LINEAR MODEL

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Contents

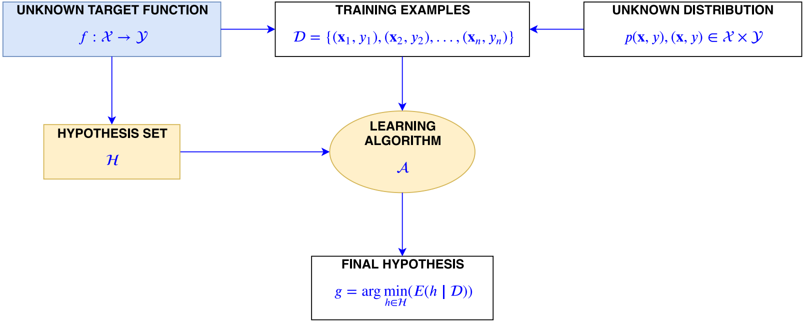
Notation

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 Goal

- Learning diagram revisited

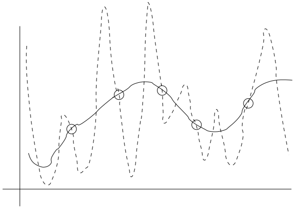


Inductive Bias

Theorem 1 (No Free Lunch Theorems)

An unbiased learner can never generalize.

- The converse of the Inductive Learning Hypothesis is that generalization only possible if we make some assumptions, or introduce some priors. We need an Inductive Bias.
- **Consider**: arbitrarily wiggly functions or random truth tables or non-smooth distributions.

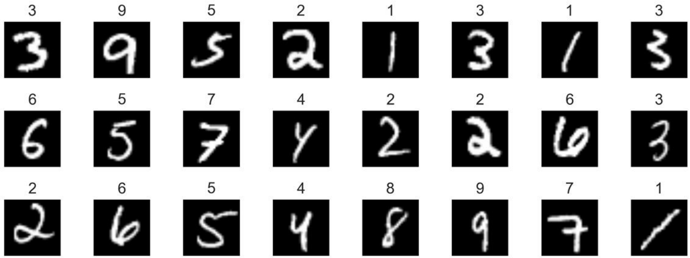


0 0 0	0
0 0 1	?
0 1 0	1
0 1 1	1
1 0 0	0
1 0 1	?
1 1 0	1
1 1 1	?

Linear 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**

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

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

- **Feature extraction**: extract useful information

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

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

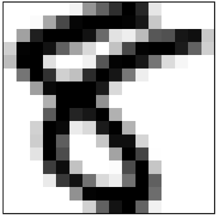
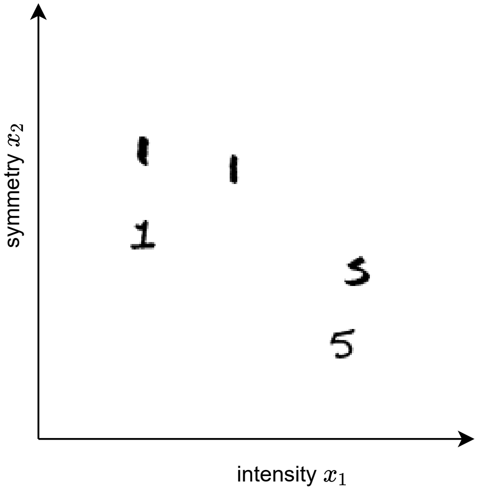
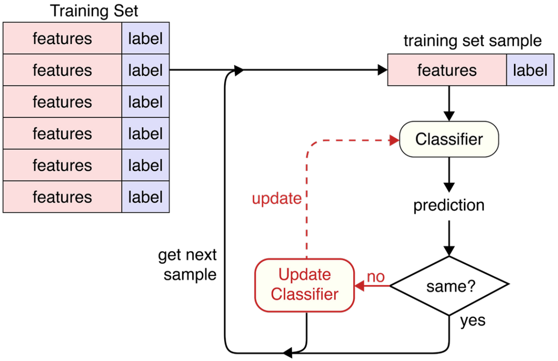


Illustration of Features



Classifier Training

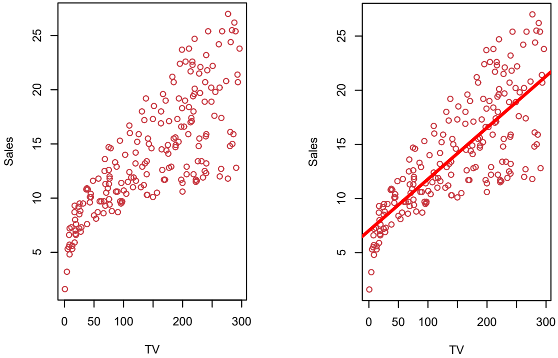
- **Select** the learning model for **classifier**, e.g., Perceptron
- **Train** the classifier



Linear Regression

Simple Problem

- 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** and **sales**



Solving Problem by Learning

- **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 $\mathcal{H}$

$$y \approx \hat{y} = h_{\boldsymbol{w}}(\mathbf{x}) = \boldsymbol{w}^\intercal \boldsymbol{x} \quad (1)$$

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

Solving Problem by Learning (cont.)

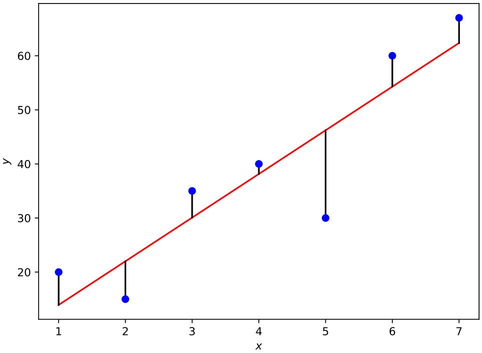
- **Task $\boldsymbol{T}$**: to predict y from $\boldsymbol{x}$ by outputting $\hat{y} = h_{\boldsymbol{w}}(\mathrm{x}) = \boldsymbol{w}^\intercal \boldsymbol{x}$
- **Performance measure $\boldsymbol{P}$**:
  The *mean squared error* MSE_{train} of the model on the train set $\mathcal{D}_{train}$ denoted as $(\boldsymbol{X}, \boldsymbol{y})$ including N samples $\{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2) \ldots (\boldsymbol{x}_N, y_N)\}$

$$MSE_{train} = \frac{1}{N} \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|^2 \tag{2}$$

Construct the matrix $\boldsymbol{X}$ and the vectors $\boldsymbol{y}$ and $\hat{\boldsymbol{y}}$

$$\underbrace{\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1^\intercal \\ \boldsymbol{x}_2^\intercal \\ \vdots \\ \boldsymbol{x}_N^\intercal \end{bmatrix}}_{\text{input data matrix}}, \quad \underbrace{\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\text{target vector}}, \quad \underbrace{\hat{\boldsymbol{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_N \end{bmatrix}}_{\text{output vector}} \tag{3}$$

Solving Problem by Learning (cont.)



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

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

Solving Problem by Learning (cont.)

Solution

- Compute the gradient of MSE_{train}

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

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

$$\begin{aligned}\nabla_{\boldsymbol{w}}(MSE_{train}) &= 0 \\ \boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{w} - \boldsymbol{X}^\top\boldsymbol{y} &= 0 \\ \boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{w} &= \boldsymbol{X}^\top\boldsymbol{y} \\ \boldsymbol{w} &= (\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}^\top\boldsymbol{y} \qquad (4)\end{aligned}$$

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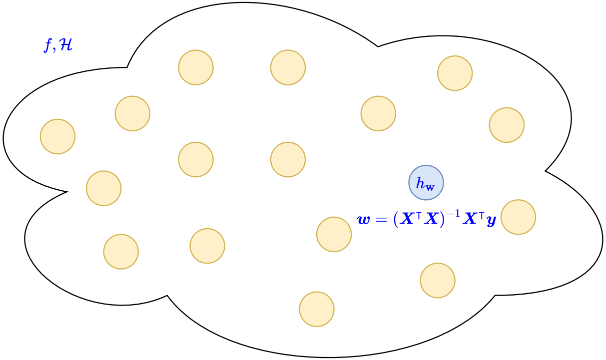
Solving Problem by Learning (cont.)



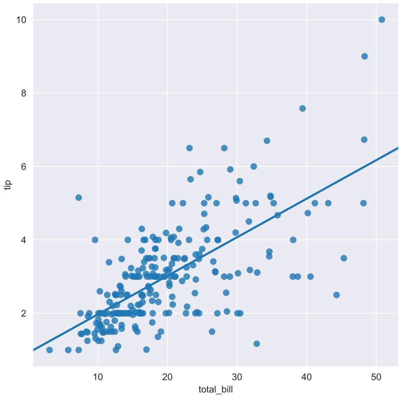
Programming Example

- 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)
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**)

Linear in What?

- **Linearity in the weights**

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = w_0 + w_1 x_1 + \ldots + w_D x_D \tag{5}$$

- We extend **the model** by introducing **linear combinations** of **fixed nonlinear functions** of the input variables

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = w_0 + w_1 \phi_1(\boldsymbol{x}) + \ldots + w_M \phi_M(\boldsymbol{x}) \tag{6}$$

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

Some types of basis functions

- Power

$$\phi_j(x) = x^j \tag{7}$$

- Gaussian

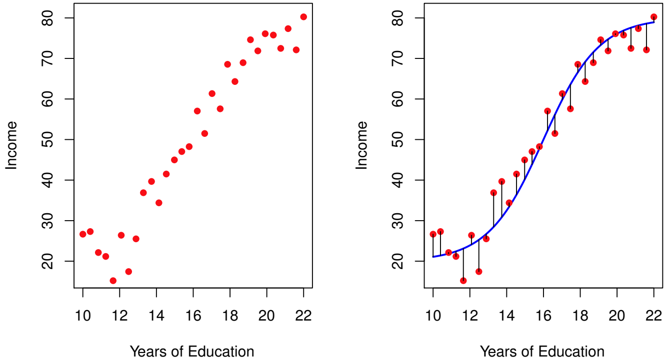
$$\phi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{s^2}\right) \tag{8}$$

- Sigmoid

$$\phi_j(x) = \frac{1}{1 + e^{-\frac{x-\mu_j}{s}}} \tag{9}$$

Another Problem

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



Solving Problem by Learning

- **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 $\mathcal{H}$

$$y \approx \hat{y} = h_{\boldsymbol{w}}(\mathbf{x}) = \boldsymbol{w}^\intercal \boldsymbol{\phi}(\boldsymbol{x}) \tag{10}$$

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

$$\boldsymbol{\phi}(\boldsymbol{x}) = \begin{bmatrix} \phi_0(\boldsymbol{x}) \\ \phi_1(\boldsymbol{x}) \\ \vdots \\ \phi_M(\boldsymbol{x}) \end{bmatrix} \tag{11}$$

Solving Problem by Learning (cont.)

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

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

Solving Problem by Learning (cont.)

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

$$\underbrace{\mathbf{\Phi} = \begin{bmatrix} \phi(\boldsymbol{x}_1)^\intercal \\ \phi(\boldsymbol{x}_2)^\intercal \\ \vdots \\ \phi(\boldsymbol{x}_N)^\intercal \end{bmatrix}}_{\text{design matrix}}, \quad \underbrace{\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\text{target vector}} \tag{12}$$

2. Calculate the vector of parameters

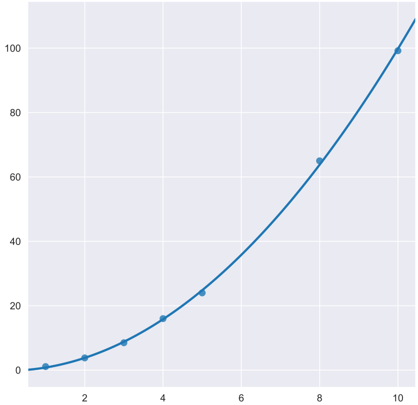
$$\boldsymbol{w} = (\mathbf{\Phi}^\intercal \mathbf{\Phi})^{-1} \mathbf{\Phi}^\intercal \boldsymbol{y} \tag{13}$$

Programming Example

```python
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)
plt.show()
```

Programming Example (cont.)



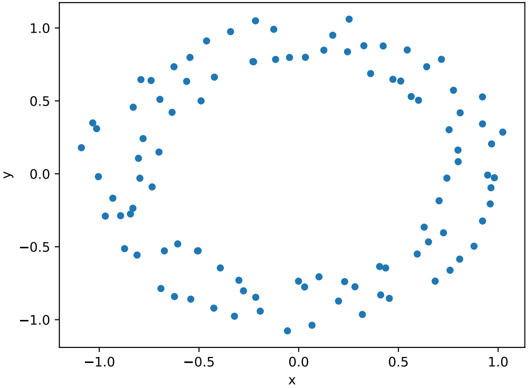
Word Example

- 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?



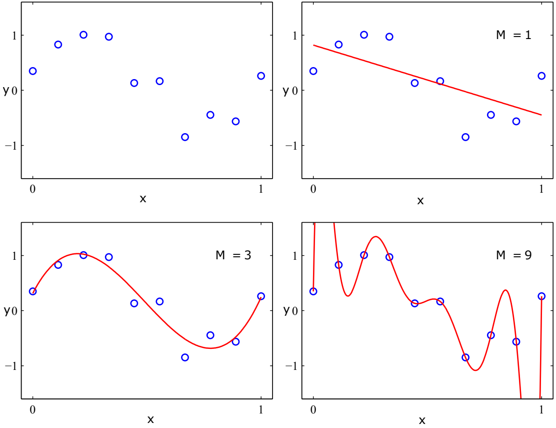
Capacity, Overfitting and Underfitting

Model Training

We consider three hypothesis sets (polynomial functions) $\mathcal{H}_1$,$\mathcal{H}_3$ and $\mathcal{H}_9$ and the results of fitting the models to the data set $\mathcal{D}$

Which one

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



Model Training (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

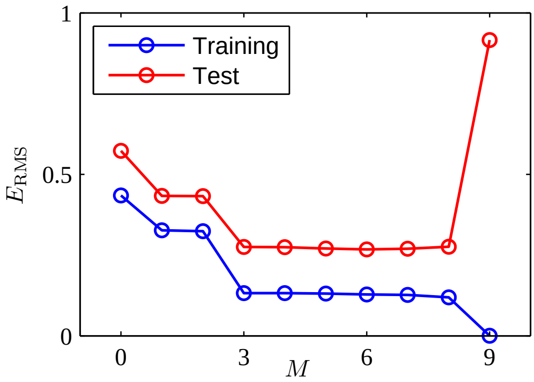


Figure 1: Graphs of the root-mean-square error evaluated on the **training set** and on an **independent test set** for various values of M

What happen if increasing N

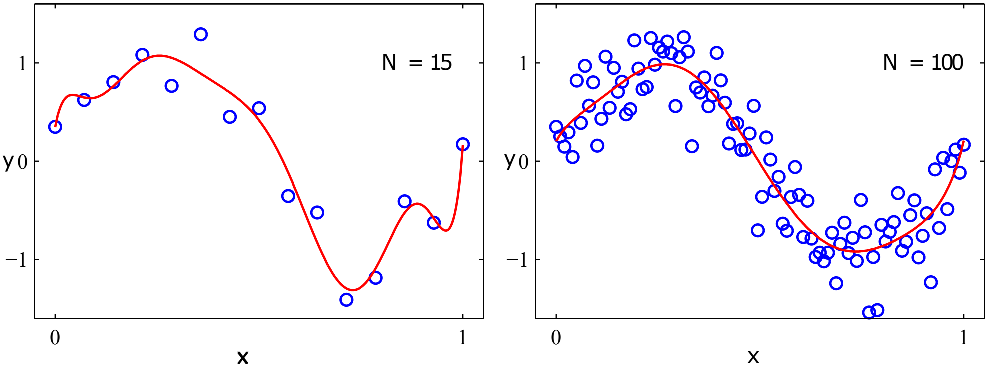
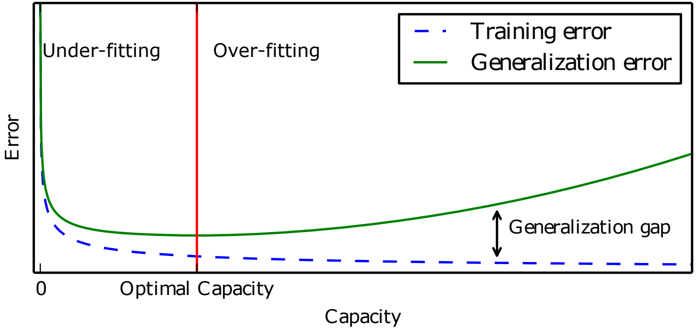


Figure 2: Using the $M = 9$ polynomial for $N = 15$ data points (left plot) and $N = 100$ data points (right plot). We see that increasing the size of the data set reduces the over-fitting problem

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.

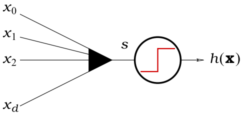


Logistic Regression

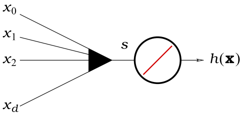
A Third Linear Model

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

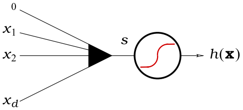
linear classification
$h(\boldsymbol{x}) = sign(s)$



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



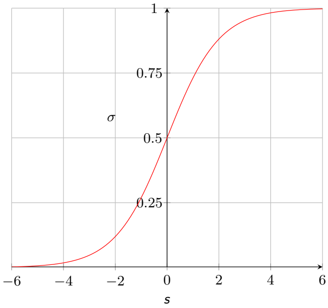
logistic regression
$h(\boldsymbol{x}) = \sigma(s)$



The logistic function

The formula

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



Some 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

Problem Statement

- The target function f is the probability

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

- Data $\mathcal{D} = \{(\boldsymbol{x}_1, y_1) ... (\boldsymbol{x}_N, y_N)\}$ with binary $y_i \in \{-1, 1\}$ generated by noisy target

$$P(y \mid \boldsymbol{x}) = \begin{cases} f(\boldsymbol{x}) & \text{for} \quad y = +1 \\ 1 - f(\boldsymbol{x}) & \text{for} \quad y = -1 \end{cases}$$

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

Error measure

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

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

where $z = h_{\boldsymbol{w}}(\boldsymbol{x}) = \sigma(\boldsymbol{w}^T\boldsymbol{x})$

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

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

Error measure (cont.)

- Maximizing Likelihood

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

- We define error measurement (*cross-entropy error*)

$$
E(h_{\boldsymbol{w}}) = -\sum_{n=1}^{N} (y_n \log z_n + (1 - y_n)\log(1 - z_n)) \tag{14}
$$

Learning Algorithm

1. Initialize the weights (parameters) at $t = 0$ $\boldsymbol{w}_0$
2. For $t = 1, 2, 3, \ldots$ do

   2.1 Compute the gradient

$$\nabla_{\boldsymbol{w}} E = -\sum_{n=1}^{N} \frac{y_n \boldsymbol{x}_n}{1 + e^{y_n \boldsymbol{w}_t^\intercal \boldsymbol{x}_n}}$$

   2.2 Update the weights

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

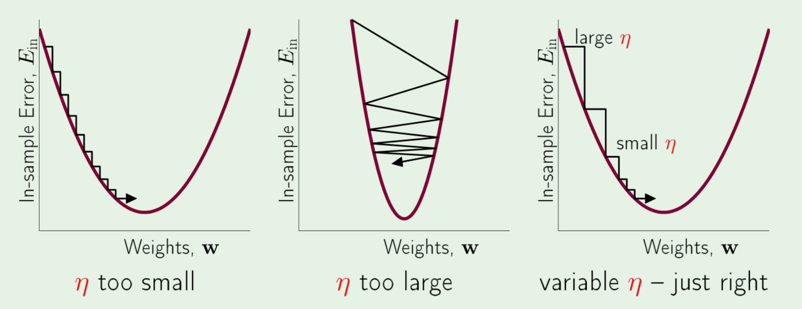
   where η is a learning rate (*hyper-parameter*)

   2.3 Iterate the next step until $\boldsymbol{w}$ is not change

3. Return the final weights $\boldsymbol{w}$

Learning Rate

- How η affects the algorithm?



Programming Example

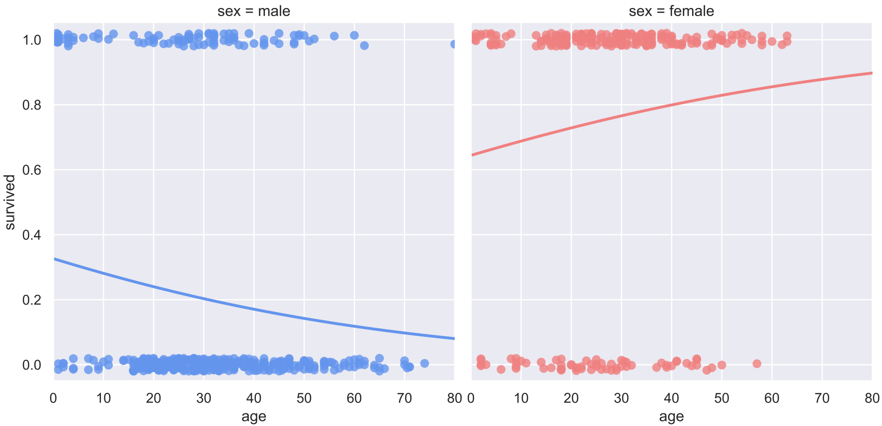
```
import matplotlib.pyplot as plt
import seaborn as sns
sns.set(style="darkgrid")

# 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.)



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