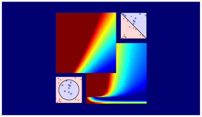
# Machine Learning Foundations
# (機器學習基石)



## Lecture 9: Linear Regression

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

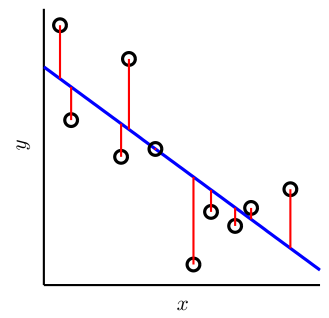
$$y \approx \sum_{i=0}^{d} w_i x_i$$

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

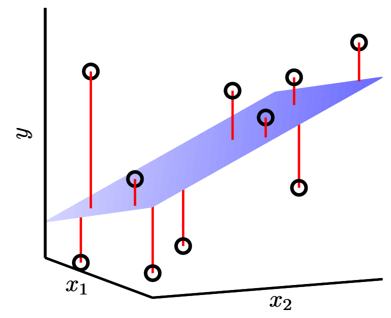
$h(\mathbf{x})$: like **perceptron**, but without the sign

# 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

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

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

# Fun Time

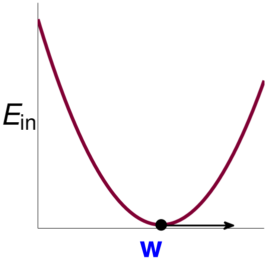
Consider using linear regression hypothesis $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ to predict the credit limit of customers $\mathbf{x}$. Which feature below shall have a positive weight in a **good hypothesis** for the task?

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

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

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

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




- $E_{\text{in}}(\mathbf{w})$: 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 $\nabla E_{\text{in}}(\mathbf{w})$

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

## 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 $\mathrm{X}$ 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**

# Is Linear Regression a 'Learning Algorithm'?

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

**No!**

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

**Yes!**

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

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