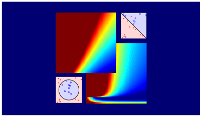
Machine Learning Foundations
(機器學習基石)



Lecture 9: Linear Regression

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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

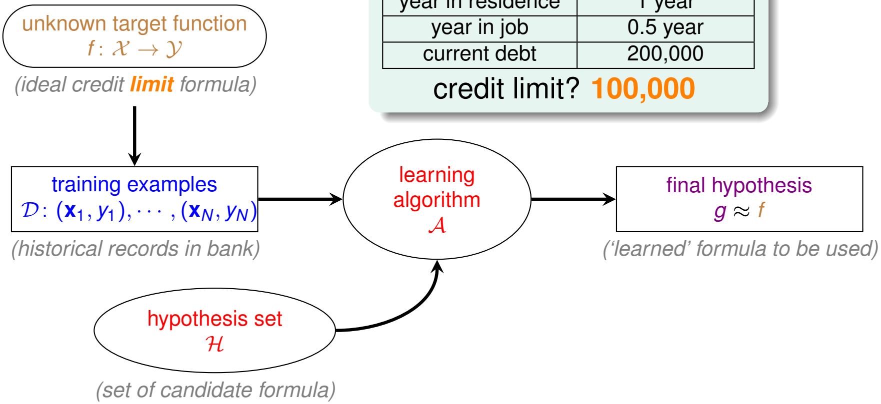
- Linear Regression Problem
- Linear Regression Algorithm
- Generalization Issue

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**



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

Linear Regression Hypothesis

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

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

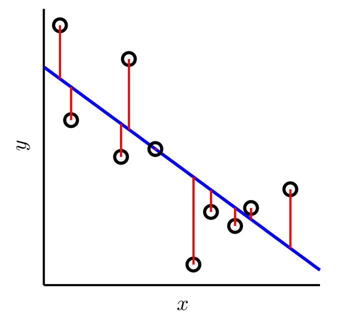
$$y \approx \sum_{i=0}^{d} w_i x_i$$

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

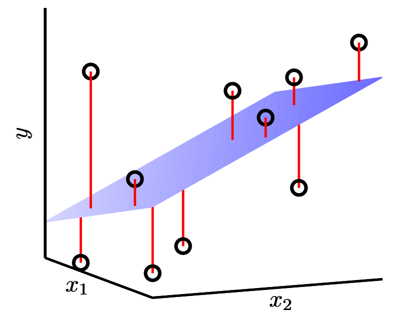
$h(\mathbf{x})$: like **perceptron**, but without the sign

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

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

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

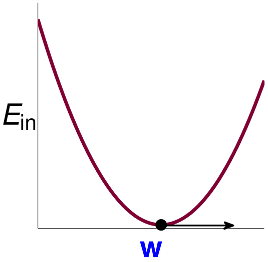
Reference Answer: ②

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' $\mathbf{w}$

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

—not possible to 'roll down'

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

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

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

one w only

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

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

simple! :-)

vector $\mathbf{w}$

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

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

similar (**derived by definition**)

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

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

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

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**

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

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

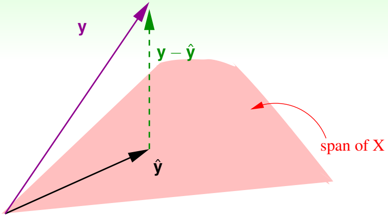
$$\overline{E_{\text{in}}} = \mathop{\mathbb{E}}_{\mathcal{D}\sim P^N}\left\{E_{\text{in}}(\mathbf{w}_{\text{LIN}} \text{ w.r.t. } \mathcal{D})\right\} \overset{\text{to be shown}}{=} \text{noise level} \cdot \left(1 - \frac{d+1}{N}\right)$$

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

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

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

Geometric View of Hat Matrix



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

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

The Hat Matrix

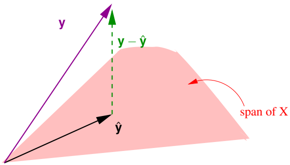
when $X^T X$ invertible, hat matrix $H = X X^\dagger = X(X^T X)^{-1} X^T$

Claim: $H^{1126} = H$

proof (when $X^T X$ invertible):

$$
\begin{aligned}
H^{1126} &= HHH^{1124} \\
&= X(X^T X)^{-1} X^T X(X^T X)^{-1} X^T H^{1124} \\
&= X(X^T X)^{-1}(X^T X)(X^T X)^{-1} X^T H^{1124} \\
&= X(X^T X)^{-1} X^T H^{1124} \\
&= H^{1125}
\end{aligned}
$$

... and you know the rest



geometrically, **projecting** 1126 **times** $\equiv$ projecting once

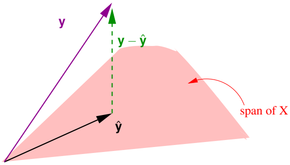
Trace of The Hat Matrix

when X^TX invertible, hat matrix $H = XX^\dagger = X(X^TX)^{-1}X^T$

Claim: $\text{trace}(H) = d + 1$ when X^TX invertible

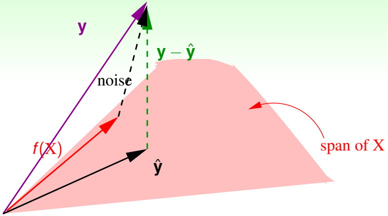
proof:

$$\begin{aligned}\text{trace}(H) &= \text{trace}(X(X^TX)^{-1}X^T)\\ &= \text{trace}(X^TX(X^TX)^{-1})\\ &= \text{trace}(I_{d+1})\\ &= d+1\end{aligned}$$



geometrically, H projects to
a $(d+1)$-dimensional subspace

An Illustrative 'Proof', Corrected



- if **y** comes from some ideal $f(\mathrm{X}) \in$ span plus **noise**
- **noise** with per-dimension 'noise level' σ^2 transformed by $\mathrm{I} - \mathrm{H}$ to be $\mathbf{y} - \hat{\mathbf{y}}$

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

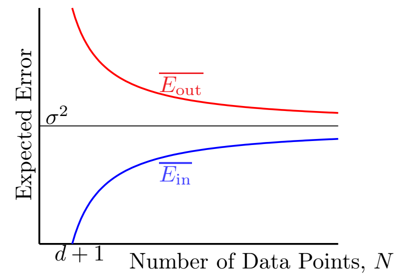
$$= \frac{1}{N}\big(N - (d+1)\big)\sigma^2$$

$$\overline{E_{\text{in}}} = \sigma^2 \cdot \left(1 - \frac{d+1}{N}\right)$$

$$\overline{E_{\text{out}}} = \sigma^2 \cdot \left(1 + \frac{d+1}{N}\right)$$ **(complicated!)**

The Learning Curve

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



- 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. $\mathrm{H}^2 = \mathrm{H}$ (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! **:-)**

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

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

4. How Can Machines Learn Better?