Machine Learning

Lecture 6
Linear Regression

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The Storyline

How Can Machines Learn?

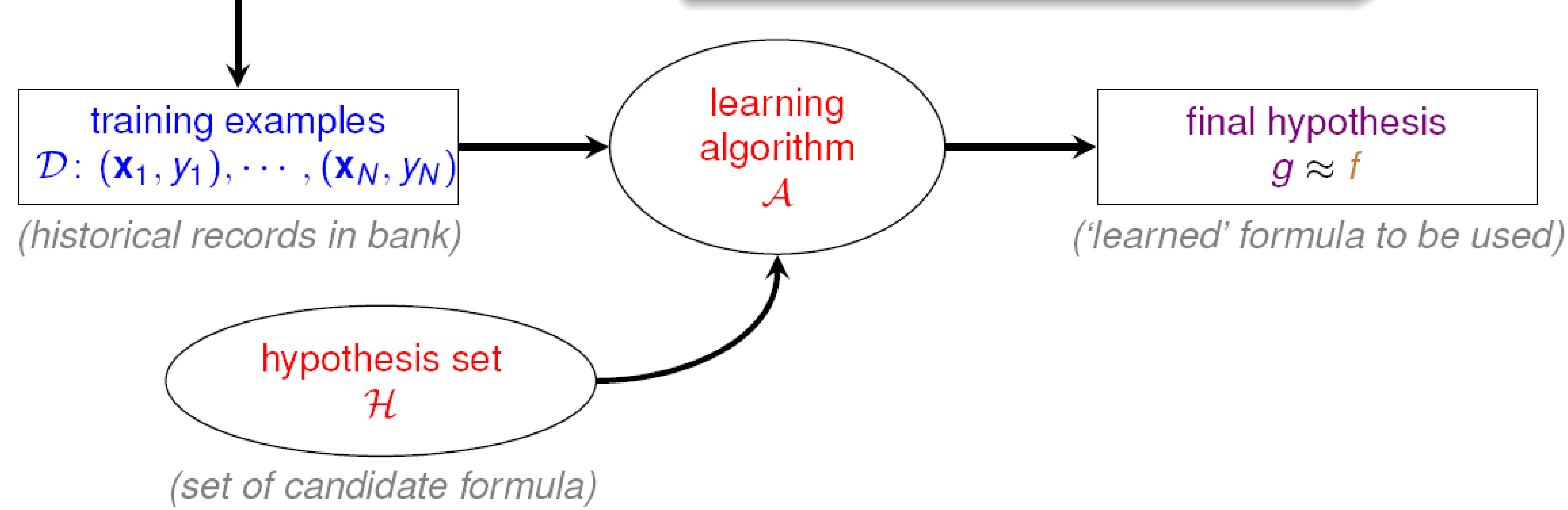
Linear Regression

- Linear Regression Problem
- Linear Regression Algorithm
- Linear Regression for Binary Classification

Credit **Limit** Problem

age	23 years
gender	female
annual salary	NTD 1,000,000
year in residence	1 year
year in job	0.5 year
current debt	200,000

credit limit? **100,000**



$\mathcal{Y} = \mathbb{R}$: **regression**

High-dimensional Data as Input

age	23 years
annual salary	NTD 1,000,000
year in job	0.5 year
current debt	200,000

- For $\mathbf{x} = (x_1, x_2, \cdots, x_d)$ '**features of customer**', compute a weighted 'score' and

$$\text{approve credit if} \quad \sum_{i=1}^{d} w_i x_i > \text{threshold}$$

$$\text{deny credit if} \quad \sum_{i=1}^{d} w_i x_i < \text{threshold}$$

- $\mathcal{Y}$: $\{+1(\textbf{good}), -1(\textbf{bad})\}$, 0 ignored—linear formula $h \in \mathcal{H}$ are

$$h(\mathbf{x}) = \text{sign}\left(\left(\sum_{i=1}^{d} w_i x_i\right) - \text{threshold}\right)$$

Vector Form of Perceptron Hypothesis

$$
\begin{aligned}
h(\mathbf{x}) &= \text{sign}\left(\left(\sum_{i=1}^{d} w_i x_i\right) - \text{threshold}\right) \\
&= \text{sign}\left(\left(\sum_{i=1}^{d} w_i x_i\right) + \underbrace{(-\text{threshold})}_{w_0} \cdot \underbrace{(+1)}_{x_0}\right) \\
&= \text{sign}\left(\sum_{i=0}^{d} w_i x_i\right) \\
&= \text{sign}\left(\mathbf{w}^T \mathbf{x}\right)
\end{aligned}
$$

- each 'tall' **w** represents a hypothesis h & is multiplied with 'tall' **x** —**will use tall versions to simplify notation**

Linear Regression Hypothesis

age	23 years
annual salary	NTD 1,000,000
year in job	0.5 year
current debt	200,000

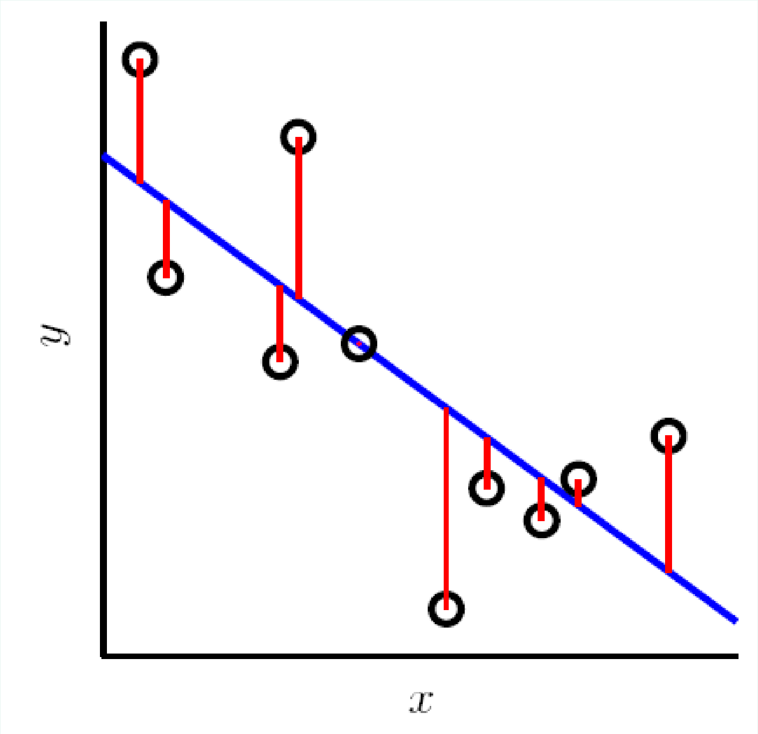
- For $\mathbf{x} = (x_0, x_1, x_2, \cdots, x_d)$ 'features of customer', approximate the desired credit limit with a weighted sum:

$$y \approx \sum_{i=0}^{d} w_i x_i$$

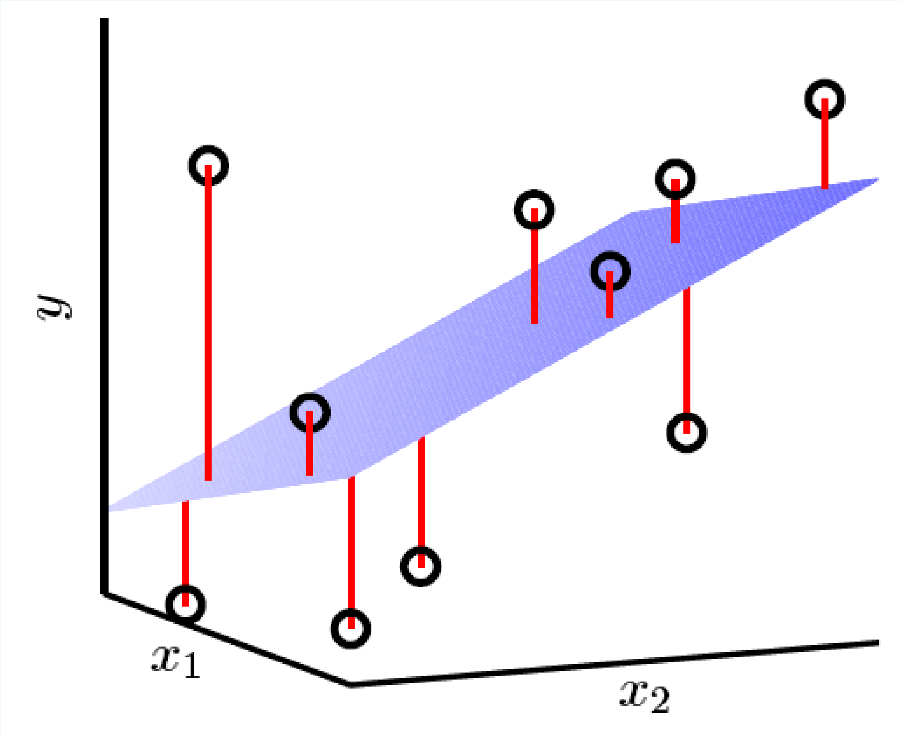
- linear regression hypothesis: $h(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$

Illustration of Linear Regression

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



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



linear regression:
find lines/hyperplanes with small residuals

The Error Measure

popular/historical error measure:

squared error $\mathrm{err}(\hat{y}, y) = (\hat{y} - y)^2$

in-sample

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(\underbrace{h(\mathbf{x}_n)}_{\mathbf{w}^T\mathbf{x}_n} - y_n)^2$$

out-of-sample

$$E_{\text{out}}(\mathbf{w}) = \underset{(\mathbf{x},y)\sim P}{\mathcal{E}}(\mathbf{w}^T\mathbf{x} - y)^2$$

next: how to minimize $E_{\text{in}}(\mathbf{w})$?

Fun Time

Consider using linear regression hypothesis $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ to predict the credit limit of customers $\mathbf{x}$. Which feature below shall have a positive weight in a **good hypothesis** for the task?

1. birth month
2. monthly income
3. current debt
4. number of credit cards owned

Matrix Form of $E_{in}(\mathbf{w})$

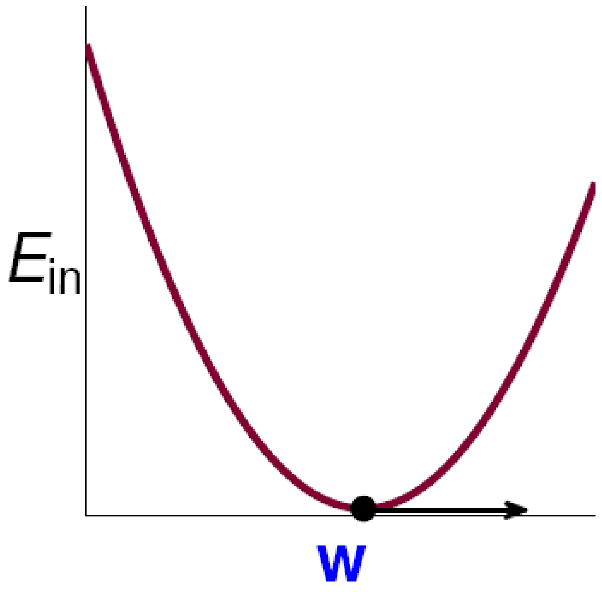
$$
\begin{aligned}
E_{\text{in}}(\mathbf{w}) &= \frac{1}{N}\sum_{n=1}^{N}(\mathbf{w}^T\mathbf{x}_n - y_n)^2 = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n^T\mathbf{w} - y_n)^2 \\
&= \frac{1}{N}\left\| \begin{matrix} \mathbf{x}_1^T\mathbf{w} - y_1 \\ \mathbf{x}_2^T\mathbf{w} - y_2 \\ \cdots \\ \mathbf{x}_N^T\mathbf{w} - y_N \end{matrix} \right\|^2 \\
&= \frac{1}{N}\left\| \begin{bmatrix} -\,-\,\mathbf{x}_1^T\,-\,- \\ -\,-\,\mathbf{x}_2^T\,-\,- \\ \cdots \\ -\,-\,\mathbf{x}_N^T\,-\,- \end{bmatrix} \mathbf{w} - \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_N \end{bmatrix} \right\|^2 \\
&= \frac{1}{N}\| \underbrace{\mathrm{X}}_{N\times d+1} \underbrace{\mathbf{w}}_{d+1\times 1} - \underbrace{\mathbf{y}}_{N\times 1} \|^2
\end{aligned}
$$

Norm

$$\|x\|_n = \sqrt[n]{\sum_{i=1}^{n} |x_i|^n}$$

- A norm is a function that assigns a strictly positive length or size to each vector in a vector space.
- $\boldsymbol{x} = (x_1, x_2, ..., x_n)$
- l_2-norm (Euclidean norm) $$\|x\|_2 = \sqrt{x_1^2 + x_2^2 + x_3^2 + \ldots + x_N^2}$$
- l_1-norm $$\|x\|_1 = \sum_{i=1}^{n} |x_i| = |x_1| + |x_2| + |x_3| + \ldots.. + |x_N|$$
- l_0-norm $$\|x\|_0 = \sqrt[0]{\sum_{i=1}^{n} |x_i|^0} = \#\left(i \mid x_i \neq 0\right)$$
- Infinite-norm $$\|x\|_\infty = \max\left(|x_1|, |x_2|, |x_3|, \ldots., |x_n|\right)$$

$$\min_{\mathbf{w}} E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\|\mathrm{X}\mathbf{w} - \mathbf{y}\|^2$$



- $E_{\text{in}}(\mathbf{w})$: continuous, differentiable, **convex**
- necessary condition of 'best' $\mathbf{w}$

$$\nabla E_{\text{in}}(\mathbf{w}) \equiv \begin{bmatrix} \frac{\partial E_{\text{in}}}{\partial w_0}(\mathbf{w}) \\ \frac{\partial E_{\text{in}}}{\partial w_1}(\mathbf{w}) \\ \cdots \\ \frac{\partial E_{\text{in}}}{\partial w_d}(\mathbf{w}) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \end{bmatrix}$$

—not possible to 'roll down'

task: find $\mathbf{w}_{\text{LIN}}$ such that $\nabla E_{\text{in}}(\mathbf{w}_{\text{LIN}}) = \mathbf{0}$

The Gradient $\nabla E_{\text{in}}(\mathbf{w})$

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\|\mathrm{X}\mathbf{w} - \mathbf{y}\|^2 = \frac{1}{N}\left(\mathbf{w}^T \underbrace{\mathrm{X}^T\mathrm{X}}_{\mathrm{A}} \mathbf{w} - 2\mathbf{w}^T \underbrace{\mathrm{X}^T\mathbf{y}}_{\mathbf{b}} + \underbrace{\mathbf{y}^T\mathbf{y}}_{c}\right)$$

one w only

$$E_{\text{in}}(w) = \frac{1}{N}\left(aw^2 - 2bw + c\right)$$

$$\nabla E_{\text{in}}(w) = \frac{1}{N}\left(2aw - 2b\right)$$

simple! :-)

vector $\mathbf{w}$

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\left(\mathbf{w}^T\mathrm{A}\mathbf{w} - 2\mathbf{w}^T\mathbf{b} + c\right)$$

$$\nabla E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\left(2\mathrm{A}\mathbf{w} - 2\mathbf{b}\right)$$

similar (**derived by definition**)

$$\nabla E_{\text{in}}(\mathbf{w}) = \frac{2}{N}\left(\mathrm{X}^T\mathrm{X}\mathbf{w} - \mathrm{X}^T\mathbf{y}\right)$$

Optimal Linear Regression Weights

task: find $\mathbf{w}_{\text{LIN}}$ such that $\frac{2}{N}\left(\mathrm{X}^T\mathrm{X}\mathbf{w} - \mathrm{X}^T\mathbf{y}\right) = \nabla E_{\text{in}}(\mathbf{w}) = \mathbf{0}$

invertible $\mathrm{X}^T\mathrm{X}$

- **easy!** unique solution

$$\mathbf{w}_{\text{LIN}} = \underbrace{\left(\mathrm{X}^T\mathrm{X}\right)^{-1}\mathrm{X}^T}_{\text{pseudo-inverse } \mathrm{X}^\dagger}\mathbf{y}$$

- often the case because $N \gg d+1$

singular $\mathrm{X}^T\mathrm{X}$

- **many** optimal solutions
- one of the solutions

$$\mathbf{w}_{\text{LIN}} = \mathrm{X}^\dagger\mathbf{y}$$

by defining $\mathrm{X}^\dagger$ in other ways

practical suggestion:

use **well-implemented $\dagger$ routine**

instead of $\left(\mathrm{X}^T\mathrm{X}\right)^{-1}\mathrm{X}^T$

for numerical stability when **almost-singular**

Linear Regression Algorithm

1. from $\mathcal{D}$, construct input matrix X and output vector $\mathbf{y}$ by

$$\mathrm{X} = \underbrace{\begin{bmatrix} --\mathbf{x}_1^T-- \\ --\mathbf{x}_2^T-- \\ \cdots \\ --\mathbf{x}_N^T-- \end{bmatrix}}_{N\times(d+1)} \quad \mathbf{y} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_N \end{bmatrix}}_{N\times 1}$$

2. calculate pseudo-inverse $\underbrace{\mathrm{X}^\dagger}_{(d+1)\times N}$

3. return $\underbrace{\mathbf{w}_{\mathrm{LIN}}}_{(d+1)\times 1} = \mathrm{X}^\dagger \mathbf{y}$

simple and efficient
with **good $\dagger$ routine**

範例

給定5組(X, Y)數據如下：

X	2	1	4	5	3
Y	1	3	7	6	3

(1) 求Y對X的迴歸直線方程式

(2) 利用迴歸直線，預測$x=8$時，y值應為多少？

$$y = ax + b = w_1 x + w_0$$

$$1 = 2w_1 + w_0$$
$$3 = 1w_1 + w_0$$
$$7 = 4w_1 + w_0$$
$$6 = 5w_1 + w_0$$
$$3 = 3w_1 + w_0$$

$$\underbrace{\begin{bmatrix}1\\3\\7\\6\\3\end{bmatrix}}_{\mathrm{y}} = \underbrace{\begin{bmatrix}2&1\\1&1\\4&1\\5&1\\3&1\end{bmatrix}}_{\mathrm{X}} \cdot \underbrace{\begin{bmatrix}w_1\\w_0\end{bmatrix}}_{\mathrm{W_{LIN}}}$$

$$\mathbf{w}_{\mathrm{LIN}} = \left(\mathrm{X}^T\mathrm{X}\right)^{-1}\mathrm{X}^T\mathbf{y}$$

$$\mathrm{W_{LIN}} = \left(\begin{bmatrix}2&1&4&5&3\\1&1&1&1&1\end{bmatrix}\cdot\begin{bmatrix}2&1\\1&1\\4&1\\5&1\\3&1\end{bmatrix}\right)^{-1}\cdot\begin{bmatrix}2&1&4&5&3\\1&1&1&1&1\end{bmatrix}\cdot\begin{bmatrix}1\\3\\7\\6\\3\end{bmatrix}=\begin{bmatrix}1.2\\0.4\end{bmatrix}$$

$$y = 1.2x + 0.4$$

Fun Time

After getting $\mathbf{w}_{\text{LIN}}$, we can calculate the predictions $\hat{y}_n = \mathbf{w}_{\text{LIN}}^T \mathbf{x}_n$. If all $\hat{y}_n$ are collected in a vector $\hat{\mathbf{y}}$ similar to how we form $\mathbf{y}$, what is the matrix formula of $\hat{\mathbf{y}}$?

1. $\mathbf{y}$
2. $\mathrm{XX}^T\mathbf{y}$
3. $\mathrm{XX}^\dagger\mathbf{y}$
4. $\mathrm{XX}^\dagger\mathrm{XX}^T\mathbf{y}$

Reference Answer: ?

HW#1 Exercise

Linear Classification vs. Linear Regression

Linear Classification

$$\begin{aligned} \mathcal{Y} &= \{-1,+1\} \\ h(\mathbf{x}) &= \mathrm{sign}(\mathbf{w}^T\mathbf{x}) \\ \mathrm{err}(\hat{y},y) &= [\![\hat{y} \neq y]\!] \end{aligned}$$

NP-hard to solve in general

Linear Regression

$$\begin{aligned} \mathcal{Y} &= \mathbb{R} \\ h(\mathbf{x}) &= \mathbf{w}^T\mathbf{x} \\ \mathrm{err}(\hat{y},y) &= (\hat{y}-y)^2 \end{aligned}$$

efficient analytic solution

[助教飛飛的重點提示]
感知器與線性迴歸
如同兩兄弟
①數學公式上的差異?
②模型表示上的差異?
③誤差評估的差異

$\{-1,+1\} \subset \mathbb{R}$: linear regression for classification?

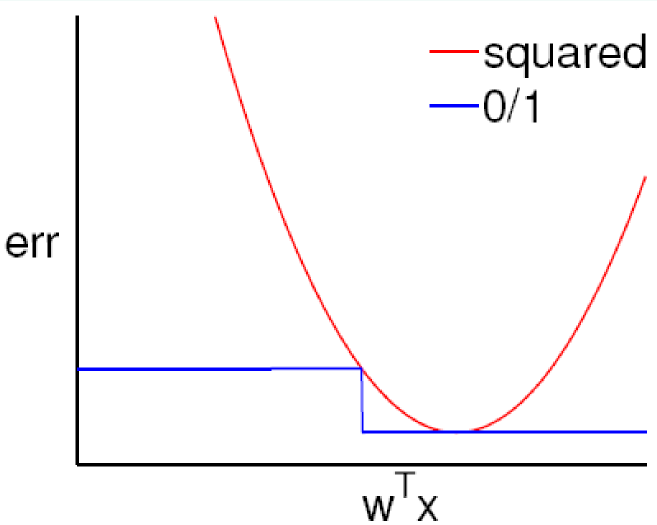
1. run LinReg on binary classification data $\mathcal{D}$ (**efficient**)
2. return $g(\mathbf{x}) = \mathrm{sign}(\mathbf{w}_{\mathrm{LIN}}^T\mathbf{x})$

but explanation of this **heuristic**?

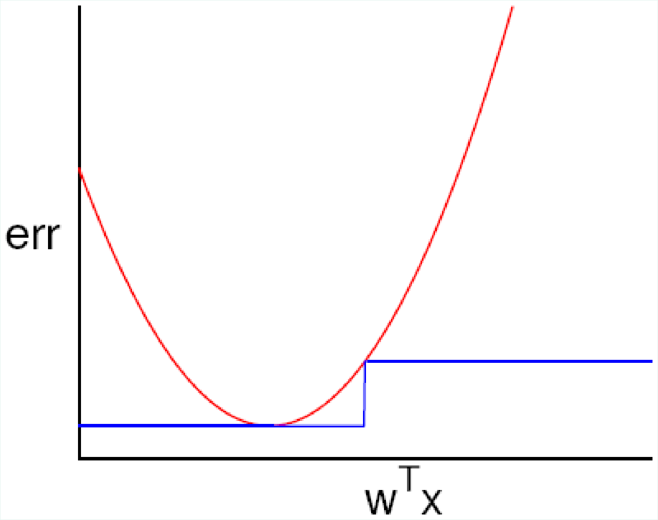
Relation of Two Errors

$$\text{err}_{0/1} = [\![\text{sign}(\mathbf{w}^T\mathbf{x}) \neq y]\!] \qquad \text{err}_{\text{sqr}} = (\mathbf{w}^T\mathbf{x} - y)^2$$

desired $y = 1$



desired $y = -1$



$$\text{err}_{0/1} \leq \text{err}_{\text{sqr}}$$

Linear Regression for Binary Classification

$$\text{err}_{0/1} \leq \text{err}_{\text{sqr}}$$

$$\begin{aligned} \text{classification } E_{\text{out}}(\mathbf{w}) &\overset{\text{VC}}{\leq} \text{classification } E_{\text{in}}(\mathbf{w}) + \sqrt{\cdots\cdots} \\ &\leq \text{regression } E_{\text{in}}(\mathbf{w}) + \sqrt{\cdots\cdots} \end{aligned}$$

- (loose) upper bound err_{sqr} as $\widehat{\text{err}}$ to approximate $\text{err}_{0/1}$
- trade **bound tightness** for **efficiency**

$\mathbf{w}_{\text{LIN}}$: useful baseline classifier,
or as **initial PLA/pocket vector**

Fun Time

Which of the following functions are upper bounds of the pointwise 0/1 error $[\![\mathrm{sign}(\mathbf{w}^T\mathbf{x}) \neq y]\!]$ for $y \in \{-1, +1\}$?

1. $\exp(-y\mathbf{w}^T\mathbf{x})$
2. $\max(0, 1 - y\mathbf{w}^T\mathbf{x})$
3. $\log_2(1 + \exp(-y\mathbf{w}^T\mathbf{x}))$
4. all of the above

Summary

How Can Machines Learn?

Linear Regression

- Linear Regression Problem
  use hyperplanes to approximate real values
- Linear Regression Algorithm
  analytic solution with pseudo-inverse
- Linear Regression for Binary Classification
  0/1 error $\leq$ squared error