Chapter 2

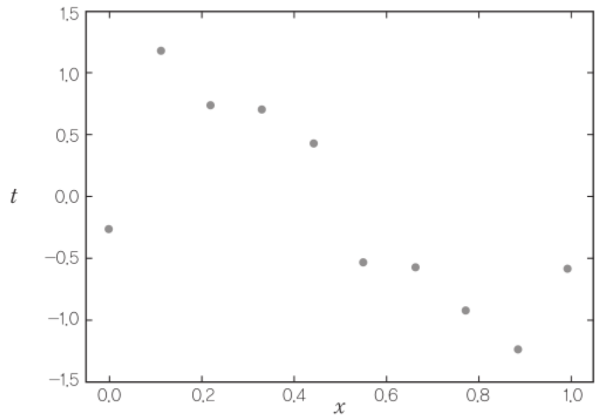
2

최소제곱법
(Least Square Method, LSM)

objective function(= □□□□)

Objective

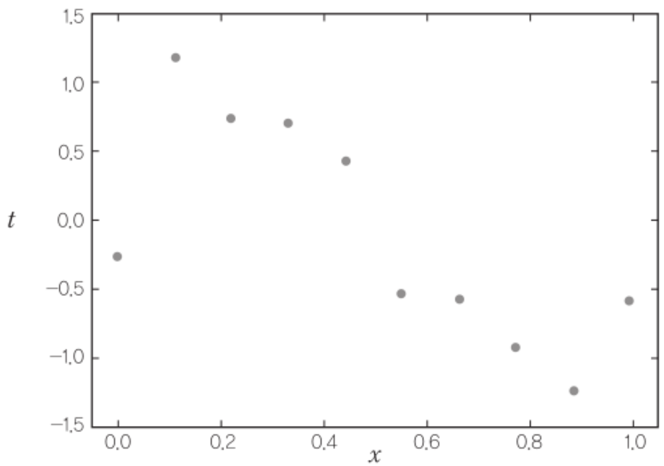
- By what function are the data points generated?



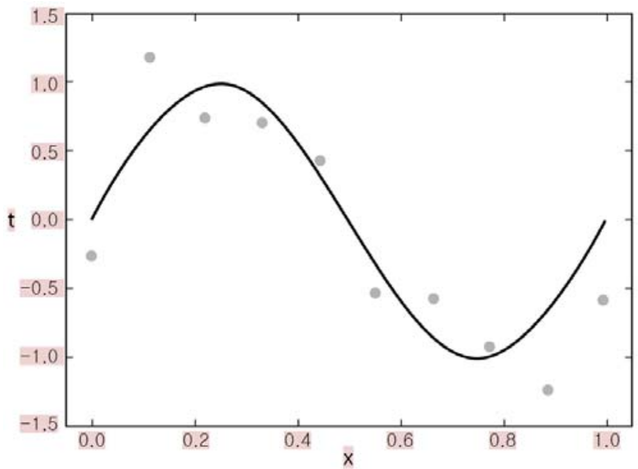
- 1) Learn the function → 2) predict the future (build model)
- The function is found in ways to minimize error between the real observed data and the predicted data

Training set

- Training set is the data set used to learn the function of the given data
- Example
  - Data: 10 data points on a *t* by *x* dimension



Learn the data to infer the function



Training in LSM

- Objective:
  - How well can we predict t (objective variable, 목적변수) using x (explanatory variable, 설명변수)
  - Use multinomial expression (다항식)

Known: x
Unknown: w, M

$$f(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M$$
$$= \sum_{m=0}^{M} w_m x^m$$

  - Estimate error of prediction
    - Predicted t – observed value x
    - $= \{f(x_1) - t_1\}^2 + \{f(x_2) - t_2\}^2 + \cdots + \{f(x_{10}) - t_{10}\}^2$
  - Final goal is to predict the optimal $\{w_m\}_{m=0}^{M}$

Measuring error of a model

- The error of a learned model is measured by

$$E_D = \frac{1}{2}\sum_{n=1}^{N}\{f(x_n) - t_n\}^2$$

$$E_D = \frac{1}{2}\sum_{n=1}^{N}\left\{\sum_{m=0}^{M} w_m x^m - t_n\right\}^2$$

- The difference of predicted and observed value is squared to remove any negative values. Hence the name "Least square method"
- Our objective is to minimize E_D

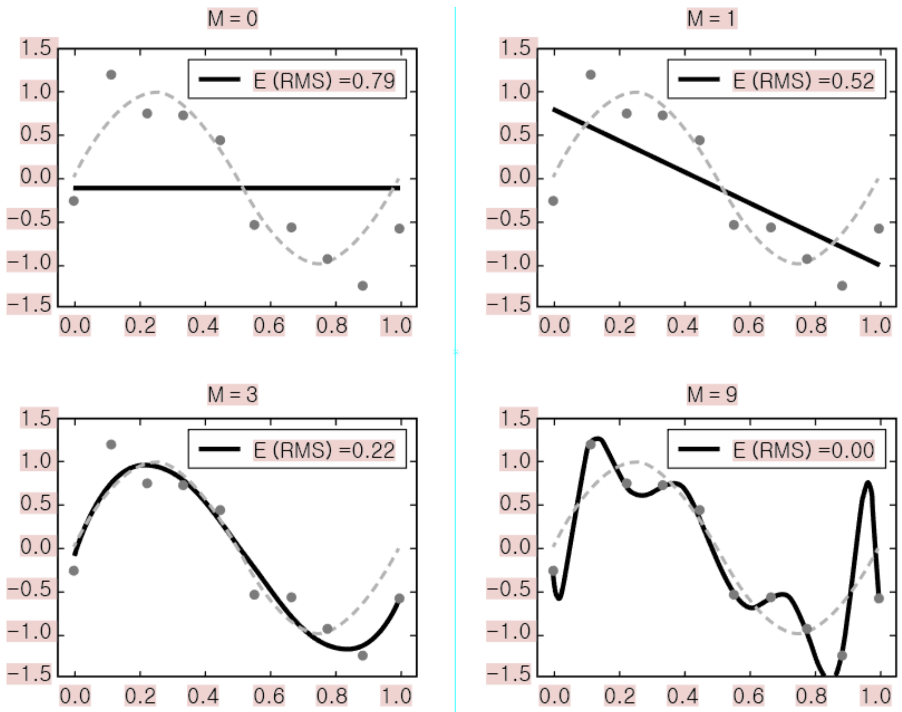
Minimizing error E_D

- [수학을 배우는 작은방] pg 50
- Differentiate E_D by w, $\frac{\partial E_D}{\partial w} = 0 \ (m = 0, \ldots, M)$
  - w is a vector, $w = (w_0, \ldots, w_M)^T$
  - $\frac{\partial E_D}{\partial w} = \sum_{m'}^{M} w_{m'} \sum_{n=1}^{N} x_n^{m'} x_n^{m} - \sum_{n=1}^{N} t_n x_n^{m} = 0$
  - If x_n^m represented as Nx(M+1) matrix θ
    - $w^T \theta^T \theta - t^T \theta = 0$
    - $w = (\theta^T \theta)^{-1} \theta^T t$
  - Where $t = (t_1, \ldots, t_N)^N$ vector of observed real values

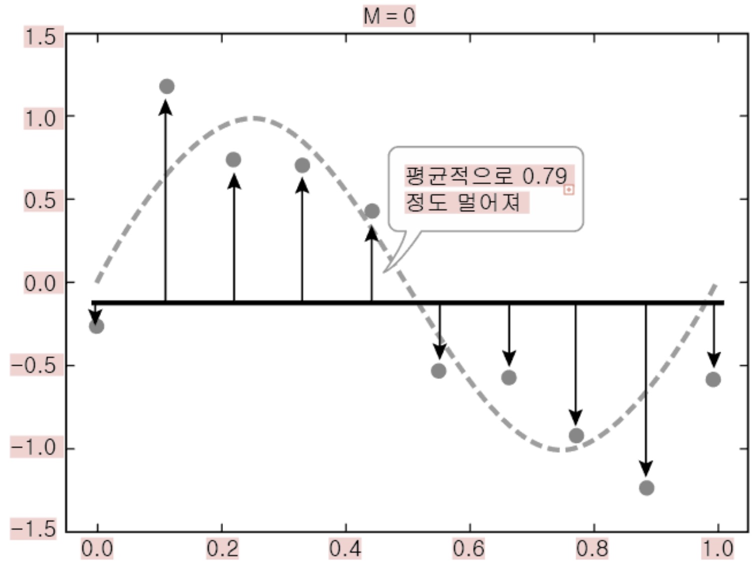
$$\theta = \begin{pmatrix} x_1^0 & x_1^1 & \cdots & x_1^M \\ x_2^0 & x_2^1 & \cdots & x_2^M \\ \vdots & \vdots & \ddots & \vdots \\ x_N^0 & x_N^1 & \cdots & x_N^M \end{pmatrix}$$

Results

- When M={0, 1, 3, 9} the learned functions are as follows
  - E(RMS-Root Mean Square)=$\sqrt{\frac{2E_D}{N}}$, which is the average error of the predicted values



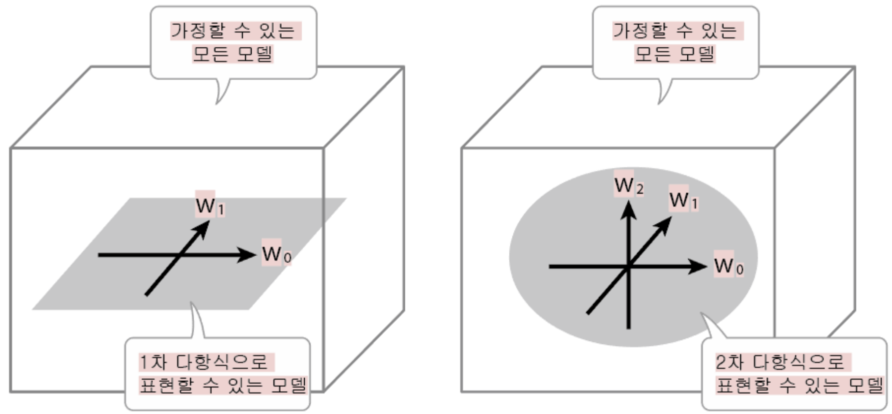
E(RMS)



The effect of M selection

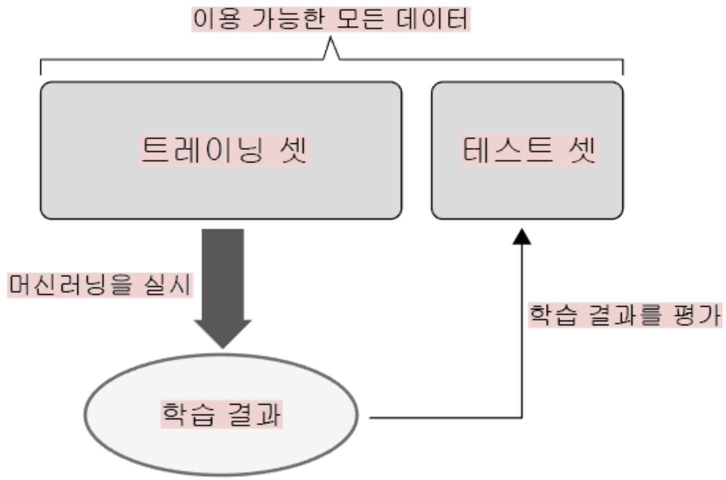
- Too small M may not represent the data well
- A large M may well represent the data
- However, a large M may cause overfitting
  - Overfitting is problem when random error or noise is represented instead of the underlying relationship
  - This is caused by lack of data or excessive use of parameters (M=9)

- Very important to select a suitable M
- Use test sets and cross validation



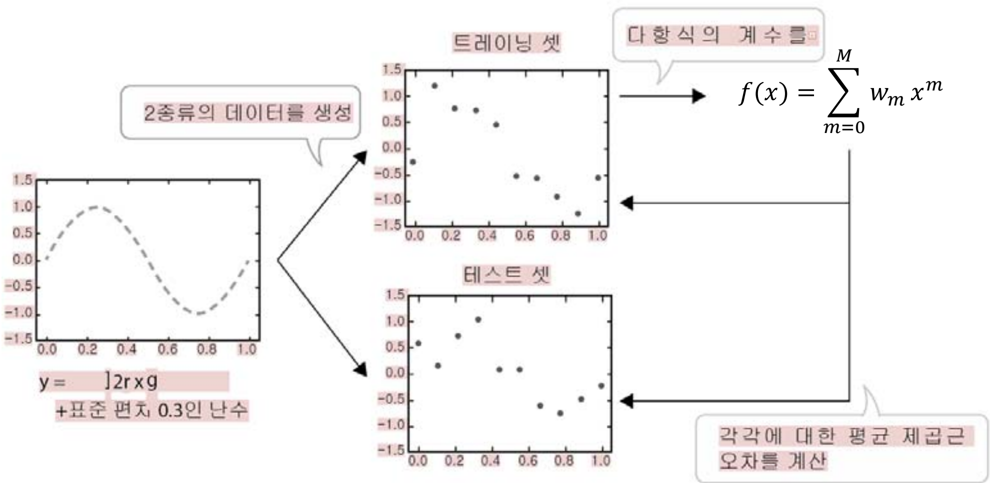
Test set

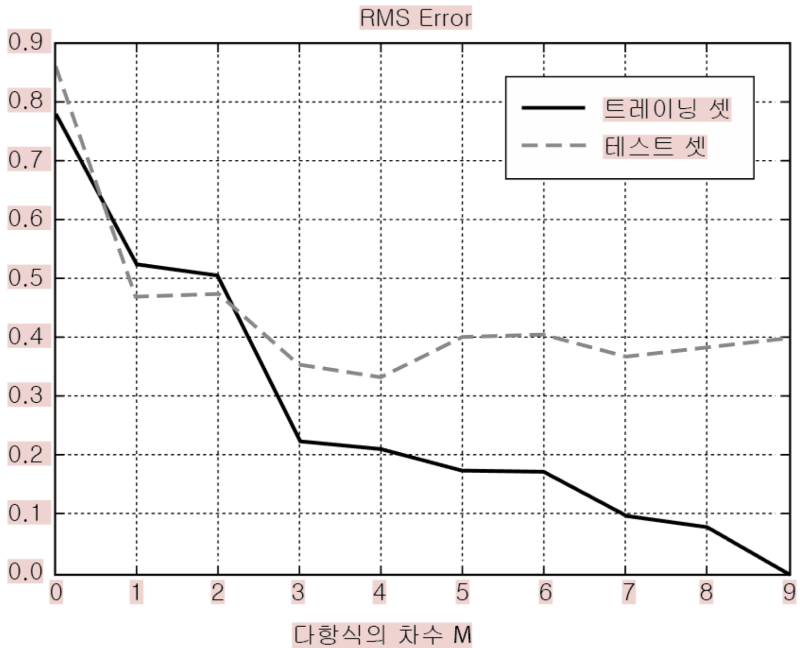
- From the collected data, split it into a **training set** and **test set**
- Use the training set to learn the function
- Use the test set to decide if overfitting has occurred



Selecting optimal M

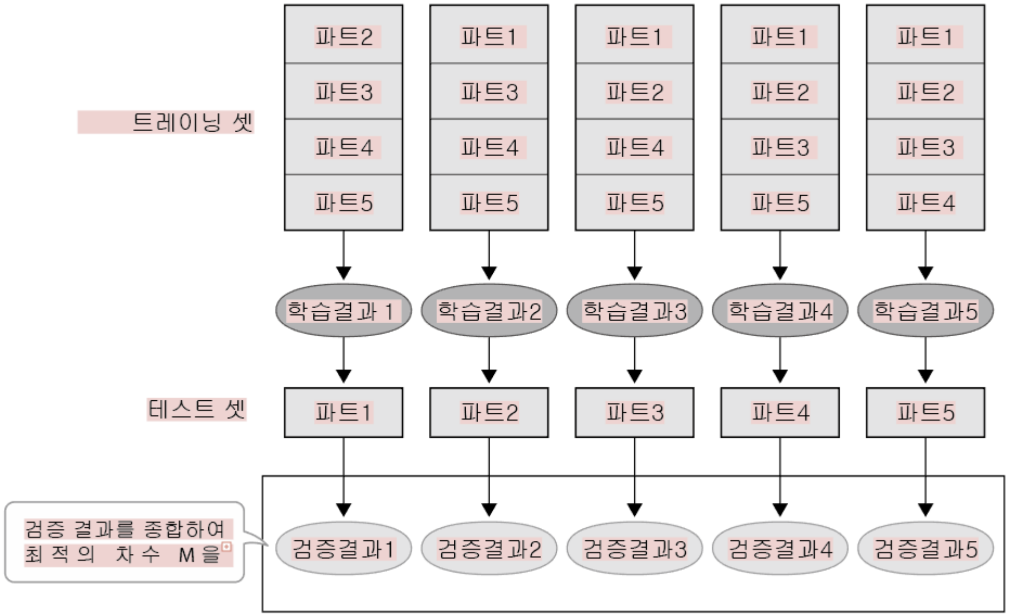
- Measure RMS of the training set and the test set independently
- With M>4, the RMS increases in the test set





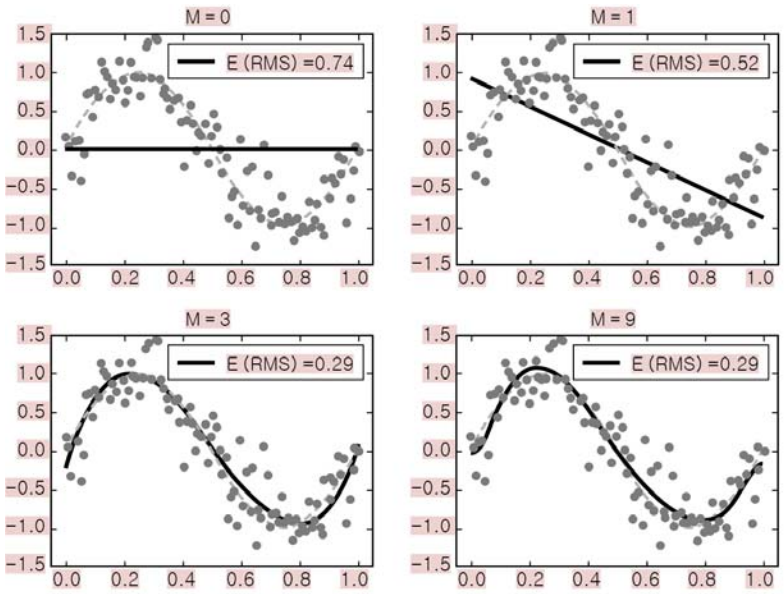
Cross validation (교차검증)

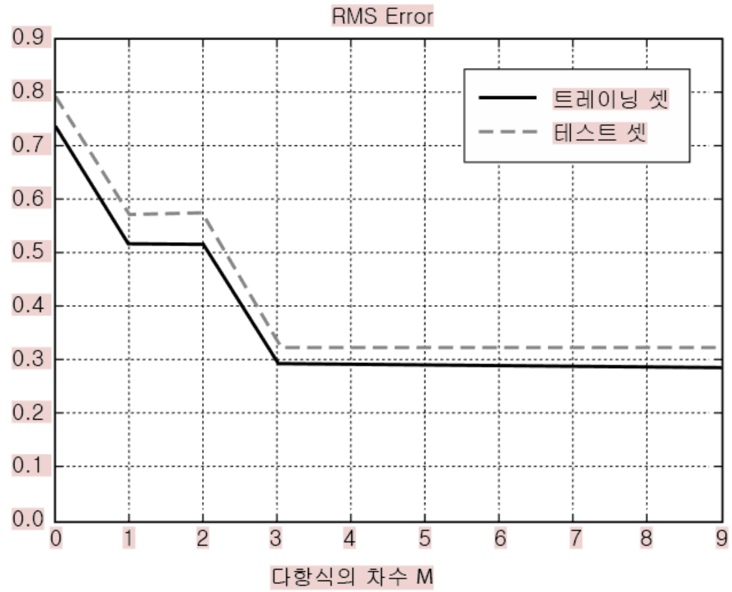
- Repeat the procedure of training/test set measurement by dividing the data set into K parts
- For each k, select k as test set and the remaining k` as training sets and measure RMS
- Select the best M, in our example it is M=4



Discussion on overfitting

- If data is large enough, we may choose large M without encountering the overfitting problem
- So the more data we have, the higher chance is that LSM will model the underlying relationship instead of random error or noise
- That's why big data is important but difficult to analyze





Chapter 3

3

최우추정법
(Maximum Likelihood Estimation)

Probability(확률)

- The measure of the likelihood that an event will occur.
- Example: normal 6-sided dice.
  - Outputs: 1, 2, 3, 4, 5, 6
  - Events: 1; 6; even
  - Probability:
    - $P(A) = \frac{\# \, of \, ways \, event \, can \, occur}{\# \, of \, possible \, outcomes}$
    - $P(1) = P(6) = 1/6$
    - $P(even) = 3/6 = 1/2$

Probability Distribution(확률 분포)

- Probability distribution: the assignment of a probability to each outcome.
  - Sum of the probabilities of all possible outcomes must be 1.
  - $\sum P(x) = 1$
- Example: normal 6-sided dice.
  - Outcomes: 1, 2, 3, 4, 5, 6
  - Probability distribution:
    - $P(x) = \frac{1}{6}, x = \{1, \ldots, 6\}$
    - $\sum P(x) = 1$

Conditional Probability(조건부확률)

- $P(i|\theta)$: the probability of event i under the condition θ.
- Example: two dices D_1, D_2
  - $P(2|D_1)$: probability of picking 2 when using dice D_1.
  - $P(2|D_2)$: probability of picking 2 when using dice D_2.

Joint Probability(결합확률)

- $P(X,Y)$: the probability of event X and Y.
- $P(X,Y) = P(X|Y)P(Y) = P(Y|X)P(X)$
- X and Y are *independent(독립)* if and only if $P(X,Y) = P(X)P(Y), P(X) \neq 0, P(Y) \neq 0$.
- Example: for two dices D_1, D_2, we first pick one dice and rolling the dice.
  - $P(D)$: probability of picking dice D_1 or D_2.
    - Ex) $P(D_1) = 0.3, P(D_2) = 0.7$
  - $P(2|D_2)$: probability of picking 2 when using dice D_2.
  - $P(1, D_1)$: probability of getting 1 while rolling dice D_1.
    - $= P(1|D_1)P(D_1)$

Independent Identically Distribution (독립동일분포)

- Independent Identically Distribution (i.i.d.):
  - Each random variable has the same probability distribution as the others and all are mutually independent.
- Example: When we get 1, 2 and 6 as the result of rolling normal dice three times.
  - All outputs have same probability distribution as we use the same dice for all trials.
  - All trials do not affect each other.
    - Getting 2 from second trial cannot be affected by the output 1 from previous trial or output 6 from later trial.
  - Therefore, the outputs (1, 2, 6) are independent identically distributed.

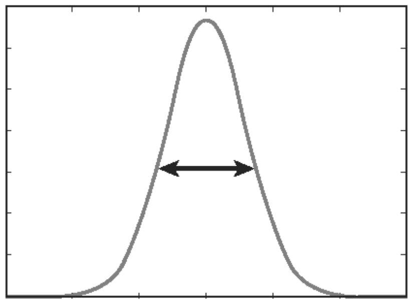
Probabilistic Model(확률 모델)

- parametric vs. non-parameteric
- 3 steps of parametric model.
    1. Define model with parameters.
    2. Define the evaluation criterion.
    3. Find the best fit parameters according to evaluation criterion.

Normal Distribution(정규분포)

- Normal distribution (Gaussian distribution) is most widely used distribution because of central limit theorem.
  - Central limit theorem establishes that when independent random variables are added, their sum tends toward a normal distribution even if the original variables themselves are not normally distributed.
- The probability distribution is defined as

$$N(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$



Remind: Least squares(최소제곱법)

- Describing Least square estimation as the 3 steps of parametric model.
  1. Define model.
     - Data: $\mathrm{D} = \{(x_n, t_n)\}_{n=1}^{N}$
     - Parameters: $\theta = \{w_m\}_{m=0}^{M}$
     - Model: $f(x; \theta) = \sum_{m=0}^{M} w_m x^m$ (M+1차 다항식)
  2. Define evaluation criterion.
     - $E_D = \frac{1}{2}\sum_{n=1}^{N}\{f(x_n) - t_n\}^2$
     - Criterion: $\underset{\theta}{argmin}\, E_D$
  3. Find parameters.

Likelihood function(우도 함수)

Likelihood function

- Function of the parameters of a model given data which is identical to the probability of observed data given parameters.
- $L(\theta; x_1, x_2, \dots, x_n) = P(x_1, x_2, \dots, x_n|\theta)$
- If $x_1, x_2, \dots, x_n$ are i.i.d from $\mathrm{P}(x|\theta)$
- $L(\theta; x_1, x_2, \dots, x_n) = P(x_1, x_2, \dots, x_n|\theta) = P(x_1|\theta)P(x_2|\theta) \dots P(x_n|\theta) = \prod_{i=1}^{n} P(x_i|\theta)$

Log likelihood function

- Since it needs a lot of multiplication of probabilities (which are usually quite small), the likelihood is likely to get very small.
- Log likelihood can alleviate this computational problem.
- $l(\theta; x_1, x_2, \dots, x_n) = \log(L(\theta; x_1, x_2, \dots, x_n)) = \sum_{i=1}^{n} \log(P(x_i|\theta))$

Maximum Likelihood Estimation(최우추정법)

- If we assume the quality of observed data is sufficiently good and not biased, the observed data is the most likely to be generated from the model.
- Therefore, maximum likelihood estimation find the parameters by maximizing the likelihood function for given observed data.

Maximum Likelihood Estimation(최우추정법)

- When we do not know parameters?
- 3 steps of parametric model.
  1. Define model.
     - Data: $\mathrm{D} = \{(x_n, t_n)\}_{n=1}^{N}$
     - Parameters: θ
     - Probability distribution: $\mathrm{P}(t_n|\theta)$ (임의의 모델)
  2. Define evaluation criterion.
     - $L(\theta; t_1, t_2, \dots, t_N) = P(t_1, t_2, \dots, t_N|\theta)$
     - Criterion: $\underset{\theta}{argmax}\, L(\theta; t_1, t_2, \dots, t_N)$ or $\underset{\theta}{argmax} \log(L(\theta; t_1, t_2, \dots, t_N))$
  3. Find parameters

Maximum Likelihood Estimation(최우추정법)

- When we know parameters of models
- Example: two dices D_1, D_2 whose probability distributions are
  - $P(1|D_1) = P(2|D_1) = \cdots = P(6|D_1) = \frac{1}{6}$
  - $P(1|D_2) = P(2|D_2) = \cdots = P(5|D_2) = \frac{1}{12}, P(6|D_2) = \frac{7}{12}.$

If one dice is randomly selected and the outputs of three rolling trials are (6, 6, 6), which dice is more likely to be selected?

  - $L(\theta_1; 6,6,6) = P(6,6,6|\theta_1) = 3P(6|\theta_1) = 3(\frac{1}{6})^3 = 3(\frac{2}{12})^3$
  - $L(\theta_2; 6,6,6) = P(6,6,6|\theta_2) = 3P(6|\theta_2) = 3(\frac{7}{12})^3$

- Dice D_2 is more likely to be selected.

Maximum Likelihood Estimation(최우추정법)

- Example of section 3.2.1 in textbook.
- Finding parameters from given data assuming that the model is *normal distribution*.
  - Data: $\mathrm{D} = \{(x_n, t_n)\}_{n=1}^{N}$
  - Parameters: $\theta = \{\mu, \sigma\}$
  - Probability distribution: $\mathrm{P}(t_n|\theta) = N(t_n|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(t_n-\mu)^2}$
  - Likelihood function: $L(\theta; t_1, t_2, \dots, t_N) = P(t_1, t_2, \dots, t_N|\theta) =$
    $\prod_{n=1}^{N} P(t_n|\theta) = \prod_{n=1}^{N} N(t_n|\mu,\sigma) = \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(t_n-\mu)^2}$

Maximum Likelihood Estimation(최우추정법)

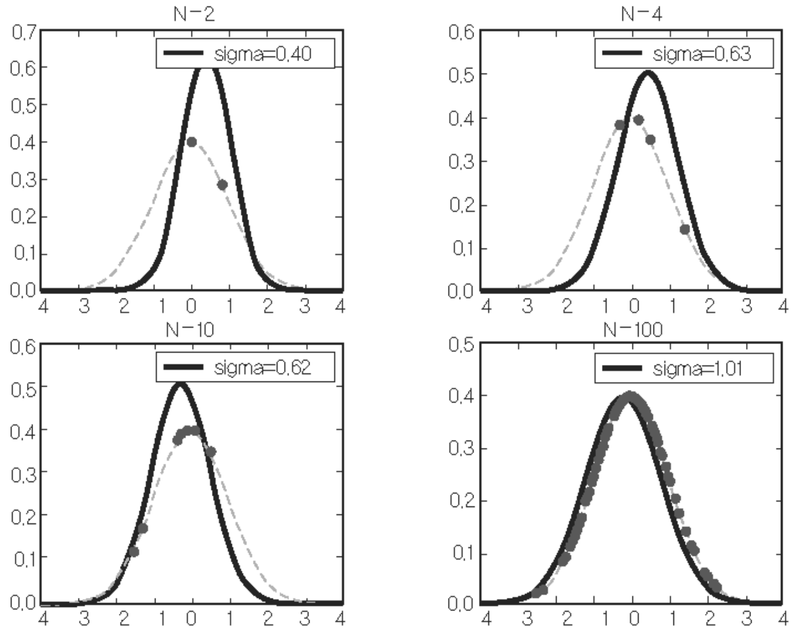
- Find parameters [P.93 수학을 배우는 작은 방 참조]
  - Find μ? -> $\underset{\mu}{argmax}\, L(\theta; t_1, t_2, \ldots, t_N) = \underset{\mu}{argmax} \log(L(\theta; t_1, t_2, \ldots, t_N))$
    - The value which satisfies $\frac{\partial L}{\partial \mu} = 0$.
  - $l = \log\big(L(\theta; t_1, t_2, \ldots, t_N)\big) = \log\left(\prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(t_n-\mu)^2}\right) = \log\left[\left(\frac{1}{2\pi\sigma^2}\right)^{\frac{N}{2}} e^{\left\{-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(t_n-\mu)^2\right\}}\right]$

$$= -\frac{N}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{n=1}^{N}(t_n - \mu)^2$$

  - $\frac{\partial l}{\partial \mu} = \frac{1}{\sigma^2}\sum_{n=1}^{N}(t_n - \mu) = \frac{1}{\sigma^2}\sum_{n=1}^{N} t_n - N\mu = 0$
  - $\therefore \hat{\mu} = \frac{1}{N}\sum_{n=1}^{N} t_n$
  - TODO: How to find σ?
- The mean of observed data is estimated as the mean of model.

Maximum Likelihood Estimation(최우추정법)

- How well the model is estimated as the number of observed data increases.
- σ is harder to estimate for small N since values far from mean are hard to be observed for small N.



Maximum Likelihood Estimation(최우추정법)

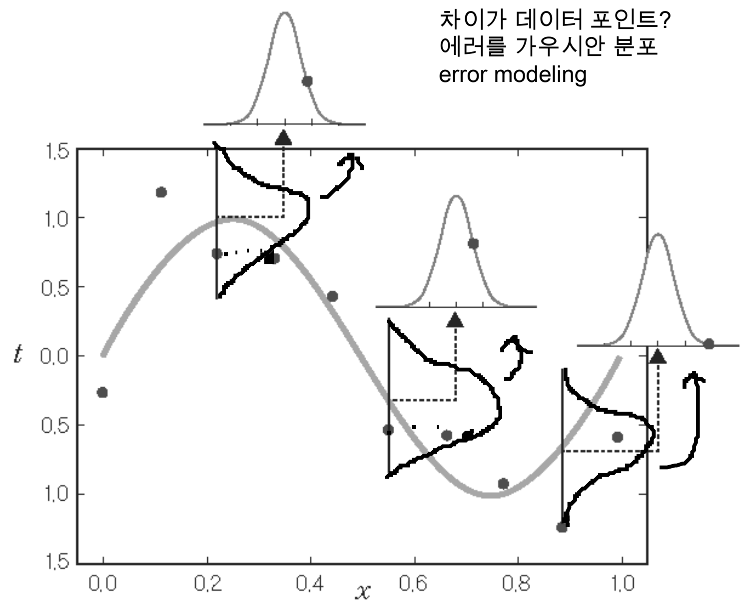
- Example of section 3.1 in textbook.
- Finding parameters from given data whose probability distribution is defined as below.
  - Data: $\mathrm{D} = \{(x_n, t_n)\}_{n=1}^{N}$
  - Parameters: $\theta = \{\{w_m\}_{m=0}^{M}, \sigma\}$
  - Probability distribution: $\mathrm{P}(t_n|\theta) = N(t_n|f(x_n), \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(t-f(x_n))^2}$

$$where\ f(x_n) = \sum_{m=0}^{M} w_m x^m$$

  - Likelihood function: $L(\theta; t_1, t_2, \dots, t_N) = P(t_1, t_2, \dots, t_N|\theta) = \prod_{n=1}^{N} P(t_n|\theta) = \prod_{n=1}^{N} N(t_n|f(x_n), \sigma) = \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(t-f(x_n))^2}$

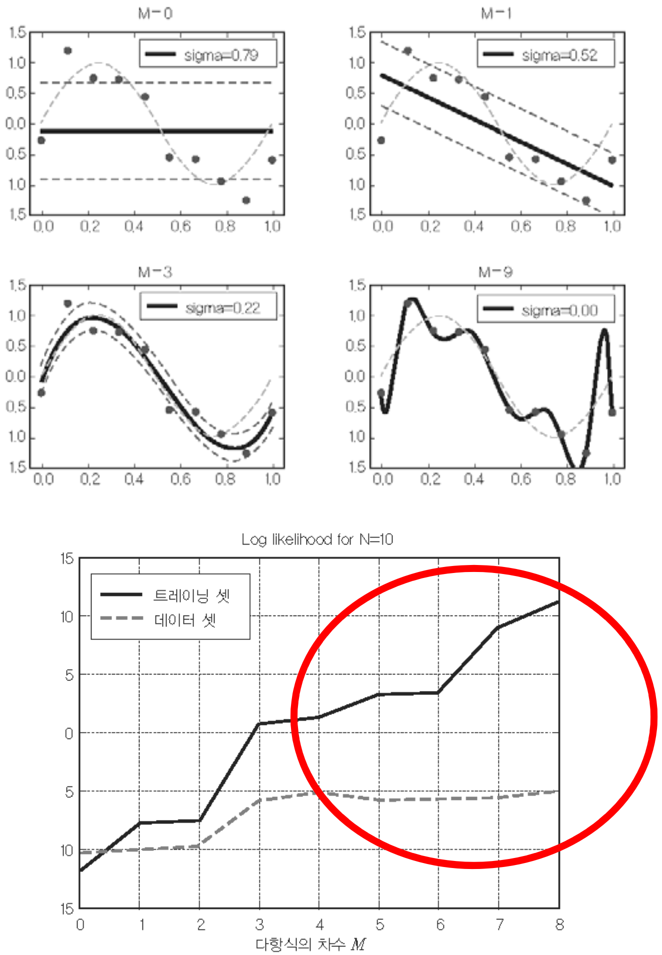
Maximum Likelihood Estimation(최우추정법)

- How this distribution looks like?
- Mean points of t each x is following polynomial $f(x_n) = \sum_{m=0}^{M} w_m x^m$.
- For each point x, output values follow normal distribution $N(t|f(x), \sigma)$.

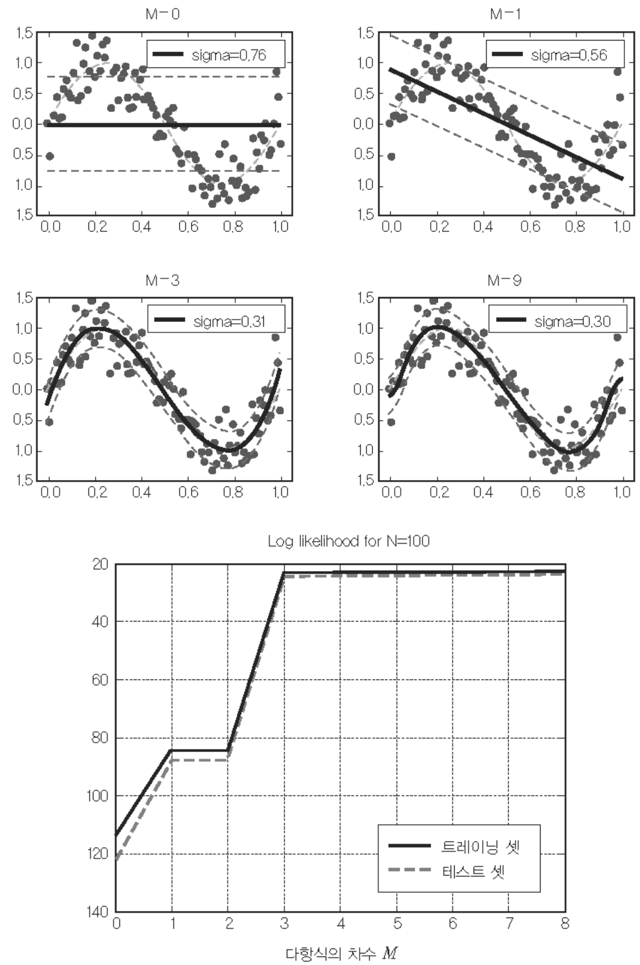


Overfitting(오버피팅)

$N = 10$



$N = 100$



The model can be overfitted if model is too complex but the number of data is not sufficient.