EE2211 Introduction to Machine Learning

Lecture 5

Semester 2
2024/2025

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Course Contents

- Introduction and Preliminaries (Xinchao)
  - Introduction
  - Data Engineering
  - Introduction to Probability and Statistics
- Fundamental Machine Learning Algorithms I (Yueming)
  - Systems of linear equations
  - Least squares, Linear regression
  - Ridge regression, Polynomial regression
- Fundamental Machine Learning Algorithms II (Yueming)
  - Over-fitting, bias/variance trade-off
  - Optimization, Gradient descent
  - Decision Trees, Random Forest
- Performance and More Algorithms (Xinchao)
  - Performance Issues
  - K-means Clustering
  - Neural Networks

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Least Squares and Linear Regression

Module II Contents

- Notations, Vectors, Matrices (introduced in L3)
- Operations on Vectors and Matrices
- Systems of Linear Equations
- Set and Functions
- Derivative and Gradient
- Least Squares, Linear Regression
- Linear Regression with Multiple Outputs
- Linear Regression for Classification
- Ridge Regression
- Polynomial Regression

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Recap: Linear and Affine Functions

Linear Functions

A function $f: \mathcal{R}^d \to \mathcal{R}$ is **linear** if it satisfies the following two properties:

- **Homogeneity** $f(\alpha \mathbf{x}) = \alpha f(\mathbf{x})$ Scaling
- **Additivity** $f(\mathbf{x} + \mathbf{y}) = f(\mathbf{x}) + f(\mathbf{y})$ Adding

Inner product function

$$f(\mathbf{x}) = \boldsymbol{a}^T \mathbf{x} = a_1 x_1 + a_2 x_2 + \cdots a_d x_d$$

Affine function (linear function + offset)

$f(\mathbf{x}) = \boldsymbol{a}^T \mathbf{x} + b$ scalar b is called the offset (or bias)

Ref: [Book4] Stephen Boyd and Lieven Vandenberghe, "Introduction to Applied Linear Algebra", Cambridge University Press, 2018 (p31)

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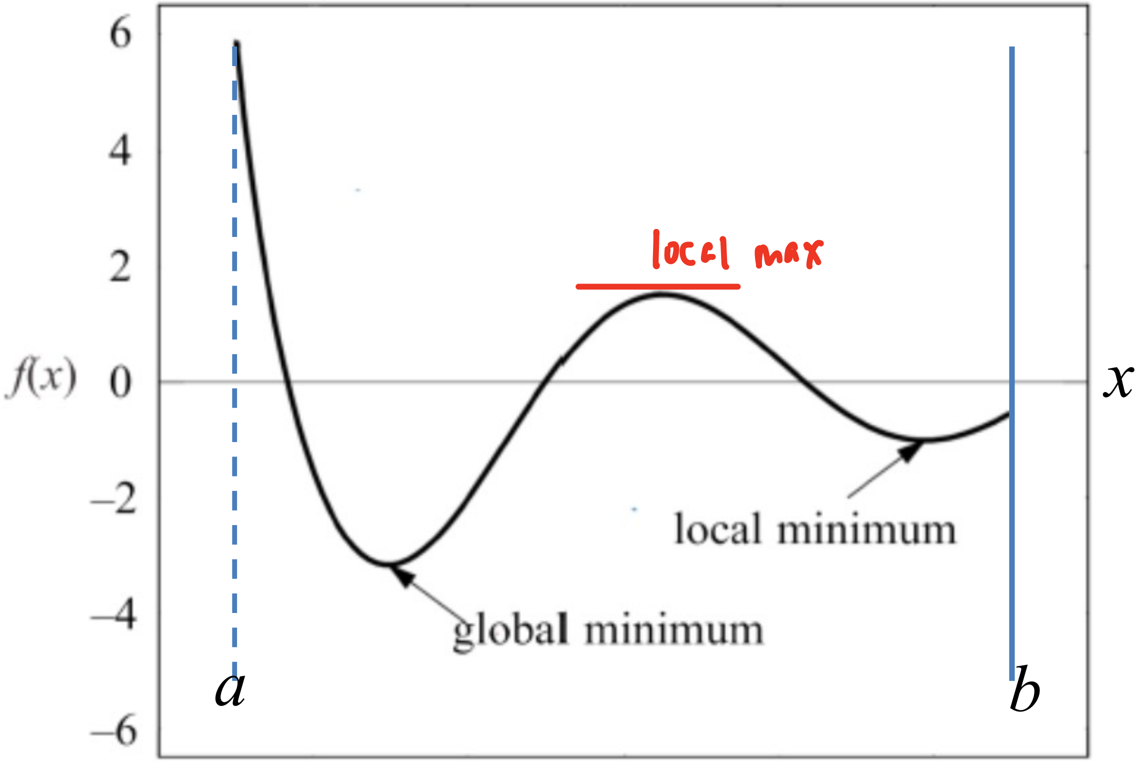
optimization (finding max/min)

Functions: Maximum and Minimum

A local and a global minima of a function



$a < x \leq b$

- $f(x)$ has a **local minimum** at $x = c$ if $f(x) \geq f(c)$ for every x in some open interval around $x = c$

- $f(x)$ has a **global minimum** at $x = c$ if $f(x) \geq f(c)$ for all x in the domain of f

Note: An interval is a set of real numbers with the property that any number that lies between two numbers in the set is also included in the set.
An **open interval** does not include its endpoints and is denoted using parentheses. E.g. (0, 1) means "all numbers greater than 0 and less than 1".

Ref: [Book1] Andriy Burkov, "The Hundred-Page Machine Learning Book", 2019 (p6-7 of chp2).

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Functions: Maximum and Minimum

Max and Arg Max

- Given a set of values $\boldsymbol{\mathcal{A}} = \{a_1,\ a_2, \dots,\ a_m\}$,
- The operator $\max_{a \in \boldsymbol{\mathcal{A}}} f(a)$ returns the highest value $f(a)$ for all elements in the set $\boldsymbol{\mathcal{A}}$
- The operator $\arg\max_{a \in \boldsymbol{\mathcal{A}}} f(a)$ returns the element of the set $\boldsymbol{\mathcal{A}}$ that maximizes $f(a)$
- When the set is **implicit** or **infinite**, we can write

$$\max_{a} f(a) \quad \text{or} \quad \arg\max_{a} f(a)$$

E.g. $f(a) = 3a,\ a \in [0,1] \rightarrow \max_{a} f(a) = 3$ and $\arg\max_{a} f(a) = 1$

max value is $3 \times [1] = 3$

the "max" element

Min and **Arg Min** operate in a similar manner

Note: **arg max** returns a value from the **domain** of the function and **max** returns from the **range (codomain)** of the function.

Ref: [Book1] Andriy Burkov, "The Hundred-Page Machine Learning Book", 2019 (p6-7 of chp2).

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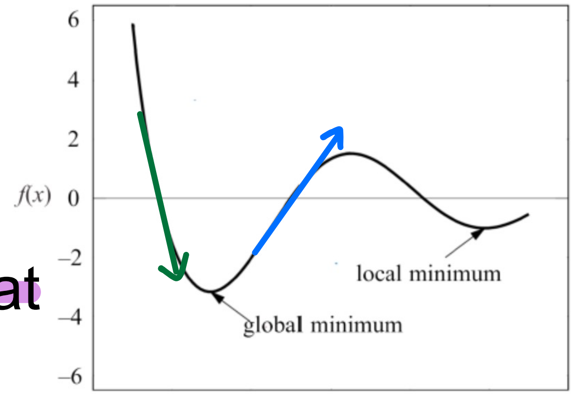
Derivative and Gradient



- The **derivative f'** of a function f is a function that describes how fast f grows (or decreases)
  - If the derivative is a constant value, e.g. 5 or −3
    - The function f grows (or decreases) constantly at any point x of its domain
  - When the derivative f' is a function
    - If f' is positive at some x, then the function f grows at this point
    - If f' is negative at some x, then the function f decreases at this point
    - The derivative of zero at x means that the function's slope at x is horizontal (e.g. maximum or minimum points) → find 2nd derivative

- The process of finding a derivative is called **differentiation.**

- **Gradient** is the generalization of derivative for functions that take several inputs (or one input in the form of a vector or some other complex structure).

Ref: [Book1] Andriy Burkov, "The Hundred-Page Machine Learning Book", 2019 (p8 of chp2).

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Derivative and Gradient

The gradient of a function is a vector of **partial derivatives**

Differentiation of a scalar function w.r.t. a vector

If $f(\mathbf{x})$ is a scalar function of *d* variables, $\mathbf{x}$ is a *d* x1 vector. Then differentiation of $f(\mathbf{x})$ w.r.t. $\mathbf{x}$ results in a *d* x1 vector

(3 input) → (1 output)

$$\frac{df(\mathbf{x})}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_d} \end{bmatrix}$$

$T : R^3 \to R^1$

(x, y, z)

3×1

This is referred to as the **gradient** of $f(\mathbf{x})$ and often written as $\nabla_{\mathbf{x}} f$.

$\nabla = \frac{\partial}{\partial x}\hat{a_x} + \frac{\partial}{\partial y}\hat{a_y} + \frac{\partial}{\partial z}\hat{a_z}$

$\nabla f = \frac{\partial f}{\partial x}\hat{a_x} + \frac{\partial f}{\partial x}\hat{a_y} + \frac{\partial f}{\partial z}\hat{a_z}$

E.g. $f(\mathbf{x}) = ax_1 + bx_2 \quad \nabla_{\mathbf{x}} f = \begin{bmatrix} a \\ b \end{bmatrix}$

Ref: Duda, Hart, and Stork, "Pattern Classification", 2001 (Appendix)

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Derivative and Gradient

Partial Derivatives

<u>Differentiation of a vector function w.r.t. a vector</u>

If $\mathbf{f}(\mathbf{x})$ is a vector function of *size* *h* x1 and $\mathbf{x}$ is a *d* x1 vector.
Then differentiation of $\mathbf{f}(\mathbf{x})$ results in a *h* x *d* matrix

$$\frac{d\mathbf{f}(\mathbf{x})}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_h}{\partial x_1} & \cdots & \frac{\partial f_h}{\partial x_d} \end{bmatrix}$$

The matrix is referred to as the **Jacobian** of $\mathbf{f}(\mathbf{x})$

Ref: Duda, Hart, and Stork, "Pattern Classification", 2001 (Appendix)

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Derivative and Gradient

$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$

$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix}$

Some Vector-Matrix Differentiation Formulae

2×1

$\begin{bmatrix} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 \end{bmatrix}$

x2 functions ⇒ Slide 9

$$\frac{d\mathbf{Ax}}{d\mathbf{x}_{3\times 1}} = \mathbf{A}_{2\times 3}$$

1×3

$$\frac{d(\boldsymbol{b}^T\mathbf{x})}{d\mathbf{x}_{3\times 1}} = \boldsymbol{b}_{1\times 3} \qquad \frac{d(\boxed{\mathbf{y}^T\mathbf{A}}\mathbf{x})}{d\mathbf{x}} = \mathbf{A}^T\mathbf{y}$$

b^T

$b^T = [b_1 \ b_2 \ b_3]$

$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$

$a = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$

$$\frac{d(\mathbf{x}^T\mathbf{Ax})}{d\mathbf{x}} = (\mathbf{A} + \mathbf{A}^T)\mathbf{x}$$

$a^T = [a_1 \ a_2 \ a_3]$

x1 function $b^T x = b_1x_1 + b_2x_2 + b_3x_3$

⇓

Slide 8 $\frac{\partial b^T x}{\partial x} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = b$

$$f(\mathbf{x}) = \boldsymbol{a}^T\mathbf{x} = a_1x_1 + a_2x_2 + \cdots a_dx_d$$

Derivations: https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf

Ref: Duda, Hart, and Stork, "Pattern Classification", 2001 (Appendix)

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Poll on PollEv.com/ymjin

Just “**skip**” if you are required to do registration

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Suppose y = 3x+5, this is a linear function. 0

1) homogeneity
2) additivity

True — 0%

False ✓ (Affine function → Linear + offset) — 0%

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When poll is active respond at **PollEv.com/ymjin**

rows

Suppose $g(x)$ is a scalar function of d variables where x is a $d \times 1$ vector, the outcome of differentiation of $g(x)$ w.r.t. x is a $d \times 1$ vector.

0

True

0%

False

0%

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Linear Regression

- **Linear regression** is a popular regression learning algorithm that learns a model which is a linear combination of features of the input example.

$$\mathbf{X}\mathbf{w} = \mathbf{y}, \quad \overset{\text{(matrix)}}{\mathbf{X} \in \mathcal{R}^{m\times d}}, \ \overset{\text{(vector)}}{\mathbf{w} \in \mathcal{R}^{d\times 1}}, \ \overset{\text{(vector)}}{\mathbf{y} \in \mathcal{R}^{m\times 1}}$$

$$\mathbf{X} = \begin{array}{c} \begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m,1} & x_{m,2} & \cdots & x_{m,d} \end{bmatrix} \\ \begin{array}{cccc} \text{feature 1} & \text{feature 2} & & \text{feature 3} \end{array} \end{array} \begin{array}{l} \text{sample 1} \\ \\ \text{sample 2} \\ \\ \end{array}, \qquad \mathbf{w} = \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

Ref: [Book1] Andriy Burkov, "The Hundred-Page Machine Learning Book", 2019 (p3 of chp3).

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Linear Regression

Don't use data from testing set when training the model!

Problem Statement: To predict the unknown y for a given $\mathbf{x}$ **(testing)**

- We have a collection of labeled examples **(training)** $\{(\mathbf{x}_i, y_i)\}_{i=1}^{m}$
  - m is the size of the collection
  - $\mathbf{x}_i$ is the d-dimensional feature vector of example $i = 1, \ldots, m$ (input)
  - y_i is a real-valued target (1-D) - output
  - Note:
    - when y_i is **continuous** valued, it is a **regression problem** (ie, like age)
    - when y_i is **discrete** valued, it is a **classification problem** (ie, like gender)

- We want to build a model $f_{\mathbf{w},b}(\mathbf{x})$ as a linear combination of features of example $\mathbf{x}$: $f_{\mathbf{w},b}(\mathbf{x}) = \mathbf{x}^T\mathbf{w} + b$

  where $\mathbf{w}$ is a d-dimensional vector of parameters and b is a real number.
- The notation $f_{\mathbf{w},b}$ means that the model f is parametrized by two values: $\mathbf{w}$ and b

Ref: [Book4] Stephen Boyd and Lieven Vandenberghe, "Introduction to Applied Linear Algebra", Cambridge University Press, 2018 (chp.14)

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Linear Regression

Learning objective function

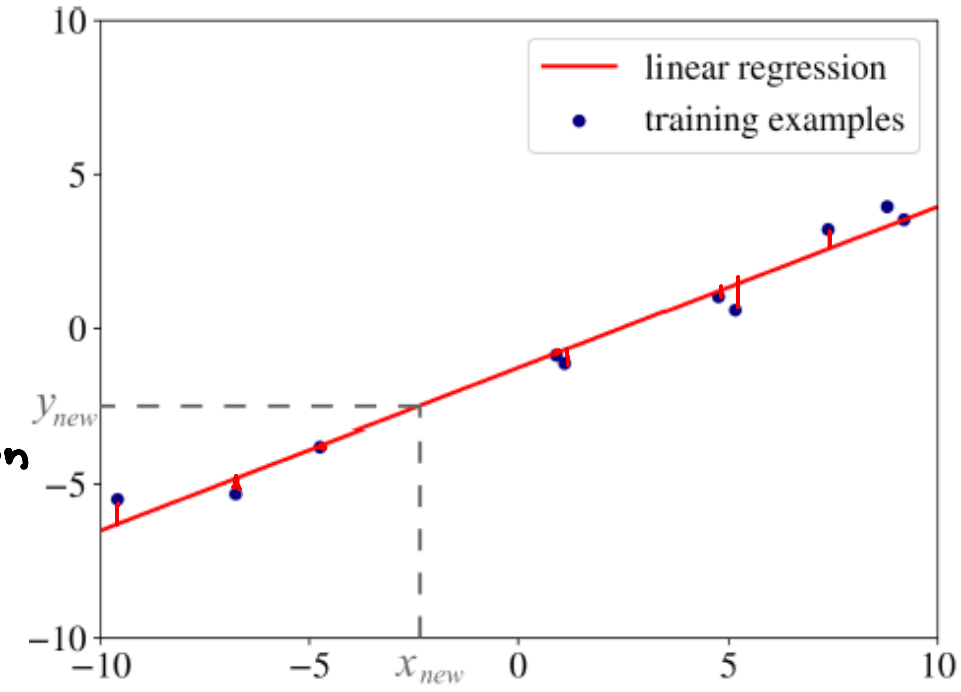
- To find the optimal values for $\mathbf{w}^*$ and b^* which **minimizes** the following expression:

ground truth

$$\boxed{\frac{1}{m}\sum_{i=1}^{m}\left(f_{\mathbf{w},b}(\mathbf{x}_i) - \mathrm{y}_i\right)^2}$$

prediction

- In mathematics, the expression we minimize or maximize is called an **objective function**, or, simply, an **objective**



$(f_{\mathbf{w}}(\mathbf{x}_i) - \mathrm{y}_i)^2$ is called the **loss function**: a measure of the difference between $f_{\mathbf{w}}(\mathbf{x}_i)$ and y_i or a penalty for misclassification of example *i*.

Ref: [Book1] Andriy Burkov, "The Hundred-Page Machine Learning Book", 2019 (chp3.1.2)

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Linear Regression

Learning objective function (using simplified notation hereon)

- To find the optimal values for $\mathbf{w}^*$ which **minimizes** the following expression:

$$\sum_{i=1}^{m} (f_{\mathbf{w}}(\mathbf{x}_i) - \mathrm{y}_i)^2$$

with $f_{\mathbf{w}}(\mathbf{x}_i) = \mathbf{x}^T\mathbf{w}$, (pg 19)

where we define $\mathbf{w} = [b, w_1, \ldots w_d]^T = [w_0, w_1, \ldots w_d]^T$,

and $\mathbf{x}_i = [1, x_{i,1}, \ldots x_{i,d}]^T = [x_{i,0}, x_{i,1}, \ldots x_{i,d}]^T$ $, i = 1, \ldots, m$

- This particular choice of the loss function is called **squared error loss**

Note: The normalization factor $\frac{1}{m}$ can be omitted as it does not affect the optimization.

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Linear Regression

$$\sum_{i=1}^{m}\left(f_{\mathbf{w},b}(\mathbf{x}_i) - y_i\right)^2$$

- All model-based learning algorithms have a **loss function**
- What we do to find the best model is **to minimize the objective** known as the **cost function**
- **Cost function** is a sum of **loss functions** over training set plus possibly some model complexity penalty (regularization)

- In linear regression, the cost function is given by the *average loss*, also called the **empirical risk** because we do not have all the data (e.g. testing data)
  - The average of all penalties is obtained by applying the model to the training data

Ref: [Book1] Andriy Burkov, "The Hundred-Page Machine Learning Book", 2019 (chp3.1.2)

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Linear Regression

Learning (Training)

- Consider the set of feature vector $\mathbf{x}_i$ and target output y_i indexed by $i = 1, \dots, m$, a linear model $f_{\mathbf{w}}(\mathbf{x}) = \mathbf{x}^T\mathbf{w}$ can be stacked as

$$\boldsymbol{f}_{\mathbf{w}}(\mathbf{X}) = \mathbf{X}\mathbf{w} \quad \Longleftrightarrow \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

Learning Model

(matrix)

(target output)

Learning target vector

$$= \begin{bmatrix} \mathbf{x}_1^T\mathbf{w} \\ \vdots \\ \mathbf{x}_m^T\mathbf{w} \end{bmatrix}$$

set of feature vectors

[pg 17]

$$\text{where} \quad \mathbf{x}_i^T\mathbf{w} = [1, x_{i,1}, \dots, x_{i,d}] \begin{bmatrix} b \\ w_1 \\ \vdots \\ w_d \end{bmatrix}$$

Note: The **bias/offset term** is responsible for **translating** the line/plane/hyperplane away from the origin.

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Linear Regression

Least Squares Regression

In vector-matrix notation, the minimization of the objective function can be written compactly using $\mathbf{e} = \mathbf{Xw} - \mathbf{y}$:

$$
\begin{aligned}
\mathrm{J}(\mathbf{w}) = {} & \mathbf{e}^T\mathbf{e} \\
& = (\mathbf{Xw} - \mathbf{y})^T(\mathbf{Xw} - \mathbf{y}) \\
& = (\mathbf{w}^T\mathbf{X}^T - \mathbf{y}^T)(\mathbf{Xw} - \mathbf{y}) \\
& = \mathbf{w}^T\mathbf{X}^T\mathbf{Xw} - \mathbf{w}^T\mathbf{X}^T\mathbf{y} - \mathbf{y}^T\mathbf{Xw} + \mathbf{y}^T\mathbf{y} \\
& = \mathbf{w}^T\mathbf{X}^T\mathbf{Xw} - 2\mathbf{y}^T\mathbf{Xw} + \mathbf{y}^T\mathbf{y}.
\end{aligned}
$$

1. Both $\mathbf{w}^T\mathbf{X}^T\mathbf{y}$ and $\mathbf{y}^T\mathbf{Xw}$ are scalars
2. Equal when transposed

$\Rightarrow \mathbf{w}^\mathrm{T}\mathbf{X}^\mathrm{T}\mathbf{y} = (\mathbf{w}^\mathrm{T}\mathbf{X}^\mathrm{T}\mathbf{y})^\mathrm{T} == \mathbf{y}^\mathrm{T}(\mathbf{X}^\mathrm{T})^\mathrm{T}(\mathbf{w}^\mathrm{T})^\mathrm{T} = \mathbf{y}^T\mathbf{Xw}$

Note: when $\boldsymbol{f}_\mathbf{w}(\mathbf{X}) = \mathbf{Xw}$, then

$$\sum_{i=1}^{m}(f_\mathbf{w}(\mathbf{x}_i) - y_i)^2 = (\mathbf{Xw} - \mathbf{y})^T(\mathbf{Xw} - \mathbf{y}).$$

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Linear Regression

Differentiating $\mathrm{J}(\mathbf{w})$ with respect to $\mathbf{w}$ and setting the result to $\mathbf{0}$:

$$\frac{\partial}{\partial \mathbf{w}} \mathrm{J}(\mathbf{w}) = \mathbf{0}$$

$$\frac{\partial}{\partial \mathbf{w}} (\mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w} - 2\mathbf{y}^T\mathbf{X}\mathbf{w} + \mathbf{y}^T\mathbf{y}) = \mathbf{0}$$

$$\Rightarrow 2\mathbf{X}^T\mathbf{X}\mathbf{w} - 2\mathbf{X}^T\mathbf{y} = \mathbf{0}$$

$$\Rightarrow \mathbf{X}^T\mathbf{X}\mathbf{w} = \mathbf{X}^T\mathbf{y}$$

$\Rightarrow$ Any minimizer $\widehat{\mathbf{w}}$ of $\mathrm{J}(\mathbf{w})$ must satisfy $\mathbf{X}^T(\mathbf{X}\mathbf{w} - \mathbf{y}) = \mathbf{0}$.

If $\mathbf{X}^T\mathbf{X}$ is invertible, then

Learning/training: $\widehat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

Prediction/testing: $\hat{f}_{\mathbf{w}}(\mathbf{X}_{new}) = \mathbf{X}_{new}\widehat{\mathbf{w}}$

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Linear Regression *****

Example 1 Training set

$\{(x_i, y_i)\}_{i=1}^{m}$

training data

$\{x=-9\} \rightarrow \{y=-6\}$
$\{x=-7\} \rightarrow \{y=-6\}$
$\{x=-5\} \rightarrow \{y=-4\}$
$\{x=1\} \rightarrow \{y=-1\}$
$\{x=5\} \rightarrow \{y=1\}$
$\{x=9\} \rightarrow \{y=4\}$

[pg 17]

*** Add 1 in front of each x

add ** offset

tall matrix - over determined

$$\underset{\mathbf{X}}{\begin{bmatrix} 1 & -9 \\ 1 & -7 \\ 1 & -5 \\ 1 & 1 \\ 1 & 5 \\ 1 & 9 \end{bmatrix}} \underset{\mathbf{w}}{\begin{bmatrix} w_0 \\ w_1 \end{bmatrix}} = \underset{\mathbf{y}}{\begin{bmatrix} -6 \\ -6 \\ -4 \\ -1 \\ 1 \\ 4 \end{bmatrix}}$$

This set of linear equations has no exact solution

However, $\mathbf{X}^T\mathbf{X}$ is invertible

Least square approximation

(left-inverse)

$$\hat{\mathbf{w}} = \mathbf{X}^\dagger \mathbf{y} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

$$= \begin{bmatrix} 6 & -6 \\ -6 & 262 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ -9 & -7 & -5 & 1 & 5 & 9 \end{bmatrix} \begin{bmatrix} -6 \\ -6 \\ -4 \\ -1 \\ 1 \\ 4 \end{bmatrix} = \begin{bmatrix} -1.4375 \\ 0.5625 \end{bmatrix}$$

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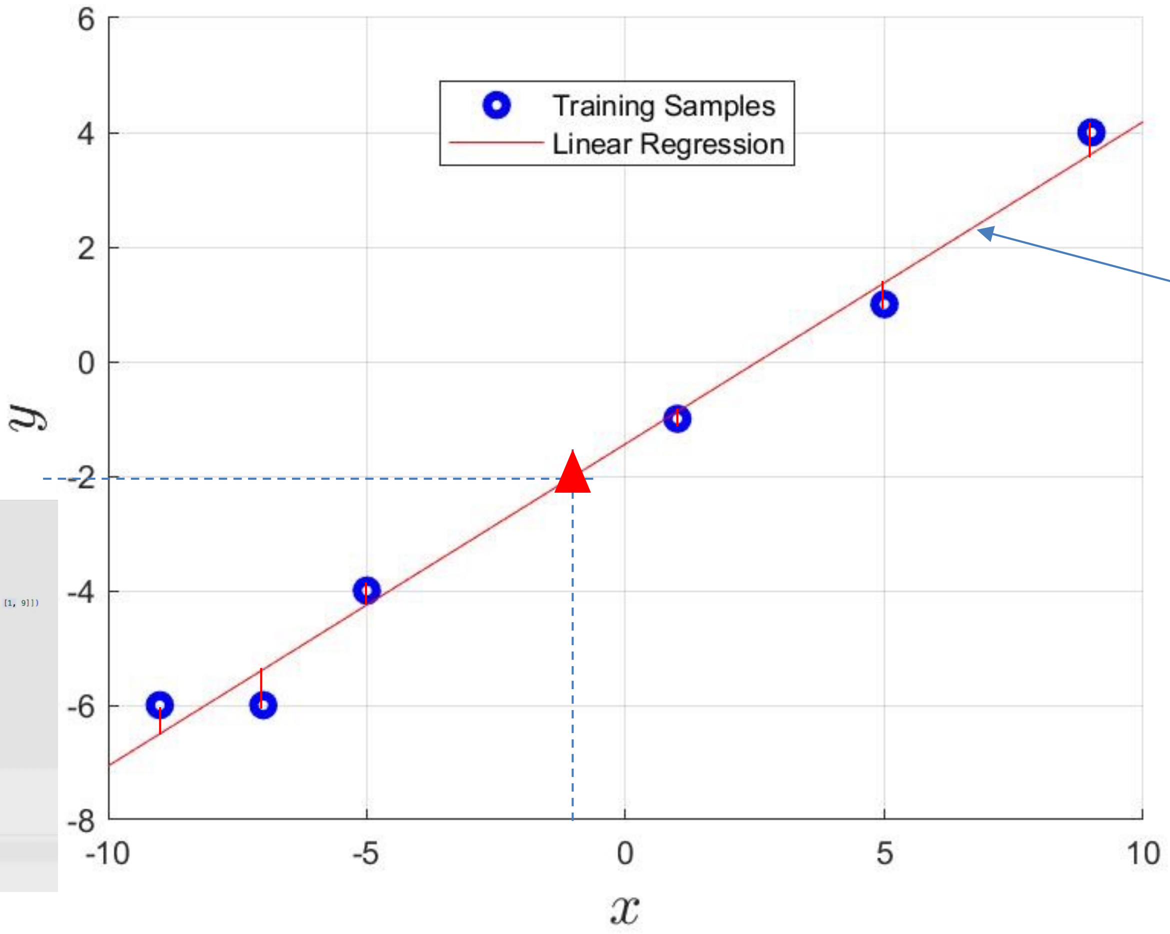
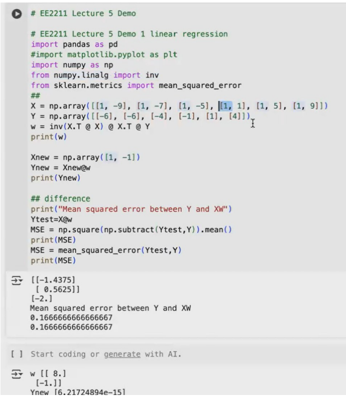
Linear Regression





```
# EE2211 Lecture 5 Demo

# EE2211 Lecture 5 Demo 1 linear regression
import pandas as pd
#import matplotlib.pyplot as plt
import numpy as np
from numpy.linalg import inv
from sklearn.metrics import mean_squared_error
##
X = np.array([[1, -9], [1, -7], [1, -5], [1, 1], [1, 5], [1, 9]])
Y = np.array([[-6], [-6], [-4], [-1], [1], [4]])
w = inv(X.T @ X) @ X.T @ Y
print(w)

Xnew = np.array([1, -1])
Ynew = Xnew@w
print(Ynew)

## difference
print("Mean squared error between Y and XW")
Ytest=X@w
MSE = np.square(np.subtract(Ytest,Y)).mean()
print(MSE)
MSE = mean_squared_error(Ytest,Y)
print(MSE)
```

```
[[-1.4375]
 [ 0.5625]]
[-2.]
Mean squared error between Y and XW
0.16666666666666667
0.16666666666666667
```

```
[ ] Start coding or generate with AI.
```

```
w [[ 8.]
 [-1.]]
Ynew [6.21724894e-15]
```

Linear Regression on one-dimensional samples

$$\hat{y} = \mathbf{X}\hat{\mathbf{w}}$$

$$= \mathbf{X}\begin{bmatrix}-1.4375\\0.5625\end{bmatrix}$$

$$y = -1.4375+0.5625x$$

Prediction:

Test set

$$\{x = -1\} \rightarrow \{y = ?\}$$

add 1 in front

$$\hat{y} = [1 \quad -1]\begin{bmatrix}-1.4375\\0.5625\end{bmatrix}$$

$$= -2$$

Python demo 1

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Linear Regression

Example 2

training data

$\{(\mathbf{x}_i, y_i)\}_{i=1}^{m}$

$\{x_1 = 1, x_2 = 1, \quad x_3 = 1\} \rightarrow \{y = 1\}$
$\{x_1 = 1, x_2 = -1, x_3 = 1\} \rightarrow \{y = 0\}$
$\{x_1 = 1, x_2 = 1, \quad x_3 = 3\} \rightarrow \{y = 2\}$
$\{x_1 = 1, x_2 = 1, \quad x_3 = 0\} \rightarrow \{y = -1\}$

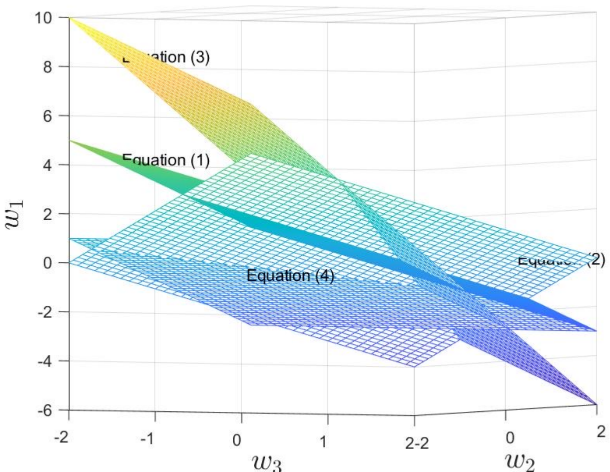
given training data
first element already 1, no need to add IN THIS CASE

Training set

no need add offset

already in training data no need add
tall matrix
- over determined

$$\overset{\mathbf{X}}{\begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 3 \\ 1 & 1 & 0 \end{bmatrix}} \overset{\mathbf{w}}{\begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}} = \overset{\mathbf{y}}{\begin{bmatrix} 1 \\ 0 \\ 2 \\ -1 \end{bmatrix}}$$



This set of linear equations has no exact solution

However, $\mathbf{X}^T\mathbf{X}$ is invertible (left inverse)

check!!

$$\hat{\mathbf{w}} = \mathbf{X}^{\dagger}\mathbf{y} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Least square approximation

↳ over-determined system

$$= \begin{bmatrix} 4 & 2 & 5 \\ 2 & 4 & 3 \\ 5 & 3 & 11 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & 3 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 2 \\ -1 \end{bmatrix} = \begin{bmatrix} -0.7500 \\ 0.1786 \\ 0.9286 \end{bmatrix}$$

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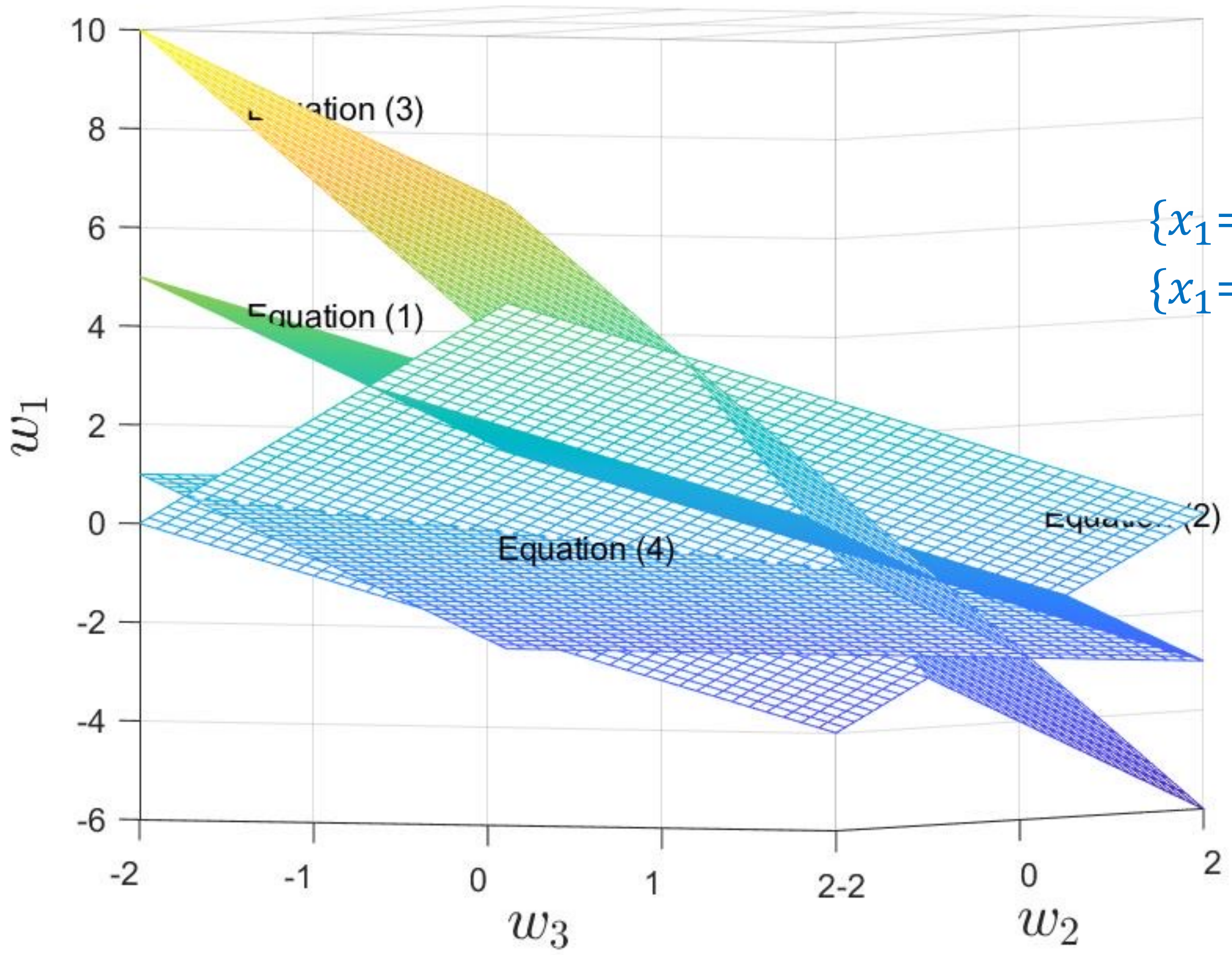
Linear Regression

The four linear equations



Prediction:

Test set

$$\{x_1 = 1, x_2 = 6, \quad x_3 = 8\} \rightarrow \{y = ?\}$$
$$\{x_1 = 1, x_2 = 0, x_3 = -1\} \rightarrow \{y = ?\}$$

$$\hat{\boldsymbol{y}} = \hat{\boldsymbol{f}}_{\mathbf{w}}(\mathbf{X}_{new}) = \mathbf{X}_{new}\hat{\mathbf{w}}$$

$$\hat{\boldsymbol{y}} = \begin{bmatrix} 1 & 6 & 8 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} -0.7500 \\ 0.1786 \\ 0.9286 \end{bmatrix}$$

$$= \begin{bmatrix} 7.7500 \\ -1.6786 \end{bmatrix}$$

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Linear Regression

Learning of Vectored Function (Multiple Outputs)

For one sample: a linear model $\mathbf{f_w}(\mathbf{x}) = \mathbf{x}^T\mathbf{W}$

Vector function

For m samples: $\mathbf{F_w}(\mathbf{X}) = \mathbf{X}\mathbf{W} = \mathbf{Y}$ → W and Y become matrix instead of vector

$$\begin{array}{l} \text{Sample } 1 \dashrightarrow \\ \vdots \\ \text{Sample } m \dashrightarrow \end{array} = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_m^T \end{bmatrix} \mathbf{W} = \begin{bmatrix} 1 & x_{1,1} & \dots & x_{1,d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{m,1} & \dots & x_{m,d} \end{bmatrix} \underbrace{\begin{bmatrix} w_{0,1} & \dots & w_{0,h} \\ w_{1,1} & \dots & w_{1,h} \\ \vdots & \ddots & \vdots \\ w_{d,1} & \dots & w_{d,h} \end{bmatrix}}_{h}$$

$$\begin{array}{l} \text{Sample 1's output} \dashrightarrow \\ \vdots \\ \text{Sample } m\text{'s output} \dashrightarrow \end{array} = \underbrace{\begin{bmatrix} y_{1,1} & \dots & y_{1,h} \\ & \vdots & \\ y_{m,1} & \dots & y_{m,h} \end{bmatrix}}_{h} \Big\} m$$

add 1   add offset

$$\mathbf{X} \in \mathcal{R}^{m\times(d+1)}, \ \mathbf{W} \in \mathcal{R}^{(d+1)\times h}, \ \mathbf{Y} \in \mathcal{R}^{m\times h}$$

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Linear Regression

Objective: $\sum_{i=1}^{m}(\mathbf{f_w}(\mathbf{x}_i) - \mathbf{y}_i)^2 = \boldsymbol{E}^T\boldsymbol{E}$

Least Squares Regression of Multiple Outputs

In matrix notation, the sum of squared errors cost function can be written compactly using $\mathbf{E} = \mathbf{XW} - \mathbf{Y}$:

$$\underbrace{\mathrm{J}(\mathbf{W})}_{\text{scalar value}} = \mathrm{trace}(\mathbf{E}^T\mathbf{E})$$

$$= \mathrm{trace}[(\mathbf{XW} - \mathbf{Y})^T(\mathbf{XW} - \mathbf{Y})]$$

If $\mathbf{X}^T\mathbf{X}$ is invertible, then

Learning/training: $\widehat{\mathbf{W}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$

Prediction/testing: $\hat{\mathbf{F}}_{\mathbf{w}}(\mathbf{X}_{new}) = \mathbf{X}_{new}\widehat{\mathbf{W}}$

Ref: Hastie, Tibshirani, Friedman, "The Elements of Statistical Learning", (2nd ed., 12th printing) 2017 (chp.3.2.4)

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Linear Regression

Least Squares Regression of Multiple Outputs

$$J(\mathbf{W}) = \mathrm{trace}(\mathbf{E}^T\mathbf{E})$$

$$= \mathrm{trace}\left(\begin{bmatrix} \mathbf{e}_1^T \\ \vdots \\ \mathbf{e}_h^T \end{bmatrix} [\mathbf{e}_1 \quad \mathbf{e}_2 \quad \dots \quad \mathbf{e}_h]\right)$$

$$= \mathrm{trace}\left(\begin{bmatrix} \mathbf{e}_1^T\mathbf{e}_1 & \mathbf{e}_1^T\mathbf{e}_2 & \dots & \mathbf{e}_1^T\mathbf{e}_h \\ \mathbf{e}_2^T\mathbf{e}_1 & \mathbf{e}_2^T\mathbf{e}_2 & \dots & \mathbf{e}_2^T\mathbf{e}_h \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{e}_h^T\mathbf{e}_1 & \mathbf{e}_h^T\mathbf{e}_2 & \dots & \mathbf{e}_h^T\mathbf{e}_h \end{bmatrix}\right) = \boxed{\sum_{k=1}^{h} \mathbf{e}_k^T\mathbf{e}_k}$$

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Linear Regression of multiple outputs

Example 3

(3 features)

Training set $\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{m}$

$\{x_1 = 1, x_2 = 1, \quad x_3 = 1\} \rightarrow \{y_1 = 1, \quad y_2 = 0\}$
$\{x_1 = 1, x_2 = -1, x_3 = 1\} \rightarrow \{y_1 = 0, \quad y_2 = 1\}$
$\{x_1 = 1, x_2 = 1, \quad x_3 = 3\} \rightarrow \{y_1 = 2, y_2 = -1\}$
$\{x_1 = 1, x_2 = 1, \quad x_3 = 0\} \rightarrow \{y_1 = -1, y_2 = 3\}$

$\mathbf{X}$ (4x3) $\quad \mathbf{W}$ (3x2) $\quad \mathbf{Y}$ (4x2)

(3 rows)

Bias

tall matrix

- over determined

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 3 \\ 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} w_{1,1} & w_{1,2} \\ w_{2,1} & w_{2,2} \\ w_{3,1} & w_{3,2} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 2 & -1 \\ -1 & 3 \end{bmatrix}$$

This set of linear equations has NO exact solution

Check if square matrix and

→ det ≠ 0

Least square approximation

↳ over-determined system

(left inverse)

$$\hat{\mathbf{W}} = \mathbf{X}^{\dagger}\mathbf{Y} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

$\mathbf{X}^T\mathbf{X}$ is invertible

$$= \begin{bmatrix} 4 & 2 & 5 \\ 2 & 4 & 3 \\ 5 & 3 & 11 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & 3 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 2 & -1 \\ -1 & 3 \end{bmatrix} = \begin{bmatrix} -0.75 & 2.25 \\ 0.1786 & 0.0357 \\ 0.9286 & -1.2143 \end{bmatrix}$$

$y_1 \qquad y_2$

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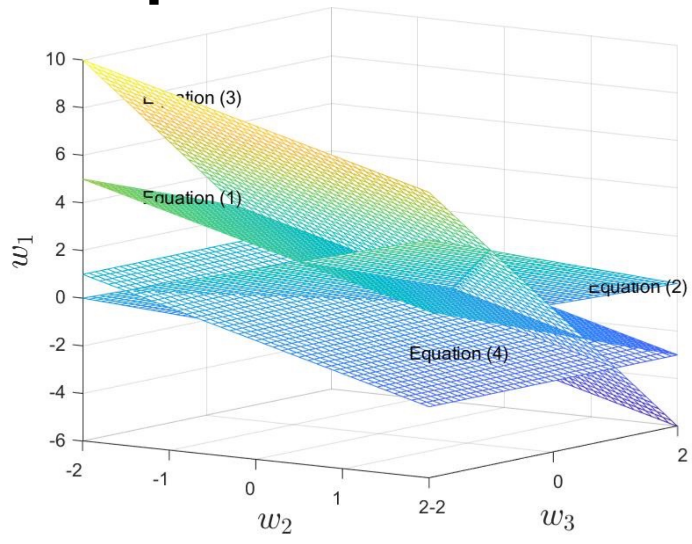
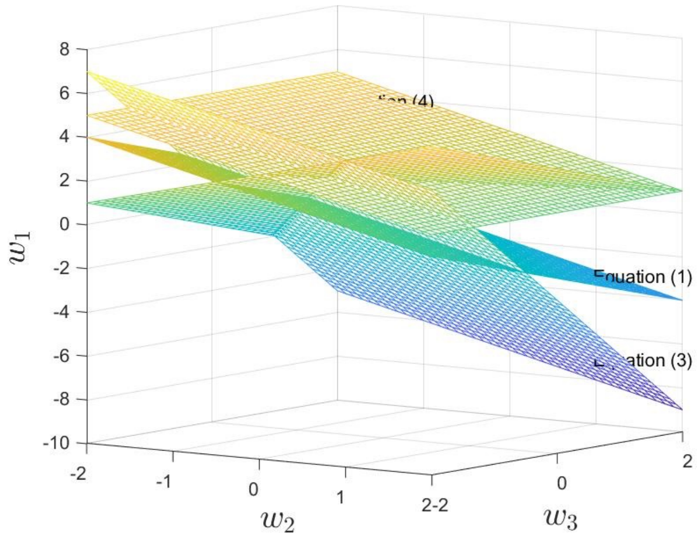
Linear Regression of multiple outputs

Example 3





Prediction:

Test set: two new samples

$$\{x_1 = 1, x_2 = 6, \quad x_3 = 8\} \rightarrow \{y_1 = ?, y_2 = ?\}$$

$$\{x_1 = 1, x_2 = 0, x_3 = -1\} \rightarrow \{y_1 = ?, y_2 = ?\}$$

$$\boxed{\hat{\mathbf{Y}} = \mathbf{X}_{new}\hat{\mathbf{W}}}$$

Bias

$$= \begin{bmatrix} 1 & 6 & 8 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} -0.75 & 2.25 \\ 0.1786 & 0.0357 \\ 0.9286 & -1.2143 \end{bmatrix}$$

$$= \begin{bmatrix} 7.75 & -7.25 \\ -1.6786 & 3.4643 \end{bmatrix}$$

```
[ ] # EE2211 Lecture 5 Demo 2
    import pandas as pd
    import matplotlib.pyplot as plt
    import numpy as np
    from numpy.linalg import inv
    from sklearn.metrics import mean_squared_error
    ##
    X = np.array([[1, 1, 1], [1, -1, 1], [1, 1, 3], [1, 1, 0]])
    Y = np.array([[1, 0], [0, 1], [2, -1], [-1, 3]])
    w = inv(X.T @ X) @ X.T @ Y
    print("the estimated w")
    print(w)

    Xnew = np.array([[1, 6, 8], [1, 0, -1]])
    Ynew = Xnew@w
    print("testing Ynew")
    print(Ynew)

    ## difference
    print("Mean squared error between Y and XW")
    Ytest=X@w
    MSE = np.square(np.subtract(Ytest,Y)).mean()
    print(MSE)
    MSE = mean_squared_error(Ytest,Y)
    print(MSE)

    the estimated w
    [[-0.75        2.25      ]
     [ 0.17857143  0.03571429]
     [ 0.92857143 -1.21428571]]
    testing Ynew
    [[ 7.75       -7.25      ]
     [-1.67857143  3.46428571]]
    Mean squared error between Y and XW
    0.3035714285714286
    0.3035714285714286
```

Python demo 2

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Linear Regression of multiple outputs

Example 4

The values of feature x and their corresponding values of multiple outputs target **y** are shown in the table below.

Based on the least square regression, what are the values of **w**?
Based on the current mapping, when x = 2, what is the value of **y**?

x	[3]	[4]	[10]	[6]	[7]
y	[0, 5]	[1.5, 4]	[-3, 8]	[-4, 10]	[1, 6]

```python
# EE2211 Lecture 5 Demo 3
import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
from numpy.linalg import inv
from sklearn.metrics import mean_squared_error
##
X = np.array([[1, 3], [1, 4], [1, 10], [1, 6], [1, 7]])
Y = np.array([[0, 5], [1.5, 4], [-3, 8], [-4, 10], [1, 6]])
w = inv(X.T @ X) @ X.T @ Y
print('W')
print(w)

Xnew = np.array([[1, 2]])

Ynew = Xnew@w

print('Ynew')
print(Xnew)
print(Xnew.shape)
print(Ynew)

Ytest= X@w
print('Ytest')
print(Ytest)
plt.plot(X[:,1], Y[:,0], 'o', label = 'Y1')
plt.plot(X[:,1], Y[:,1], 'x', label = 'Y2')
plt.plot(X[:,1], Ytest[:,0])
plt.plot(X[:,1], Ytest[:,1])
plt.xlabel('X')
plt.ylabel('Y')
plt.show()
```

$$\hat{\mathbf{W}} = \mathbf{X}^{\dagger}\mathbf{Y} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} = \begin{bmatrix} 1.9 & 3.6 \\ -0.4667 & 0.5 \end{bmatrix}$$

Python demo 3

$$\widehat{\mathbf{Y}_{new}} = \mathbf{X}_{new}\,\hat{\mathbf{W}} = [1 \quad 2]\,\hat{\mathbf{W}} = [0.9667 \quad 4.6]$$

Prediction

↳ add 1

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Summary

- Notations, Vectors, Matrices
- Operations on Vectors and Matrices
  - Dot-product, matrix inverse
- Systems of Linear Equations $\boldsymbol{f}_{\mathbf{w}}(\mathbf{X}) = \mathbf{X}\mathbf{w} = \mathbf{y}$
  - Matrix-vector notation, linear dependency, invertible
  - Even-, over-, under-determined linear systems
- Functions, Derivative and Gradient
  - Inner product, linear/affine functions
  - Maximum and minimum, partial derivatives, gradient
- Least Squares, Linear Regression
  - Objective function, loss function
  - Least square solution, training/learning and testing/prediction
  - Linear regression with multiple outputs

Learning/training $\hat{\mathbf{w}} = (\mathbf{X}_{train}^T \mathbf{X}_{train})^{-1} \mathbf{X}_{train}^T \mathbf{y}_{train}$

Prediction/testing $\mathbf{y}_{test} = \mathbf{X}_{test}\, \hat{\mathbf{w}}$

- Classification
- Ridge Regression
- Polynomial Regression

Python packages: numpy, pandas, matplotlib.pyplot, numpy.linalg, and sklearn.metrics (for mean_squared_error), numpy.linalg.pinv

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