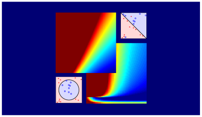
Machine Learning Foundations
(機器學習基石)



Lecture 9: Linear Regression

Hsuan-Tien Lin (林軒田)

htlin@csie.ntu.edu.tw

Department of Computer Science
& Information Engineering

National Taiwan University
(國立台灣大學資訊工程系)

Roadmap

1. When Can Machines Learn?
2. Why Can Machines Learn?

Lecture 8: Noise and Error

learning can happen
with **target distribution** $P(y|\mathbf{x})$ and **low** E_{in} **w.r.t.** $\mathbf{err}$

3. **How** Can Machines Learn?

Lecture 9: Linear Regression

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

4. How Can Machines Learn Better?

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**

unknown target function
$f\colon \mathcal{X} \to \mathcal{Y}$

*(ideal credit **limit** formula)*

training examples
$\mathcal{D}\colon (\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$

(historical records in bank)

learning algorithm
$\mathcal{A}$

final hypothesis
$g \approx f$

('learned' formula to be used)

hypothesis set
$\mathcal{H}$

(set of candidate formula)

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

Linear Regression Hypothesis

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

(for bias)
+1

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

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

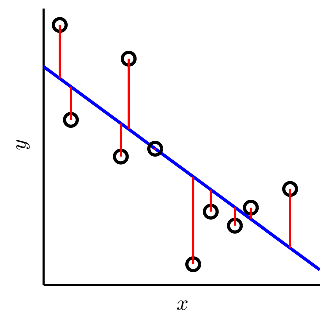
- linear regression hypothesis: $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$

$h(\mathbf{x})$: like **perceptron**, but without the sign

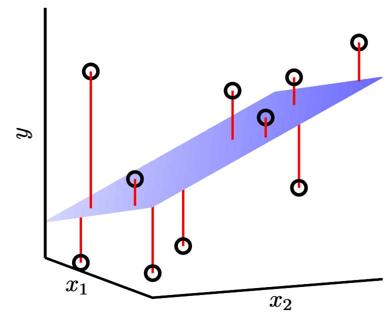
sign(Σwx)

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

minimize

The Error Measure

popular/historical error measure:

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

We want to use w to define. (Less confusing)

in-sample

$E_{in}(h)$

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

out-of-sample

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

We may have noise.

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

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

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

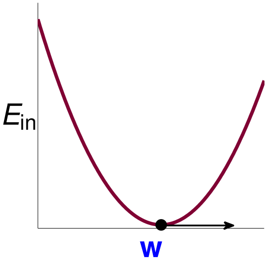
Reference Answer: 2

Customers with higher monthly income should naturally be given a higher credit limit, which is captured by the positive weight on the 'monthly income' feature.

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

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

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



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

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

—not possible to 'roll down'

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

LIN: linear regression

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

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

scalar

one w only

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

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

simple! :-)

vector $\mathbf{w}$

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

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

similar (**derived by definition**)

A is a symmetric matrix.

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

Optimal Linear Regression Weights

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

First scenario:

invertible $X^TX_{(d+1,\,d+1)}$ $\leftarrow X_{(N,\,d+1)}$

- **easy!** unique solution

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

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

Second scenario:

singular X^TX

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

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

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

practical suggestion: Don't try to classify two scenarios.
use **well-implemented $\dagger$ routine**
instead of $\left(X^TX\right)^{-1}X^T$
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 $\underbrace{\mathbf{w}_{\text{LIN}}}_{(d+1)\times 1} = \mathrm{X}^\dagger\mathbf{y}$

simple and efficient
with **good † routine**

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. $\mathrm{X}\mathrm{X}^T\mathbf{y}$
3. $\mathrm{X}\mathrm{X}^\dagger\mathbf{y}$
4. $\mathrm{X}\mathrm{X}^\dagger\mathrm{X}\mathrm{X}^T\mathbf{y}$

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. $\mathrm{X}\mathrm{X}^T\mathbf{y}$
3. $\mathrm{X}\mathrm{X}^\dagger\mathbf{y}$
4. $\mathrm{X}\mathrm{X}^\dagger\mathrm{X}\mathrm{X}^T\mathbf{y}$

Reference Answer: 3

Note that $\hat{\mathbf{y}} = \mathrm{X}\mathbf{w}_{\text{LIN}}$. Then, a simple substitution of $\mathbf{w}_{\text{LIN}}$ reveals the answer.

Is Linear Regression a 'Learning Algorithm'?

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

No!

- analytic (**closed-form**) solution, 'instantaneous'
- not improving E_{in} nor E_{out} iteratively

Yes!

- good E_{in}? **yes, optimal!**
- good E_{out}? **yes, finite d_{VC} like perceptrons**
- improving iteratively? **somewhat, within an iterative pseudo-inverse routine**

Conclusion: if $E_{\text{out}}(\mathbf{w}_{\text{LIN}})$ is good, **learning 'happened'**!

Benefit of Analytic Solution: 'Simpler-than-VC' Guarantee

$$\overline{E_{\text{in}}} = \underset{\mathcal{D}\sim P^N}{\mathcal{E}}\left\{E_{\text{in}}(\mathbf{w}_{\text{LIN}} \text{ w.r.t. } \mathcal{D})\right\} \overset{\text{to be shown}}{=} \text{noise level} \cdot \left(1 - \frac{d+1}{N}\right)$$

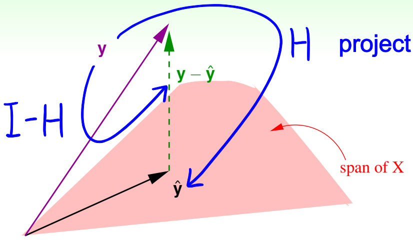
$$E_{\text{in}}(\mathbf{w}_{\text{LIN}}) = \frac{1}{N}\|\mathbf{y} - \underbrace{\hat{\mathbf{y}}}_{\text{predictions}}\|^2 = \frac{1}{N}\|\mathbf{y} - \mathrm{X}\underbrace{\mathrm{X}^{\dagger}\mathbf{y}}_{\mathbf{w}_{\text{LIN}}}\|^2$$

$$= \frac{1}{N}\|(\underbrace{\mathrm{I}}_{\text{identity}} - \mathrm{X}\mathrm{X}^{\dagger})\mathbf{y}\|^2$$

call $\mathrm{X}\mathrm{X}^{\dagger}$ the hat matrix H
because it puts $\wedge$ on $\mathbf{y}$

Geometric View of Hat Matrix

residual transform $\mathrm{I}-\mathrm{H}$



H project

in $\mathbb{R}^N$

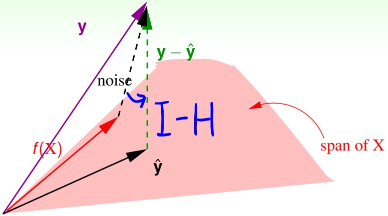
- $\hat{\mathbf{y}} = \mathrm{X}\mathbf{w}_{\text{LIN}}$ within the span of X columns
- $\mathbf{y} - \hat{\mathbf{y}}$ smallest: $\mathbf{y} - \hat{\mathbf{y}} \perp$ span
- H: project $\mathbf{y}$ to $\hat{\mathbf{y}} \in$ span
- $\mathrm{I} - \mathrm{H}$: transform $\mathbf{y}$ to $\mathbf{y} - \hat{\mathbf{y}} \perp$ span

$$\begin{bmatrix} | & | & & | \\ x_0 & x_1 & \cdots & x_d \\ | & | & & | \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}$$

$$= w_0 \begin{bmatrix} | \\ x_0 \\ | \end{bmatrix} + w_1 \begin{bmatrix} | \\ x_1 \\ | \end{bmatrix} + \cdots$$

claim: $\text{trace}(\mathrm{I} - \mathrm{H}) = N - (d+1)$. **Why? :-)**

An Illustrative 'Proof'



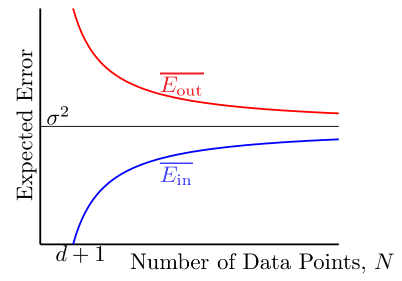
- if **y** comes from some ideal $f(\mathrm{X}) \in$ span plus **noise**
- **noise** transformed by $\mathrm{I} - \mathrm{H}$ to be $\mathbf{y} - \hat{\mathbf{y}}$

$$E_{\text{in}}(\mathbf{w}_{\text{LIN}}) = \frac{1}{N}\|\mathbf{y} - \hat{\mathbf{y}}\|^2 = \frac{1}{N}\|(\mathrm{I} - \mathrm{H})\textbf{noise}\|^2$$
$$= \frac{1}{N}\big(N - (d+1)\big)\|\textbf{noise}\|^2$$

$$\overline{E_{\text{in}}} = \textbf{noise level} \cdot \left(1 - \frac{d+1}{N}\right)$$
$$\overline{E_{\text{out}}} = \textbf{noise level} \cdot \left(1 + \frac{d+1}{N}\right) \textbf{ (complicated!)}$$

The Learning Curve

$$\overline{E_{\text{out}}} = \textbf{noise level} \cdot \left(1 + \frac{d+1}{N}\right)$$
$$\overline{E_{\text{in}}} = \textbf{noise level} \cdot \left(1 - \frac{d+1}{N}\right)$$



- both converge to σ^2 (**noise** level) for $N \to \infty$
- expected generalization error: $\frac{2(d+1)}{N}$
  —**similar to worst-case guarantee from VC**

linear regression (LinReg):
learning 'happened'!

Fun Time

Which of the following property about H is not true?

1. H is symmetric
2. $H^2 = H$ (double projection = single one)
3. $(I - H)^2 = I - H$ (double residual transform = single one)
4. none of the above

Fun Time

Which of the following property about H is not true?

1. H is symmetric
2. $\mathrm{H}^2 = \mathrm{H}$ (double projection = single one)
3. $(\mathrm{I} - \mathrm{H})^2 = \mathrm{I} - \mathrm{H}$ (double residual transform = single one)
4. none of the above

Reference Answer: 4

You can conclude that 2 and 3 are true by their physical meanings! **:-)**

Linear Classification vs. Linear Regression

Linear Classification

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

NP-hard to solve in general

Linear Regression

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

efficient analytic solution

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

Can we treat {-1, +1} as real numbers and apply linear regression on classification problem?

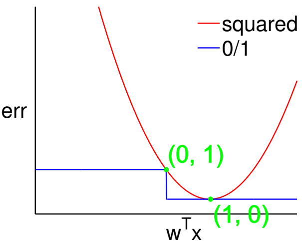
1. run LinReg on binary classification data $\mathcal{D}$ (**efficient**)
2. return $g(\mathbf{x}) = \text{sign}(\mathbf{w}_{\text{LIN}}^T\mathbf{x})$

but explanation of this **heuristic**?

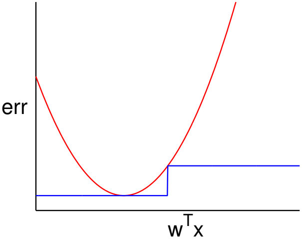
Relation of Two Errors

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

desired $y = 1$



desired $y = -1$



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

Linear Regression for Binary Classification

$$\mathrm{err}_{0/1} \le \mathrm{err}_{\text{sqr}}$$

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

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

$\mathbf{w}_{\text{LIN}}$: useful baseline classifier,
or as **initial PLA/pocket vector** $\mathbf{w}_0$

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

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

Reference Answer: 4

Plot the curves and you'll see. Thus, all three can be used for binary classification. In fact, all three functions connect to very important algorithms in machine learning and we will discuss one of them soon in the next lecture. **Stay tuned. :-)**

Summary

1. When Can Machines Learn?
2. Why Can Machines Learn?

Lecture 8: Noise and Error

3. **How** Can Machines Learn?

Lecture 9: Linear Regression

- Linear Regression Problem
  use hyperplanes to approximate real values
- Linear Regression Algorithm
  analytic solution with pseudo-inverse
- Generalization Issue
  $E_{\text{out}} - E_{\text{in}} \approx \frac{2(d+1)}{N}$ **on average**
- Linear Regression for Binary Classification
  0/1 error $\leq$ squared error

- **next: binary classification, regression, and then?**

4. How Can Machines Learn Better?