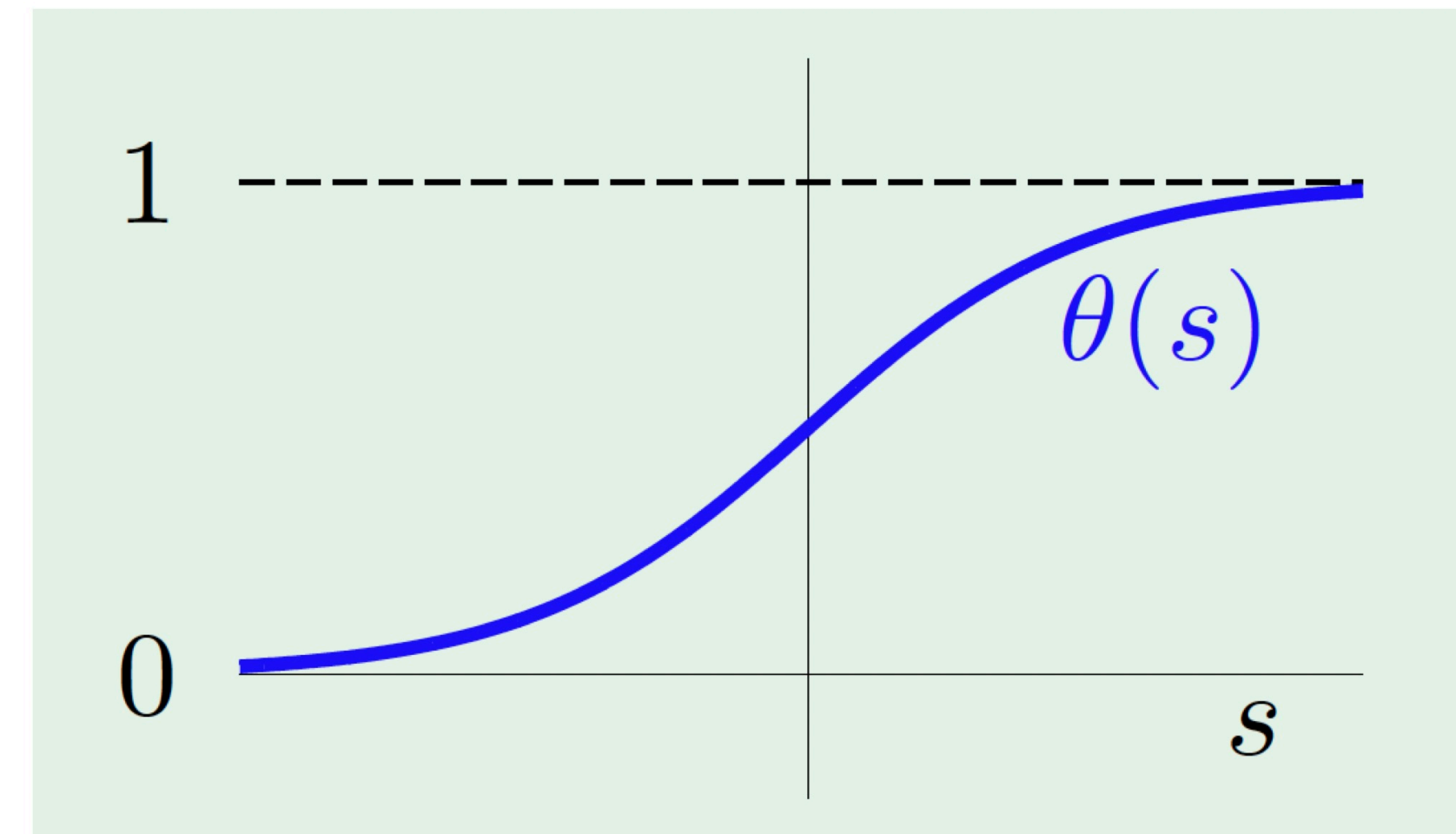
- It is called sigmoid function



Logistic Regression

Binary Classification

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- **Logistic hypothesis:**
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 - Where $\theta(s) = \frac{e^s}{1 + e^s} = \frac{1}{1 + e^{-s}}$
- How about $P(y = -1 | x)$?



Logistic Regression

Binary Classification

- Assume **linear** scoring function: $s = f(x) = w^T x$

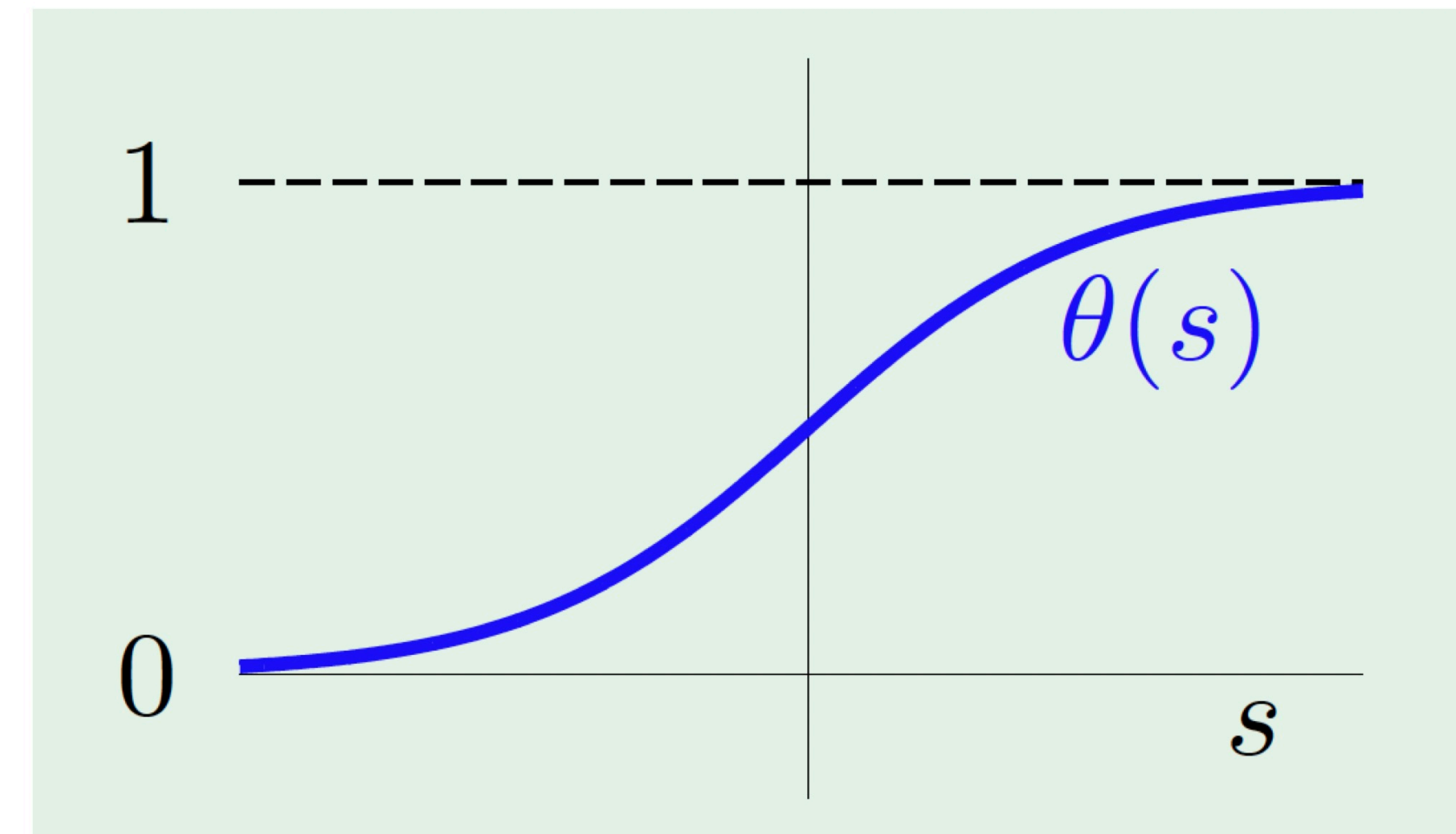
- **Logistic hypothesis:**

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- Where $\theta(s) = \frac{e^s}{1 + e^s} = \frac{1}{1 + e^{-s}}$

- How about $P(y = -1 | x)$?

- $P(y = -1 | x) = 1 - \frac{1}{1 + e^{-w^T x}} = \frac{1}{1 + e^{w^T x}} = \theta(-w^T x)$



Logistic Regression

Binary Classification

- Assume **linear** scoring function: $s = f(x) = w^T x$
- **Logistic hypothesis**:
 - $P(y = 1 | x) = \theta(w^T x)$,
 - Where $\theta(s) = \frac{e^s}{1 + e^s} = \frac{1}{1 + e^{-s}}$
- How about $P(y = -1 | x)$?
 - $P(y = -1 | x) = 1 - \frac{1}{1 + e^{-w^T x}} = \frac{1}{1 + e^{w^T x}} = \theta(-w^T x)$
- Therefore, $P(y | x) = \theta(yw^T x)$

Logistic Regression

Maximizing the likelihood

- Likelihood of $\mathcal{D} = (x_1, y_1), \dots, (x_N, y_N)$:

$$\bullet \prod_{n=1}^N P(y_n | x_n) = \prod_{n=1}^N \theta(y_n w^T x_n)$$

Logistic Regression

Maximizing the likelihood

- Likelihood of

$$\mathcal{D} = (x_1, y_1), \dots, (x_N, y_N):$$

$$\bullet \prod_{n=1}^N P(y_n | x_n) = \prod_{n=1}^N \theta(y_n w^T x_n)$$

- Find w to maximize the likelihood!

$$\max_w \prod_{n=1}^N \theta(y_n w^T x_n)$$

$$\Leftrightarrow \max_w \log\left(\prod_{n=1}^N \theta(y_n w^T x_n)\right)$$

$$\Leftrightarrow \min_w - \sum_{n=1}^N \log(\theta(y_n w^T x_n))$$

$$\bullet \Leftrightarrow \min_w \sum_{n=1}^N \log(1 + e^{-y_n w^T x_n})$$

Logistic Regression

Empirical Risk Minimization (linear)

- Linear classification/regression:

- $$\min_w \frac{1}{N} \sum_{n=1}^N \text{loss}(\underbrace{w^T x_n}_{\hat{y}_n}, y_n)$$

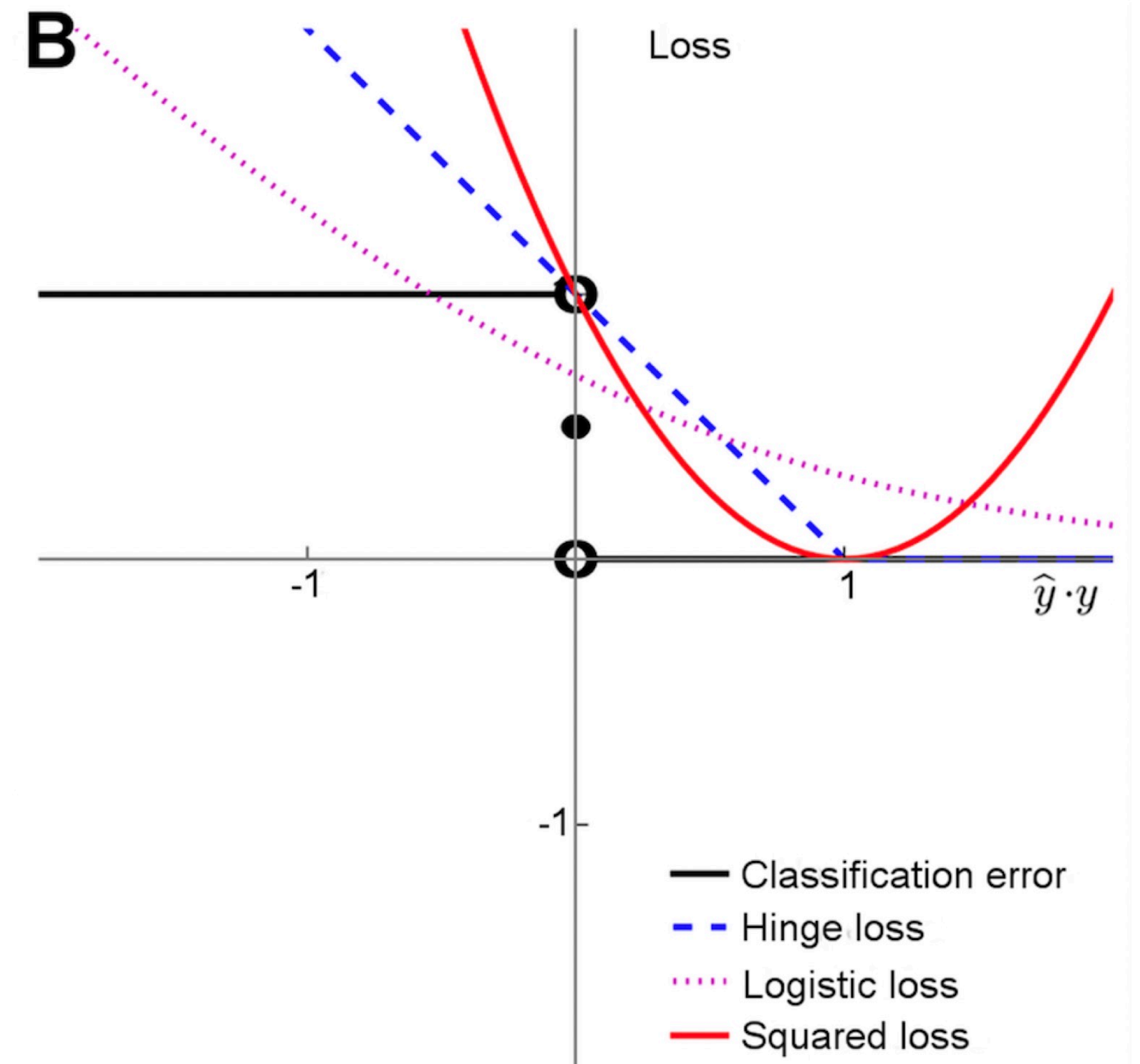
\hat{y}_n : the predicted score

- Linear regression:

$$\text{loss}(h(x_n), y_n) = (w^T x_n - y_n)^2$$

- Logistic regression:

$$\text{loss}(h(x_n), y_n) = \log(1 + e^{-y_n w^T x_n})$$

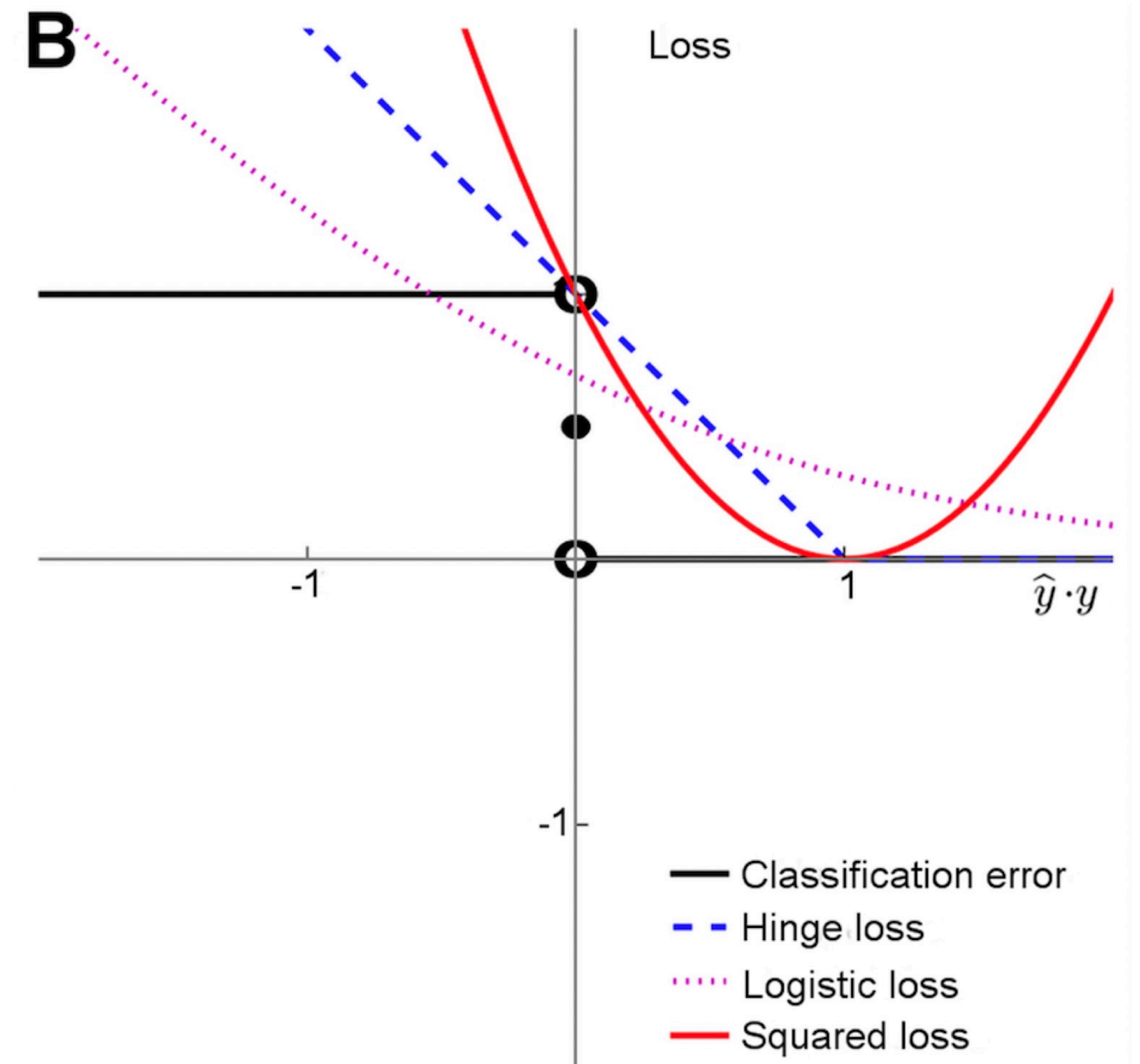


Support Vector Machines

Hinge loss

- Replace the logistic loss by hinge loss:

$$\min_w \frac{1}{N} \sum_{n=1}^N \max(0, 1 - y_n w^T x_n)$$



Logistic Regression

Empirical Risk Minimization (general)

- Assume $f_W(x)$ is the decision function to be learned
 - (W is the parameters of the function)

- General empirical risk minimization

- $$\min_W \frac{1}{N} \sum_{n=1}^N \text{loss}(f_W(x_n), y_n)$$

- Example: Neural network ($f_W(\cdot)$ is the network)