LINEAR MODEL

Bùi Tiến Lên

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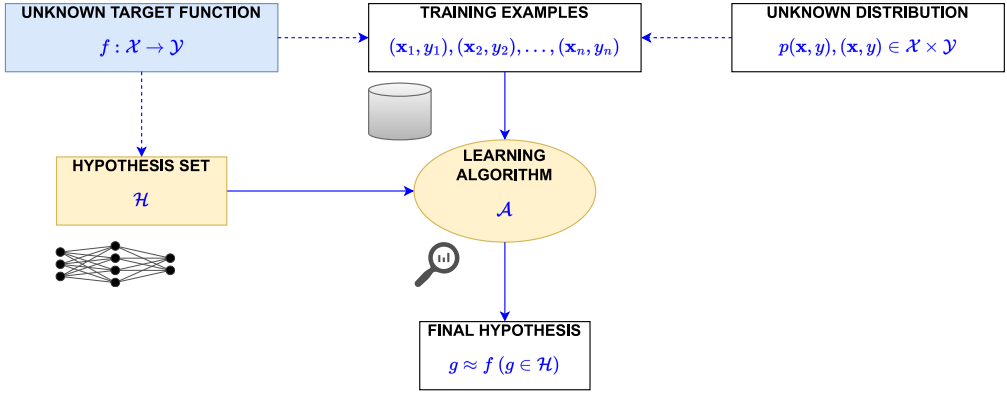
Contents

Notation

symbol	meaning
$a, b, c, N \ldots$	scalar number
$\boldsymbol{w}, \boldsymbol{v}, \boldsymbol{x}, \boldsymbol{y} \ldots$	column vector
$\boldsymbol{X}, \boldsymbol{Y} \ldots$	matrix
$\mathbb{R}$	set of real numbers
$\mathbb{Z}$	set of integer numbers
$\mathbb{N}$	set of natural numbers
$\mathbb{R}^D$	set of vectors
$\mathcal{X}, \mathcal{Y}, \ldots$	set
$\mathcal{A}$	algorithm

operator	meaning
$\boldsymbol{w}^\mathsf{T}$	transpose
$\boldsymbol{X}\boldsymbol{Y}$	matrix multiplication
$\boldsymbol{X}^{-1}$	inverse

Learning diagram

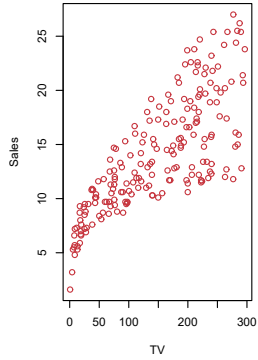


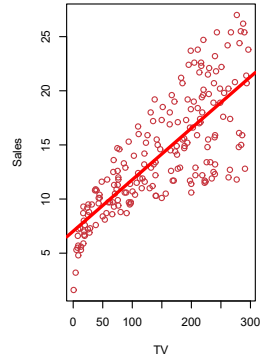
Linear Regression

- Simple Linear Model
- Weighted Linear Model
- Linear Basis Function Model

Problem 1

- Consider the Advertising data set $\mathcal{D}_{train}$ consists of the **sales** of that product in 200 different markets, along with advertising budgets for the product in each of those markets for the media **TV**. Find the *relationship* between **TV** (input) and **sales** (output)





Linear Regression Model

Concept 1

A **linear regression** is a model that assumes a **linear relationship** between **inputs** and the **output**.

Problem Statement

- **The requirement** is to build a system that can take a vector $\boldsymbol{x} \in \mathbb{R}^{D+1}$ as **input** and **predict** the value of a scalar $y \in \mathbb{R}$ as its **output**
- **The hypothesis set** $\mathcal{H}$

$$y \approx \hat{y} = h_{\boldsymbol{w}}(\mathbf{x}) = \boldsymbol{w}^{\mathsf{T}}\boldsymbol{x} \tag{1}$$

where $\hat{y}$ be the value that our model (function) predicts y and $\boldsymbol{w} \in \mathbb{R}^{D+1}$ is a *vector of parameters* of the model

Problem Statement (cont.)

- **Task** $\boldsymbol{T}$: to predict y from $\boldsymbol{x}$ by outputting $\hat{y} = h_{\boldsymbol{w}}(\mathbf{x}) = \boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}$
- The train set $\mathcal{D}_{train}$ denoted as $(\boldsymbol{X}, \boldsymbol{y})$ including N samples $\{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2) \dots (\boldsymbol{x}_N, y_N)\}$, construct the matrix $\boldsymbol{X}$ and the vectors $\boldsymbol{y}$ and $\hat{\boldsymbol{y}}$

$$\underbrace{\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1^{\mathsf{T}} \\ \boldsymbol{x}_2^{\mathsf{T}} \\ \vdots \\ \boldsymbol{x}_N^{\mathsf{T}} \end{bmatrix}}_{\text{input data matrix}}, \quad \underbrace{\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\text{target vector}}, \quad \underbrace{\hat{\boldsymbol{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_N \end{bmatrix}}_{\text{output vector}} \tag{2}$$

Problem Statement (cont.)

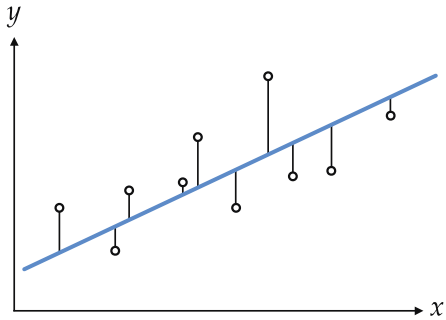
- **Performance measure P**:

Concept 2

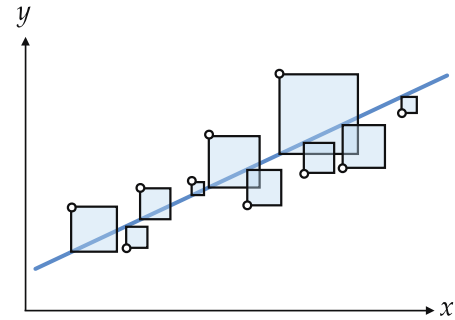
The *mean squared error* MSE_{train} of the model on the train set $\mathcal{D}_{train}$

$$MSE_{train} = \frac{1}{N} \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|^2 = \frac{1}{N} \sum_{n=1}^{N} (\hat{y}_n - y_n)^2 \tag{3}$$

Problem Statement (cont.)



MAE



MSE

Problem Statement (cont.)

- **The learning goal**: find the vector of parameter $\boldsymbol{w}$ such that

$$\boldsymbol{w} = \arg\min_{\boldsymbol{w}}(MSE_{train}) \tag{4}$$

Solving Problem

Solution

- Compute the gradient of MSE_{train}

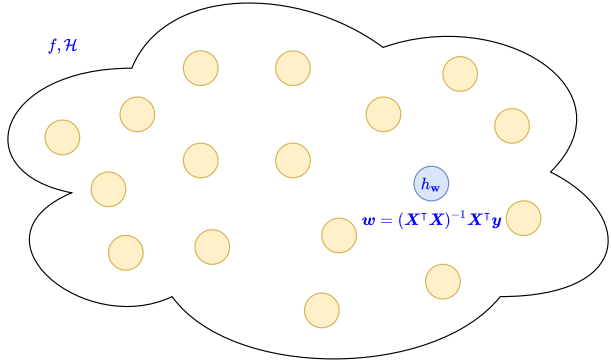
$$\begin{aligned} \nabla_{\boldsymbol{w}}(MSE_{train}) &= \nabla_{\boldsymbol{w}}(\boldsymbol{w}^\top \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{w} - \boldsymbol{w}^\top \boldsymbol{X}^\top \boldsymbol{y} - \boldsymbol{y}^\top \boldsymbol{X}\boldsymbol{w} + \boldsymbol{y}^\top \boldsymbol{y}) \\ &= 2\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{w} - 2\boldsymbol{X}^\top \boldsymbol{y} \end{aligned} \tag{5}$$

- If MSE_{train} reach the min value then $\nabla_{\boldsymbol{w}}(MSE_{train}) = 0$

$$\begin{aligned} \nabla_{\boldsymbol{w}}(MSE_{train}) &= 0 \\ \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{w} - \boldsymbol{X}^\top \boldsymbol{y} &= 0 \\ \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{w} &= \boldsymbol{X}^\top \boldsymbol{y} \\ \boldsymbol{w} &= (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y} \end{aligned} \tag{6}$$

■

Solving Problem (cont.)



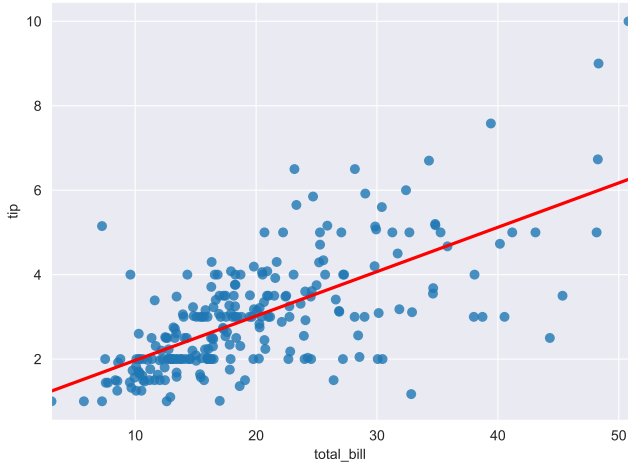
Programming Example

- Use `seaborn` to read `tips` dataset and find the linear relationship between `total_bill` and `tip`

```
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt

sns.set_style("darkgrid")
tips = sns.load_dataset("tips")
sns.regplot(x="total_bill", y="tip", data=tips, ci=None, line_kws
    ={'color':'red'})
plt.show()
```

Programming Example (cont.)



Word Example

1. Find the linear regression function $y = f(x) = w_0 + w_1 x$ given the following data set $\mathcal{D}$

input x	target y
1	2
2	3
3	3
4	5

2. Find the linear regression function $y = f(\boldsymbol{x}) = f(x_1, x_2) = w_0 + w_1 x_1 + w_2 x_2$ given the following data set $\mathcal{D}$

input $\boldsymbol{x}$	target y
(1, 1)	1
(2, 3)	3
(3, 4)	4
(4, 3)	5

Discussion

- D is a large number
- Online learning
- Limitations of **the model** (**hypothesis set**)

Weighted Linear Model

- In some cases the observations may be weighted; for example, they may not be equally reliable. In this case, we find the vector of parameters $\boldsymbol{w}$ to minimize the weighted sum of squares of errors

$$E_{train} = \sum_{n=1}^{N} a_n (\hat{y}_n - y_n)^2 \tag{7}$$

Solving Problem

1. Construct the matrices $\boldsymbol{X}, \boldsymbol{A}$ and the vector $\boldsymbol{y}$

$$\underbrace{\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1^\top \\ \boldsymbol{x}_2^\top \\ \vdots \\ \boldsymbol{x}_N^\top \end{bmatrix}}_{\text{input data matrix}}, \quad \underbrace{\boldsymbol{A} = \begin{bmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_N \end{bmatrix}}_{\text{weight matrix}}, \quad \underbrace{\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\text{target vector}} \tag{8}$$

2. Calculate the vector of parameters

$$\boldsymbol{w} = (\boldsymbol{X}^\top \boldsymbol{A} \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{A} \boldsymbol{y} \tag{9}$$

Linear in What?

- **Linearity in the weights**

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = w_0 + w_1 x_1 + \ldots + w_D x_D \tag{10}$$

Biến đổi phi tuyến

Concept 3

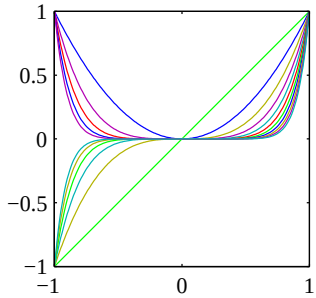
A linear basis function model is a linear combination of **fixed nonlinear functions** of the input variables

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = w_0\phi_0(\boldsymbol{x}) + w_1\phi_1(\boldsymbol{x}) + ... + w_M\phi_M(\boldsymbol{x}) \tag{11}$$

where $\phi_i(\boldsymbol{x})$ are basis functions

Some types of basis functions

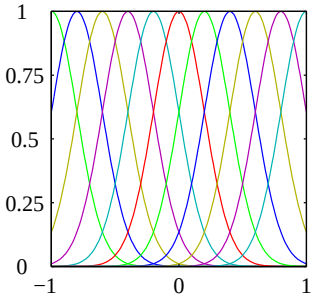
- Polynomial



$$\phi_j(x) = x^j \tag{12}$$

Some types of basis functions (cont.)

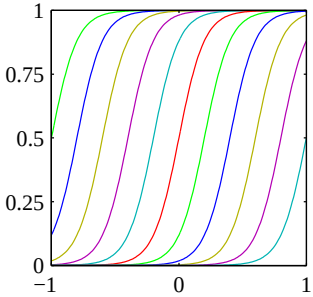
- Gaussian



$$\phi_j(x;\mu_j,s_j)=\exp\left(-\frac{(x-\mu_j)^2}{s_j^2}\right) \quad (13)$$

Some types of basis functions (cont.)

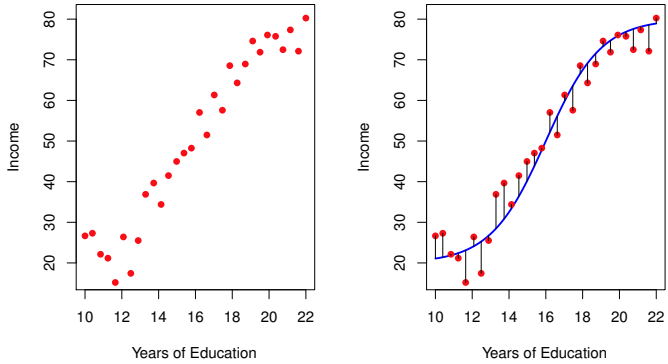
- Sigmoid



$$\phi_j(x; \mu_j, s_j) = \frac{1}{1 + e^{-\frac{x-\mu_j}{s_j}}} \qquad (14)$$

Problem 2

- Find the relationship between `Years of Education` and `Income` based on the given data



Problem Statement

- **The requirement** is to build a system that can take a vector $\boldsymbol{x} \in \mathbb{R}^D$ as **input** and **predict** the value of a scalar $y \in \mathbb{R}$ as its **output**
- The hypothesis set $\mathcal{H}$

$$y \approx \hat{y} = h_{\boldsymbol{w}}(\mathbf{x}) = \boldsymbol{w}^{\mathsf{T}} \boldsymbol{\phi}(\boldsymbol{x}) \tag{15}$$

where $\hat{y}$ be the value that our model (function) predicts y, $\boldsymbol{w} \in \mathbb{R}^{M+1}$ is a *vector of parameters* of the model and $\boldsymbol{\phi}$ is a set of $M+1$ basis functions

$$\boldsymbol{\phi}(\boldsymbol{x}) = \begin{bmatrix} \phi_0(\boldsymbol{x}) \\ \phi_1(\boldsymbol{x}) \\ \vdots \\ \phi_M(\boldsymbol{x}) \end{bmatrix} \tag{16}$$

Problem Statement (cont.)

- **Task T**: to predict y from $\boldsymbol{x}$ by outputting $\hat{y} = h_{\boldsymbol{w}}(\mathbf{x}) = \boldsymbol{w}^{\mathsf{T}}\boldsymbol{\phi}(\boldsymbol{x})$
- **Performance measure P**:
  The *mean squared error* MSE_{train} of the model on the train set $\mathcal{D}_{train}$ including N samples $\{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2) \dots (\boldsymbol{x}_N, y_N)\}$
- **The learning goal**: find the vector of parameter $\boldsymbol{w}$ such that

$$\boldsymbol{w} = \arg\min_{\boldsymbol{w}}(MSE_{train})$$

Solving Problem

1. Construct the matrix $\boldsymbol{\Phi}$ and the vector $\boldsymbol{y}$

$$\underbrace{\boldsymbol{\Phi} = \begin{bmatrix} \phi(\boldsymbol{x}_1)^\intercal \\ \phi(\boldsymbol{x}_2)^\intercal \\ \vdots \\ \phi(\boldsymbol{x}_N)^\intercal \end{bmatrix}}_{\text{design matrix}}, \quad \underbrace{\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\text{target vector}} \tag{17}$$

2. Calculate the vector of parameters

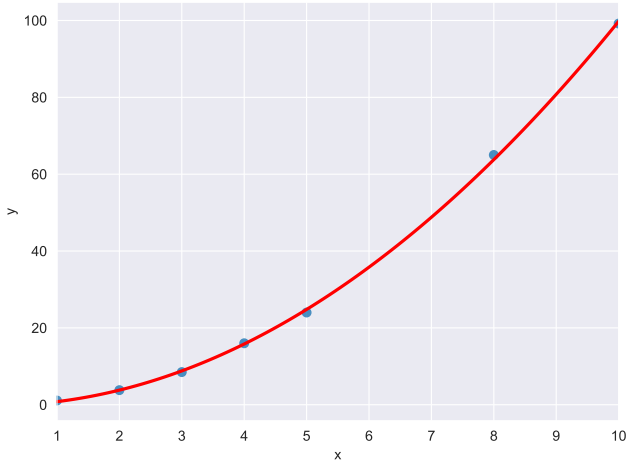
$$\boldsymbol{w} = (\boldsymbol{\Phi}^\intercal \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^\intercal \boldsymbol{y} \tag{18}$$

Programming Example

```
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt

sns.set_style("darkgrid")
x = [1, 2, 3, 4, 5, 8, 10]
y = [1.1, 3.8, 8.5, 16, 24, 65, 99.2]
sns.regplot(x, y, order=2, ci=None, line_kws={'color':'red'})
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```

Programming Example (cont.)



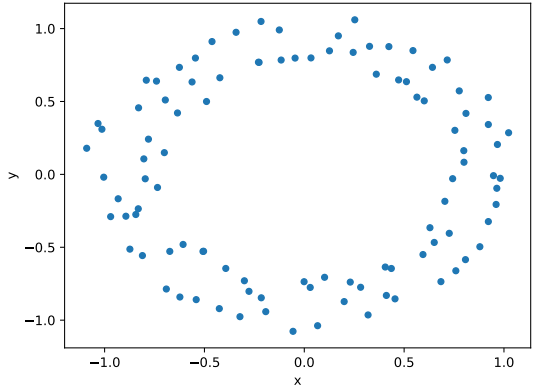
Word Example

- Find a polynomial regression function $y = f(x) = w_0 + w_1 x + w_2 x^2$ given the data set $\mathcal{D}$

input x	target y
1	2
2	3
3	3
4	5

Puzzle

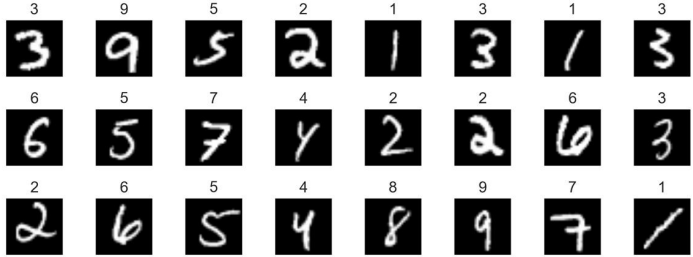
- What basis functions?



Classification

A real data set

- Some 16-by-16 pixel grayscale image from the MNIST database



Input representation

Input representation or **feature extraction**

- **"raw" input**

  pixels $\quad \boldsymbol{x}^\mathsf{T} = \begin{pmatrix} x_0 & x_1 & \dots & x_{256} \end{pmatrix}$

  linear model $\quad \boldsymbol{w}^\mathsf{T} = \begin{pmatrix} w_0 & w_1 & \dots & w_{256} \end{pmatrix}$

- **Feature extraction**: extract useful information

  intensity and symmetry $\quad \boldsymbol{x}^\mathsf{T} = \begin{pmatrix} x_1 & x_2 \end{pmatrix}$

  linear model $\quad \boldsymbol{w}^\mathsf{T} = \begin{pmatrix} w_1 & w_2 \end{pmatrix}$

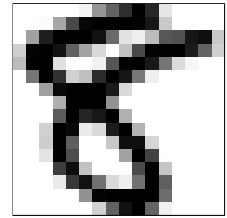
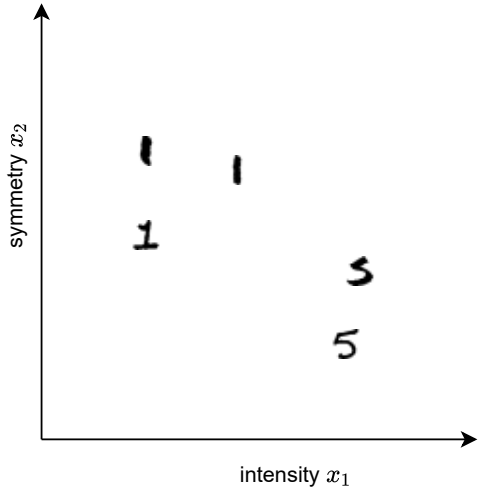


Illustration of Features



The Problem with Categorical Data

- Some algorithms can work with categorical data directly.
  - For example, a decision tree can be learned directly from categorical data with no data transform required
- Many machine learning algorithms cannot operate on label data directly.
  - They require all input variables and output variables to be numeric.
- There are two common types of conversion: integer encoding and one-hot encoding

Integer Encoding

- For categorical variables where no such ordinal relationship exists, the integer encoding is not enough.

id	color
1	red
2	green
3	blue
4	red
...	...

Integer encoding

id	color
1	1
2	2
3	3
4	1
...	...

One-Hot Encoding

- One-hot encoding ensures that machine learning does not assume that higher numbers are more important.

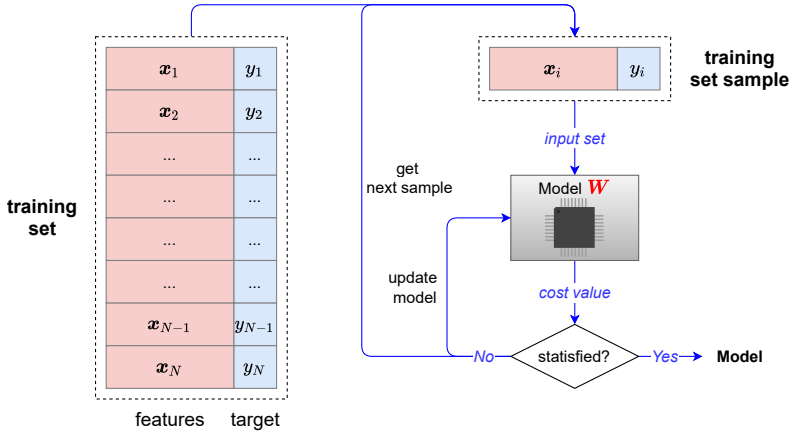
id	color
1	red
2	green
3	blue
4	red
...	...

One-hot encoding

id	color_red	color_green	color_blue
1	1	0	0
2	0	1	0
3	0	0	1
4	1	0	0
...	...	...	...

Classifier Training

- **Select** the learning model for **classifier**, e.g., Perceptron
- **Train** the classifier/model using a training set $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_N, y_N)\}$



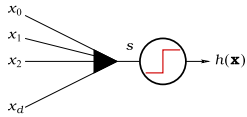
Logistic Regression

- Binary Classification
- Evaluation
- Multi-class Classification

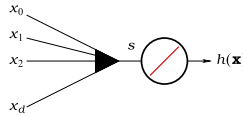
A Third Linear Model

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

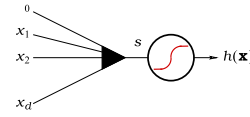
linear classification
$h(\boldsymbol{x}) = sign(s)$



linear regression
$h(\boldsymbol{x}) = s$



logistic regression
$h(\boldsymbol{x}) = \sigma(s)$



The logistic function

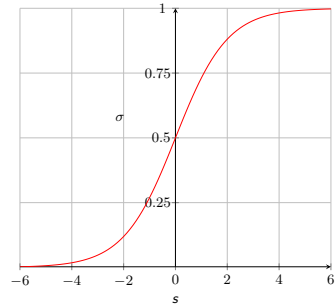
- The formula

$$\sigma(s) = \frac{1}{1 + e^{-s}} \qquad (19)$$

- The **logistic function** converts a score to a probability
- Properties

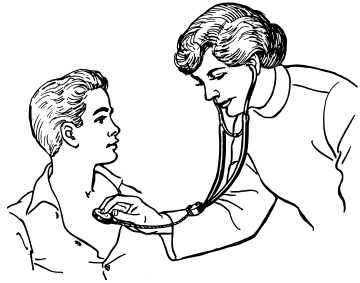
$$\sigma(-s) = 1 - \sigma(s)$$

$$\sigma'(s) = \sigma(s)(1 - \sigma(s))$$



Probability Interpretation

- $h(\boldsymbol{x}) = \sigma(s)$ can be interpreted as a probability
- For example, prediction of heart attacks
  - Input $\boldsymbol{x}$: cholesterol level, age, weight, etc.
  - The signal $s = \boldsymbol{w}^T\boldsymbol{x}$: risk score
  - $\sigma(s)$: probability of a heart attack



score → probability of heart attack

Problem Statement

- The target function f is the probability distribution

$$f : \mathbb{R}^D \to [0, 1]$$

- Hypothesis set $h_{\boldsymbol{w}}(\boldsymbol{x}) = \sigma(\boldsymbol{w}^T \boldsymbol{x})$ and the conditional probability

$$P(y \mid \boldsymbol{x}, \boldsymbol{w}) = \begin{cases} h_{\boldsymbol{w}}(\boldsymbol{x}) & \text{for} \quad y = 1 \\ 1 - h_{\boldsymbol{w}}(\boldsymbol{x}) & \text{for} \quad y = 0 \end{cases} \tag{20}$$

Error measure

We define error measurement based on likelihood

- For each $(\boldsymbol{x}, y)$, y is generated by probability $h_{\boldsymbol{w}}(\boldsymbol{x})$.
- Plausible error measure based on **likelihood** of y given $\boldsymbol{x}$ and $\boldsymbol{w}$

$$P(y \mid \boldsymbol{x}, \boldsymbol{w}) = z^y (1-z)^{1-y} \tag{21}$$

where

$$z = h_{\boldsymbol{w}}(\boldsymbol{x}) = \sigma(\boldsymbol{w}^\intercal \boldsymbol{x}) \tag{22}$$

- Likelihood of $\mathcal{D} = \{(\boldsymbol{x}_1, y_1) ... (\boldsymbol{x}_N, y_N)\}$ given $\boldsymbol{w}$ is

$$\prod_{n=1}^{N} P(y_n \mid \boldsymbol{x}_n, \boldsymbol{w}) \tag{23}$$

Error measure (cont.)

- **Learning goal**: maximizing likelihood

$$\begin{array}{lll} & \text{Maximize} & \prod_{n=1}^{N} P(y_n \mid \boldsymbol{x}_n, \boldsymbol{w}) \\ \Leftrightarrow & \text{Minimize} & -\log \prod_{n=1}^{N} P(y_n \mid \boldsymbol{x}_n, \boldsymbol{w}) \\ \Leftrightarrow & \text{Minimize} & -\sum_{n=1}^{N} (y_n \log z_n + (1-y_n)\log(1-z_n)) \end{array} \tag{24}$$

Learning Algorithm (Gradient Descent)

1. Initialize the weights (parameters) at $t = 0$ $\boldsymbol{w}_0$
2. For $t = 1, 2, 3, \ldots$ do
   - **2.1** Compute the outputs z_n for each $\boldsymbol{x}_n$ $(n = 1, \ldots, N)$

$$z_n = \sigma(\boldsymbol{w}_t^T \boldsymbol{x}_n) \tag{25}$$

   - **2.2** Compute the gradient

$$\nabla_{\boldsymbol{w}} E = \frac{1}{N} \sum_{n=1}^{N} \boldsymbol{x}_n (z_n - y_n) \tag{26}$$

   - **2.3** Update the weights

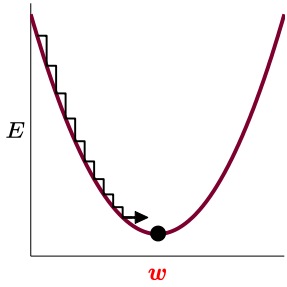
$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \eta \nabla_{\boldsymbol{w}} E \tag{27}$$

     where η is a learning rate (*hyper-parameter*)

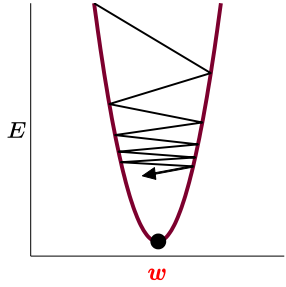
   Iterate the next step until $\boldsymbol{w}$ is not changes
3. Return the final weights $\boldsymbol{w}$

Learning Rate

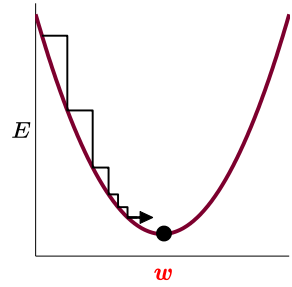
- How η affects the algorithm?



η too small



η too large



η right

Programming Example

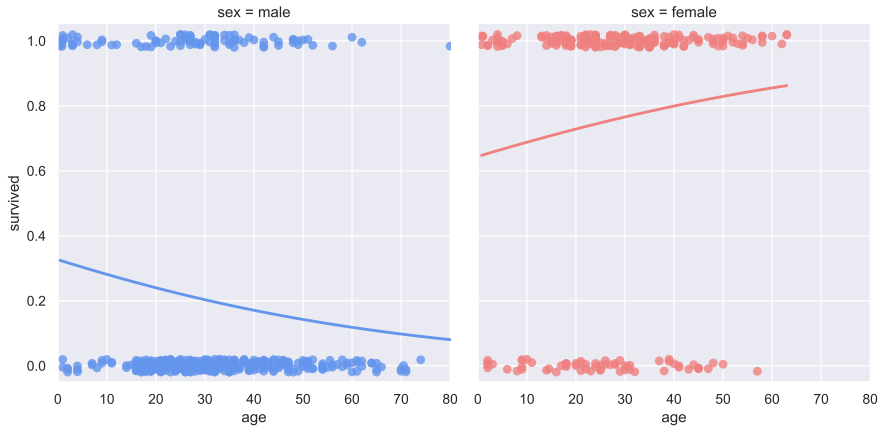
```
import matplotlib.pyplot as plt
import seaborn as sns
sns.set(style="darkgrid")

# Load the example titanic dataset
df = sns.load_dataset("titanic")

# Make a custom palette with gendered colors
pal = dict(male="#6495ED", female="#F08080")

# Show the survival proability as a function of age and sex
g = sns.lmplot(x="age", y="survived", col="sex", hue="sex", data=df,
    palette=pal, y_jitter=.02, logistic=True, ci=None)
g.set(xlim=(0, 80), ylim=(-.05, 1.05))
plt.show()
```

Programming Example (cont.)



Evaluation

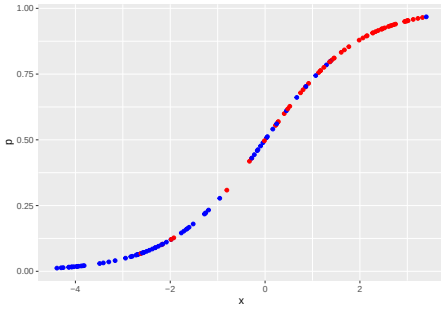
- Consider two-class problem with two classes $\oplus$ and $\ominus$
- The performance of logistic regression model is based on a threshold *th*

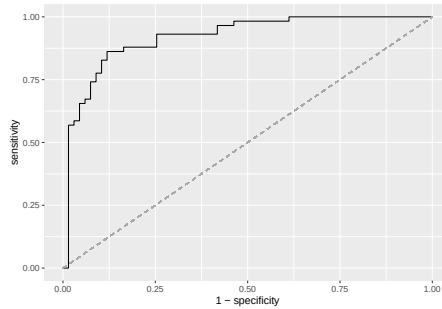
$$
\begin{aligned}
y \text{ is } \oplus \text{ if } P(y \mid \boldsymbol{x}) &\geq th \\
y \text{ is } \ominus \text{ if } P(y \mid \boldsymbol{x}) &< th
\end{aligned}
\tag{28}
$$

  - High threshold: high specificity, low sensitivity
  - Low threshold: low specificity, high sensitivity
- We should select the best threshold for the trade-off between the cost of *false positives* vs *false negatives*

ROC Curve

- The receiver operating characteristic (*ROC*) curve is plot which shows the performance of a binary classifier as function of its cut-off threshold.
- It essentially shows the *true positive rate* (*sensitivity*) against the *false positive rate* (1-*specificity*) for various threshold values.
- The area under the curve (*AUC*) is an aggregated measure of performance.

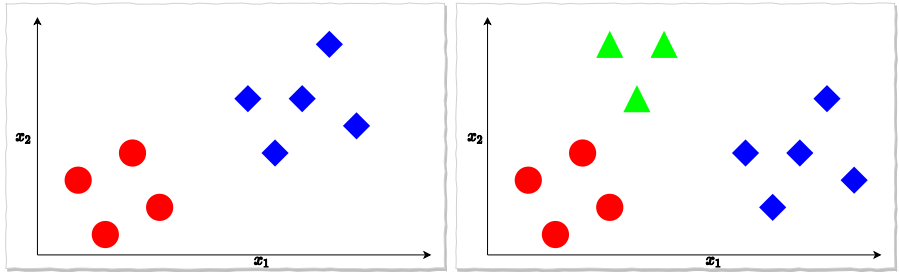




Multi-class classification problems

- **Email foldering/tagging**: Work (1), Friends (2), Family (3), Hobby (4)
- **Medical diagrams**: Not ill, Cold, Flu
- **Weather**: Sunny, Cloudy, Rain, Snow

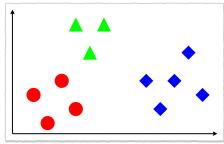
Visual of Binary vs Multi-class classification

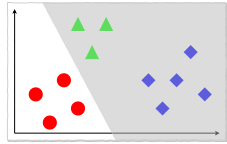


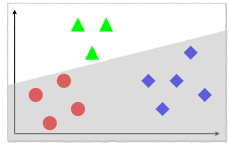
Approaches

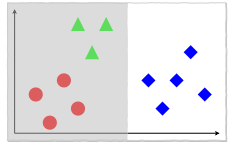
- One-vs-one
- Hierarchical
- **One-vs-all**

One-vs-all









- Class ○ (1):

$$h^{(1)}(\boldsymbol{x}) = P(y = 1 \mid \boldsymbol{x}, \boldsymbol{w}_1)$$

- Class △ (2):

$$h^{(2)}(\boldsymbol{x}) = P(y = 2 \mid \boldsymbol{x}, \boldsymbol{w}_2)$$

- Class ♢ (3):

$$h^{(3)}(\boldsymbol{x}) = P(y = 3 \mid \boldsymbol{x}, \boldsymbol{w}_3)$$

One-vs-all (cont.)

Learning

- Train a logistic regression classifier $h^{(i)}(\boldsymbol{x})$ for each class i to predict the probability that $y = i$.

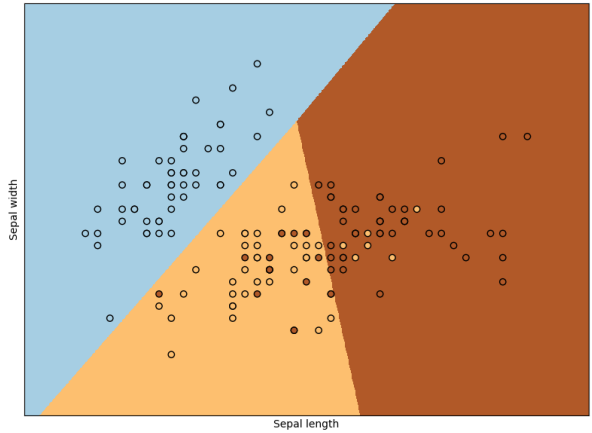
Prediction

- On a new input $\boldsymbol{x}$, to make a prediction, pick the class i that maximizes

$$\arg\max_i (h^{(i)}(\boldsymbol{x})) \tag{29}$$

Decision boundaries and decision regions

- Logistic regression for **Iris** dataset



Softmax Regression

- Softmax Regression
- Cross Entropy vs. MSE

Softmax Regression

Concept 4

Softmax regression is a generalization of logistic regression that we can use for multi-class classification

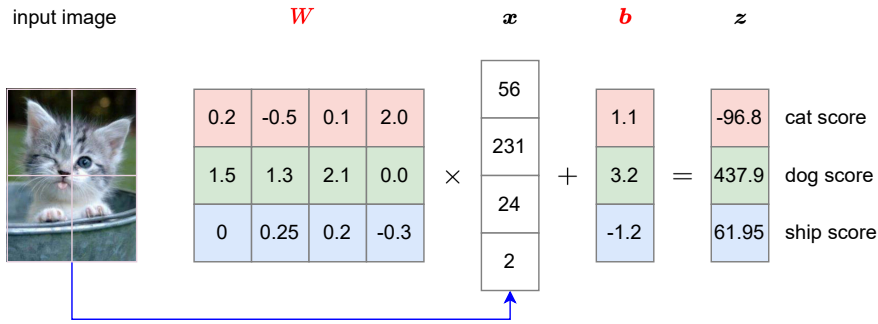
- In Softmax regression, we replace the sigmoid function by the so-called softmax function $\boldsymbol{\phi}(\cdot) = \{\phi_1, ..., \phi_C\}$.

Score function

Concept 5

The **score function** f that maps the raw features to class scores.

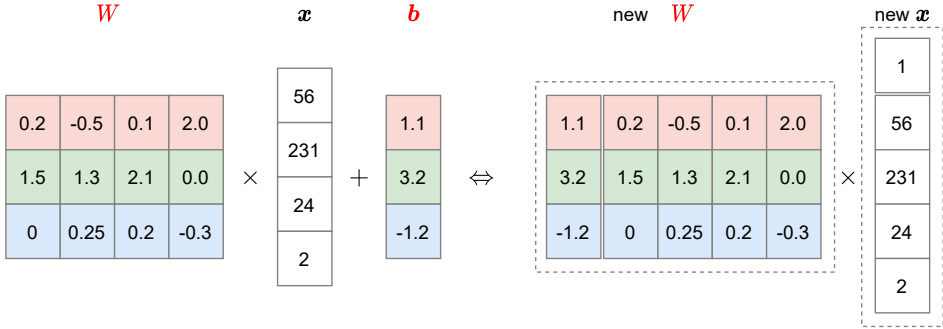
$$\boldsymbol{z} = f(\boldsymbol{x}; W, \boldsymbol{b}) = W\boldsymbol{x} + \boldsymbol{b} \tag{30}$$



Score function (cont.)

- Use bias trick $W_0 = \boldsymbol{b}$ to represent the two parameters $W, \boldsymbol{b}$ as one

$$\boldsymbol{z} = f(\boldsymbol{x}; W) = W\boldsymbol{x} \tag{31}$$



Softmax function

Concept 6

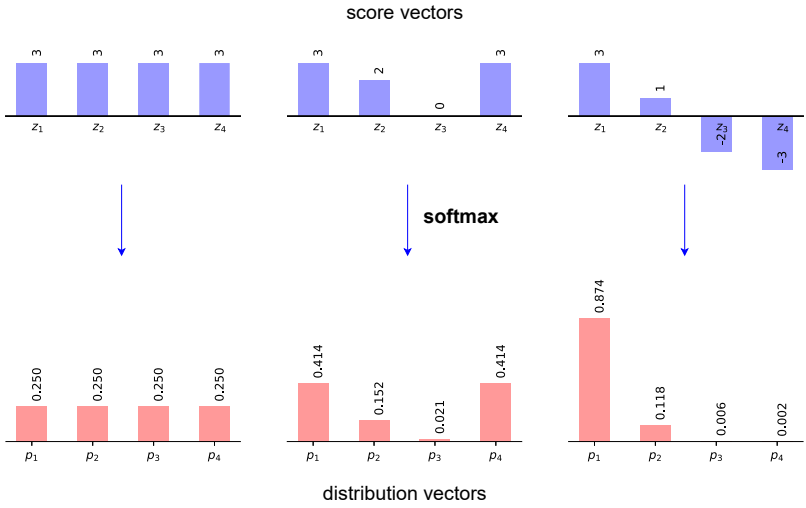
The **softmax function** converts a score vector $\boldsymbol{z} = (z_1, ..., z_C)$ to a discrete distribution vector $\boldsymbol{p} = (p_1, ..., p_C)$

$$p_i = P(y = i \mid \boldsymbol{z}) = \phi_i(\boldsymbol{z}) = \frac{e^{z_i}}{\sum_{j=1}^{C} e^{z_j}}, \ i \in [1, ..., C] \tag{32}$$

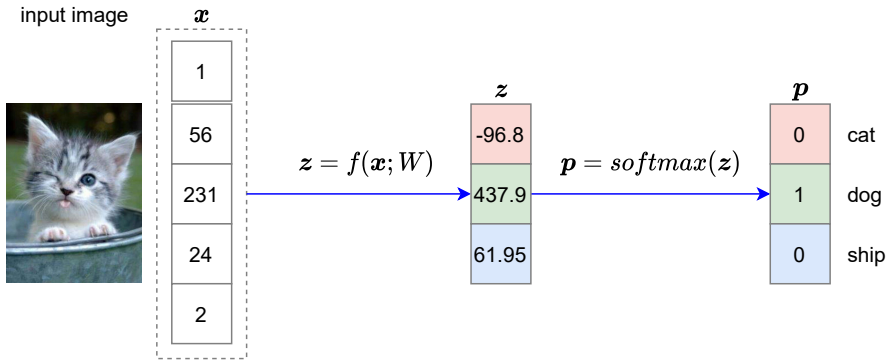
where

$$z_i = w_{i0} + w_{i1}x_1 + ... + w_{iD}x_D = \boldsymbol{w}_i^{\mathsf{T}}\boldsymbol{x} \tag{33}$$

Softmax function (cont.)



Softmax function (cont.)



Problem Statement

- Given $\mathcal{D} = \{(\boldsymbol{x}_1, y_1)...(\boldsymbol{x}_N, y_N)\}$ where $y_n \in \{1, ..., C\}$.
- Denote $\boldsymbol{t}_n$ is a **one-hot encoding** of y_n (or target discrete distribution)
- **Learning goal**: Find a softmax function $\boldsymbol{\phi}_W(\cdot) = \{\phi_1, ..., \phi_C\}$ that minimize

$$\arg\min_W E(\boldsymbol{\phi}_W) = \arg\min_W \sum_{n=1}^{N} CE(\boldsymbol{p}_n, \boldsymbol{t}_n) \tag{34}$$

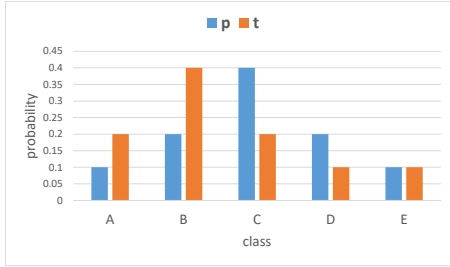
Cross Entropy

Concept 7

Cross-entropy (CE) is a measure of the difference between two probability distributions. The cross-entropy between a "true" distribution $\boldsymbol{t} = (t_1, ..., t_C)$ and an estimated distribution $\boldsymbol{p} = (p_1, ..., p_C)$ is defined as

$$CE(\boldsymbol{p}, \boldsymbol{t}) = -\sum_{i=1}^{C} t_i \log p_i \tag{35}$$

Cross Entropy (cont.)



$$\left.\begin{array}{l} \boldsymbol{p} = (0.1, 0.2, 0.4, 0.2, 0.1) \\ \boldsymbol{t} = (0.2, 0.4, 0.2, 0.1, 0.1) \end{array}\right\} \rightarrow CE(\boldsymbol{p}, \boldsymbol{t}) = 1.678$$

- $CE > 0$
- $CE(\boldsymbol{p}, \boldsymbol{t}) \neq CE(\boldsymbol{t}, \boldsymbol{p})$
- CE minimize if $p_i = t_i, \forall i$

MSE

Concept 8

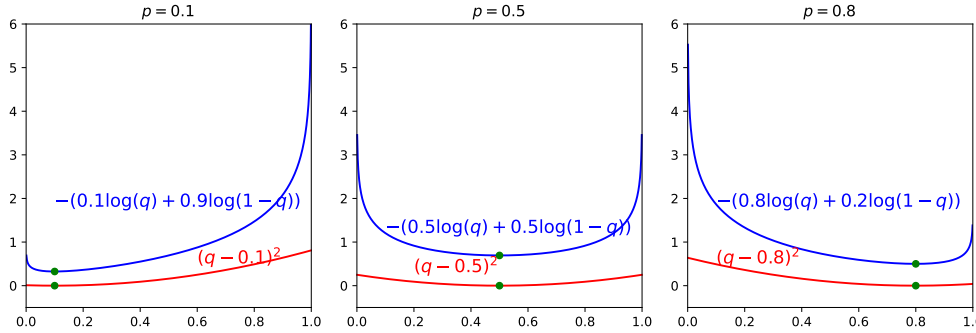
Mean squared error (MSE) is a measure of the average of the squares of the errors.

$$MSE(\boldsymbol{p}, \boldsymbol{t}) = \frac{1}{C}\sum_{i=1}^{C}(p_i - t_i)^2 \tag{36}$$

- $MSE \geq 0$
- $MSE(\boldsymbol{p}, \boldsymbol{t}) = MSE(\boldsymbol{t}, \boldsymbol{p})$
- $MSE = 0$ if $p_i = t_i, \forall i$

Cross Entropy vs. MSE

- Consider three "true" binary distributions $\boldsymbol{p} = (0.1, 0.9), (0.5, 0.5)$ and $(0.8, 0.2)$



Learning Algorithm

1. Initialize the weights W_0 (parameters) at $t = 0$
2. For $t = 1, 2, 3, \ldots$ do
   - **2.1** Compute the ouput distribution $\boldsymbol{p}_n$ for each $\boldsymbol{x}_n$ $(n = 1 \ldots N)$

$$\boldsymbol{p}_n = softmax(W_t \boldsymbol{x}_n) \tag{37}$$

   - **2.2** Compute the gradient

$$\nabla_W E = \frac{1}{N} \sum_{n=1}^{N} (\boldsymbol{p}_n - \boldsymbol{t}_n) \boldsymbol{x}_n^\intercal \tag{38}$$

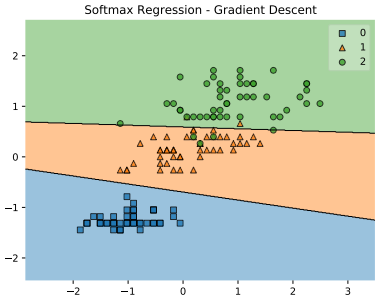
   - **2.3** Update the weights

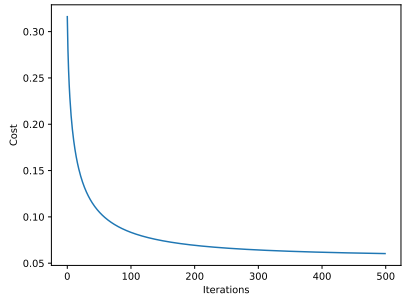
$$W_{t+1} = W_t - \eta \nabla_W E \tag{39}$$

   Iterate the next step until W is not change
3. Return the final weights W

Example

- Softmax regression for **Iris** dataset





Capacity, Overfitting and Underfitting

- Model Capacity
- Model vs. Data
- Bias-Variance
- Tradeoff of Capacity
- Regularization
- Tradeoff of Regularization

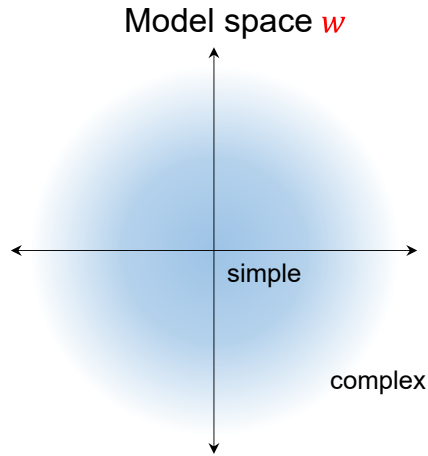
Model Capacity

Concept 9

Capacity is model complexity.

The most common ways to estimate the capacity of a model:

- VC dimension
- The number of parameters
- The norm of parameters



Model vs. Data

Concept 10

Data is divided into three sets: **training set**, **validation set** and **test set**.

Concept 11

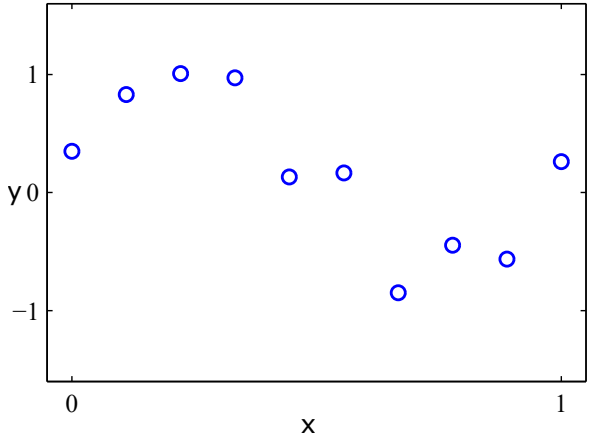
Models can be too limited. We can't find a function that fits the data well. This is called **underfitting**.

Concept 12

Models can also be too rich. We don't just model the data, but also the underlying noise. This is called **overfitting**.

Model vs. Data (cont.)

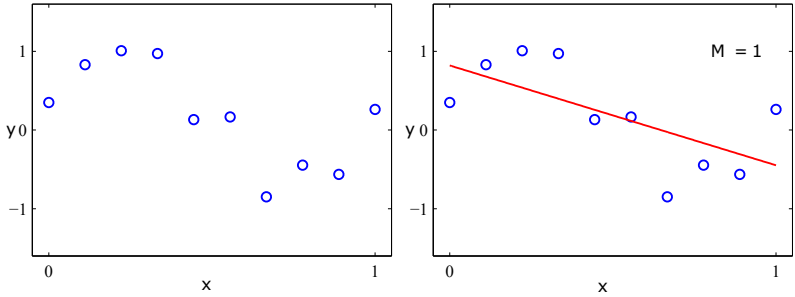
- Given the data set $\mathcal{D} = \{(x_1, y_1), ...(x_{10}, y_{10})\}$ shown in the following figure, find the best regression function to the data



Model vs. Data (cont.)

- Consider the simple hypothesis set

$$\mathcal{H}_1 = \{h \mid y = h(x) = w_0 + w_1 x\} \tag{40}$$

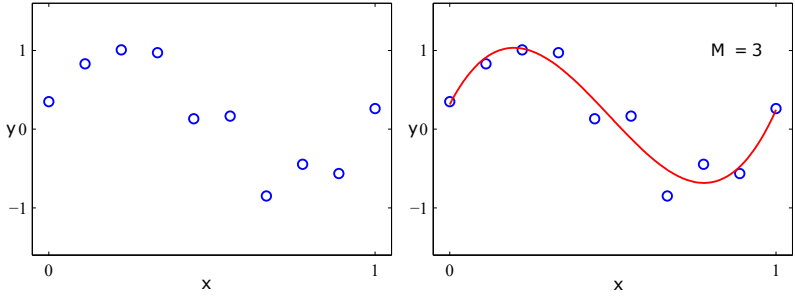


Model vs. Data (cont.)

- Consider the hypothesis set

$$\mathcal{H}_3 = \{h \mid y = h(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3\} \tag{41}$$

(note that $\mathcal{H}_1 \subset \mathcal{H}_3$)

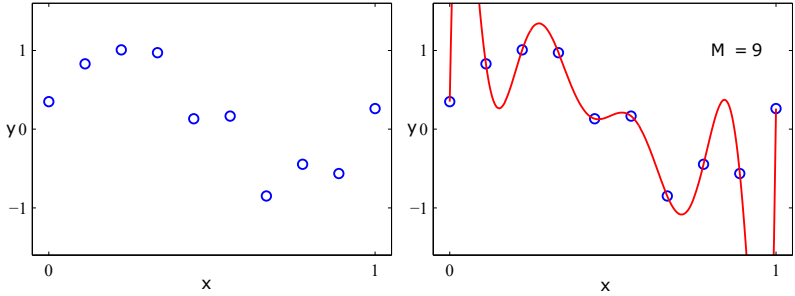


Model vs. Data (cont.)

- Consider the hypothesis set

$$\mathcal{H}_9 = \{h \mid y = h(x) = w_0 + w_1 x + w_2 x^2 + ... + w_9 x^9\} \tag{42}$$

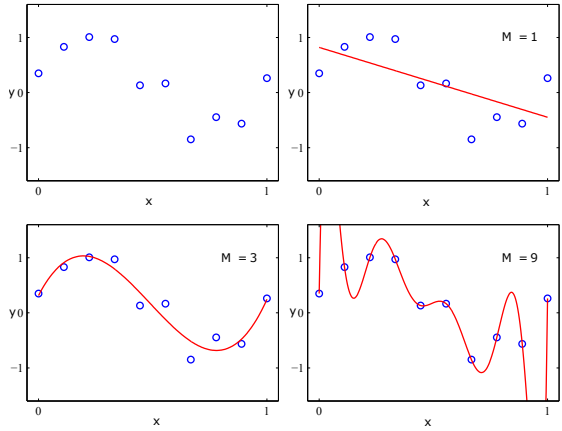
(note that $\mathcal{H}_1 \subset \mathcal{H}_3 \subset \mathcal{H}_9$)



Model vs. Data (cont.)

Which one

- Under-fitting
- Over-fitting
- **Appropriate fitting**



Model vs. Data (cont.)

	$M = 1$	$M = 3$	$M = 9$
w_0	0.82	0.31	0.35
w_1	-1.27	7.99	232.37
w_2		-25.43	-5321.83
w_3		17.37	48568.31
w_4			-231639.30
w_5			640042.26
w_6			-1061800.52
w_7			1042400.18
w_8			-557682.99
w_9			125201.43

Model Performance

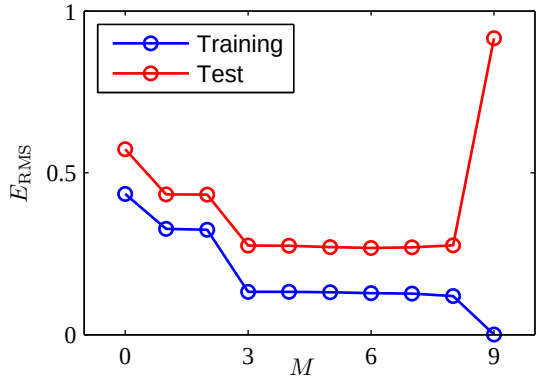


Figure 1: Graphs of the root-mean-square error evaluated on the **training set** and on an **independent test set** for various values of M

What happen if increasing N

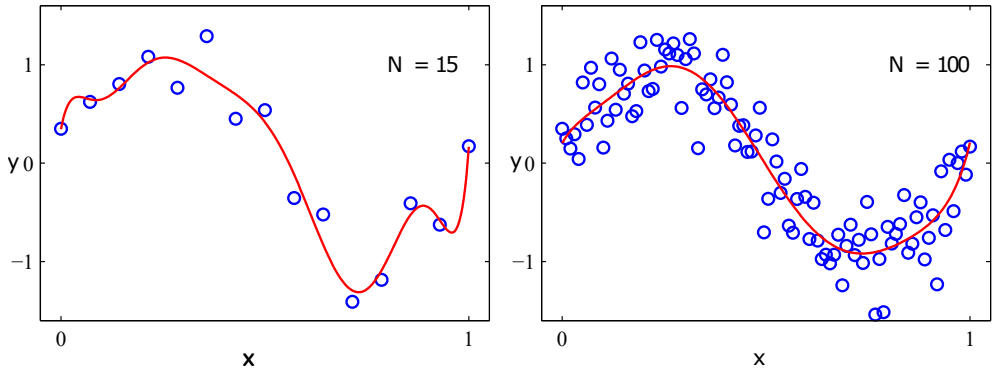


Figure 2: Using the $M = 9$ polynomial for $N = 15$ data points (left plot) and $N = 100$ data points (right plot). We see that increasing the size of the data set reduces the over-fitting problem

Errors in Learning Model

- **Bias errors**: error due to assumption in the model
  - High bias to signify underfitting
- **Variance errors**: It measures the variability in the results given by model when the dataset is changed
  - High variance to signify overfitting

$$\text{Expected error} = \text{Bias} + \text{Variance} + \text{Irreducible Error} \tag{43}$$

Errors in Learning Model (cont.)

Concept 13

Given a learning model $\langle \mathcal{H}, \mathcal{A} \rangle$, we define the "average" hypothesis $\overline{g}(x)$

$$\overline{g}(x) = \mathbb{E}_{\mathcal{D}}\left[g_{\mathcal{D}}(x)\right] \tag{44}$$

where $g_{\mathcal{D}}(x)$ is the "**best**" hypothesis given the data set $\mathcal{D}$

- Bias of learning model

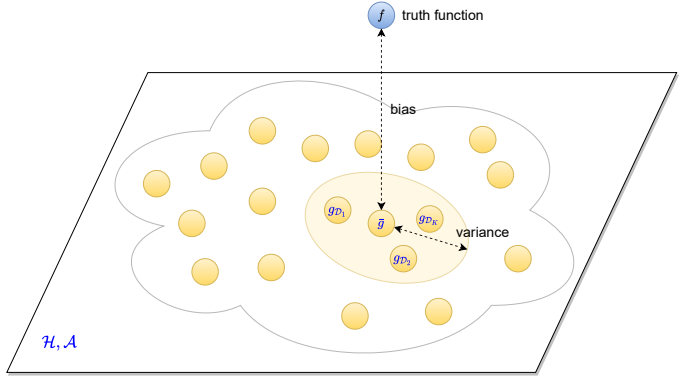
$$\text{Bias} = \mathbb{E}_x\left[\left(\overline{g}(x) - f(x)\right)^2\right] \tag{45}$$

  where $f(x)$ is the "**truth**" function

- Variance of learning model

$$\text{Variance} = \mathbb{E}_x\left[\mathbb{E}_{\mathcal{D}}\left[\left(g_{\mathcal{D}}(x) - \overline{g}(x)\right)^2\right]\right] \tag{46}$$

Errors in Learning Model (cont.)



- Given many independent data sets $\mathcal{D}_1, \mathcal{D}_2, ..., \mathcal{D}_K$, we can estimate $\overline{g}(x)$ by

$$\overline{g}(x) \approx \frac{1}{K} \sum_{i=1}^{K} g_{\mathcal{D}_i}(x) \tag{47}$$

Example: two learning models

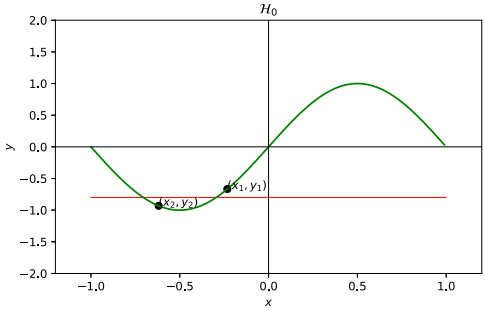
- Consider a target function sine

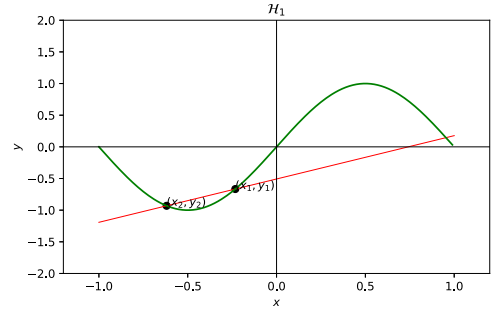
$$\begin{array}{rccc} f & : & [-1,1] & \rightarrow & \mathbb{R} \\ & & x & \rightarrow & \sin(\pi x) \end{array} \tag{48}$$

- We generate 100 data sets $\{\mathcal{D}_i\}, i = 1, ..., 100$, each containing $N = 2$ data points, independently from the sinusoidal curve $f(x) = \sin(\pi x)$. For each data set $\mathcal{D}_i$, we fit the data using one of two models
  - $\mathcal{H}_0$: set of all lines of the form $h(x) = b$
  - $\mathcal{H}_1$: set of all lines of the form $h(x) = ax + b$
  - Note that $\mathcal{H}_0 \subset \mathcal{H}_1$

Example: two learning models (cont.)

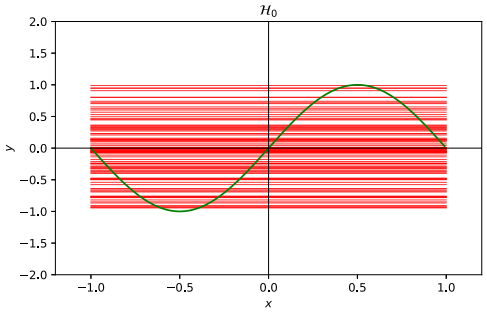
- Given a data set $\mathcal{D}_i = \{(x_1, y_1), (x_2, y_2)\}$.
  - For $\mathcal{H}_0$, we choose the constant hypothesis that best fits the data (the horizontal line at the midpoint, $b = (y_1 + y_2)/2$).
  - For $\mathcal{H}_1$, we choose the line that passes through the two data points (x_1, y_1) and (x_2, y_2).

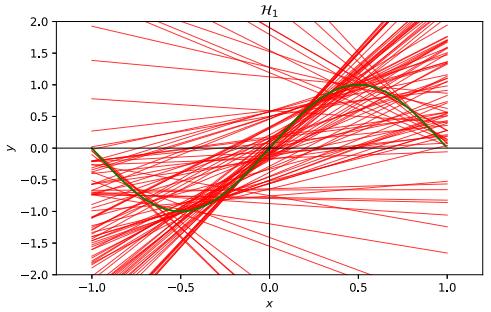




Example: two learning models (cont.)

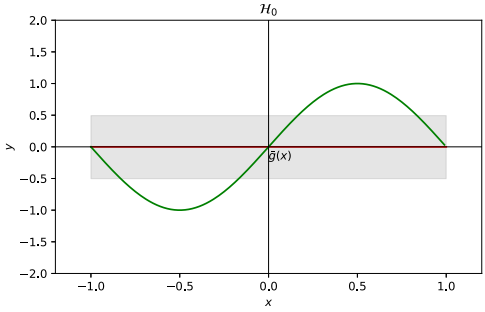
- Repeating this process with 100 data sets $\{\mathcal{D}_i\}, i = 1, ..., 100,$



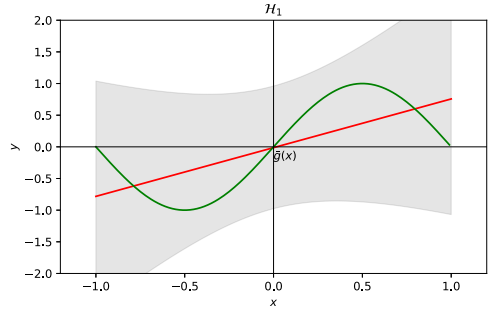


Example: two learning models (cont.)

- The bias-variance for each learning model



- bias=0.50
- var=**0.25**

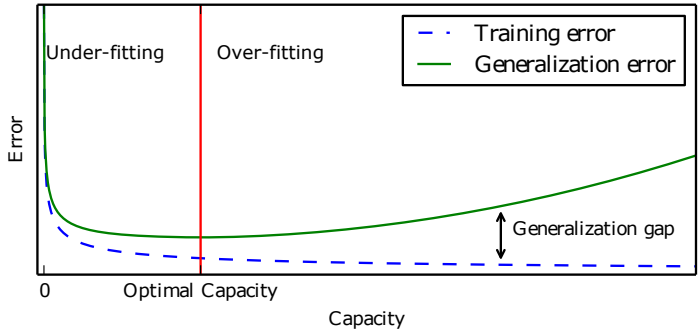


- bias=**0.21**
- var=1.69

Generalization and Capacity

The criteria determining how well a machine learning model will perform:

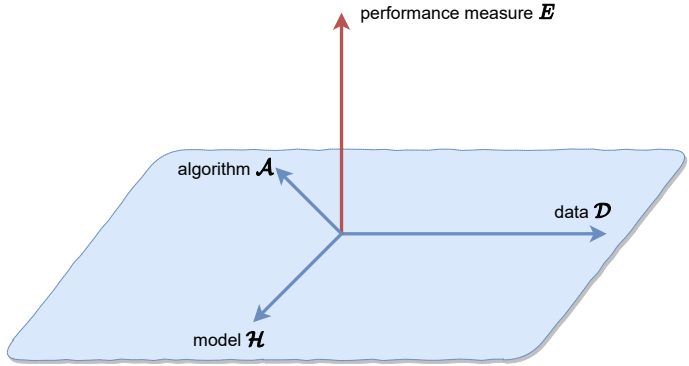
1. Make the training error small.
2. Make the gap between training and test (generalization) error small.



Regularization

Concept 14

Regularization is any modification we make to a learning model that is intended to reduce its generalization error but not its training error.



Addressing

High bias	High variance
Obtain more features	Decrease number of features
Decrease regularization λ	Increase regularization λ
Extend model	Obtain more data
Train longer	Stop early
New model architecture	New model architecture

Regularization for Linear Regression

- Using regularized MSE_{train} for linear regression

$$\boldsymbol{w} = \arg\min_{\boldsymbol{w}} \left[MSE_{train} + \lambda \left(\frac{1}{N} \boldsymbol{w}^T \boldsymbol{w} \right) \right] \tag{49}$$

  where λ is the regularization coefficient (*hyper-parameter*) that controls the relative importance of the data-dependent error MSE_{train} and the regularization term $\lambda \left(\frac{1}{N} \boldsymbol{w}^T \boldsymbol{w} \right)$

- Solving for $\boldsymbol{w}$, we obtain

$$\boldsymbol{w} = (\boldsymbol{X}^\intercal \boldsymbol{X} + \lambda \boldsymbol{I})^{-1} \boldsymbol{X}^\intercal \boldsymbol{y} \tag{50}$$

Example: one learning model

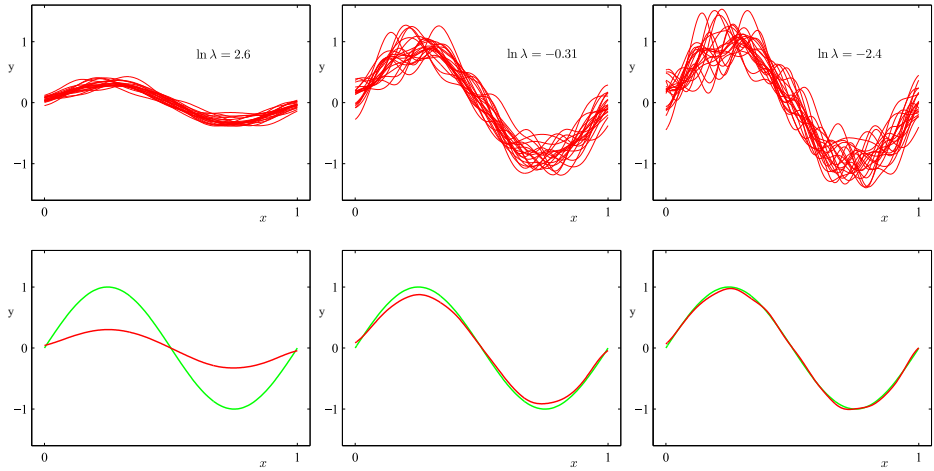
- Consider a target function sine

$$\begin{array}{rccc} f & : & [-1,1] & \rightarrow & \mathbb{R} \\ & & x & \rightarrow & \sin(2\pi x) \end{array} \tag{51}$$

- We generate 100 data sets $\{\mathcal{D}_i\}, i = 1, ..., 100$, each containing $N = 25$ data points, independently from the sinusoidal curve $f(x) = \sin(2\pi x)$. For each data set $\mathcal{D}_i$, we fit a model with 24 Gaussian basis functions by minimizing the regularized error function

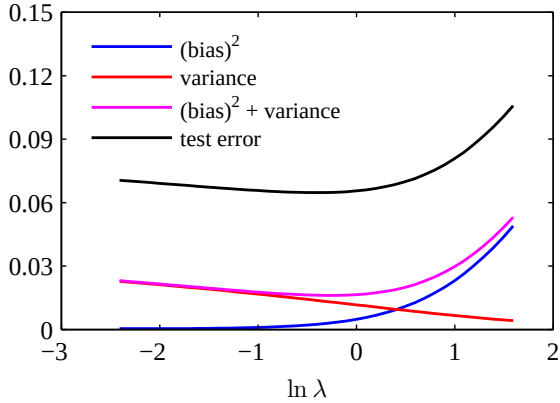
Example: one learning model (cont.)

- Illustration of the dependence of bias and variance on model regularization coefficient



Example: one learning model (cont.)

- Summary of the dependence of bias and variance on model regularization coefficient



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