Pattern Information Processing: Linear Models and Least-Squares

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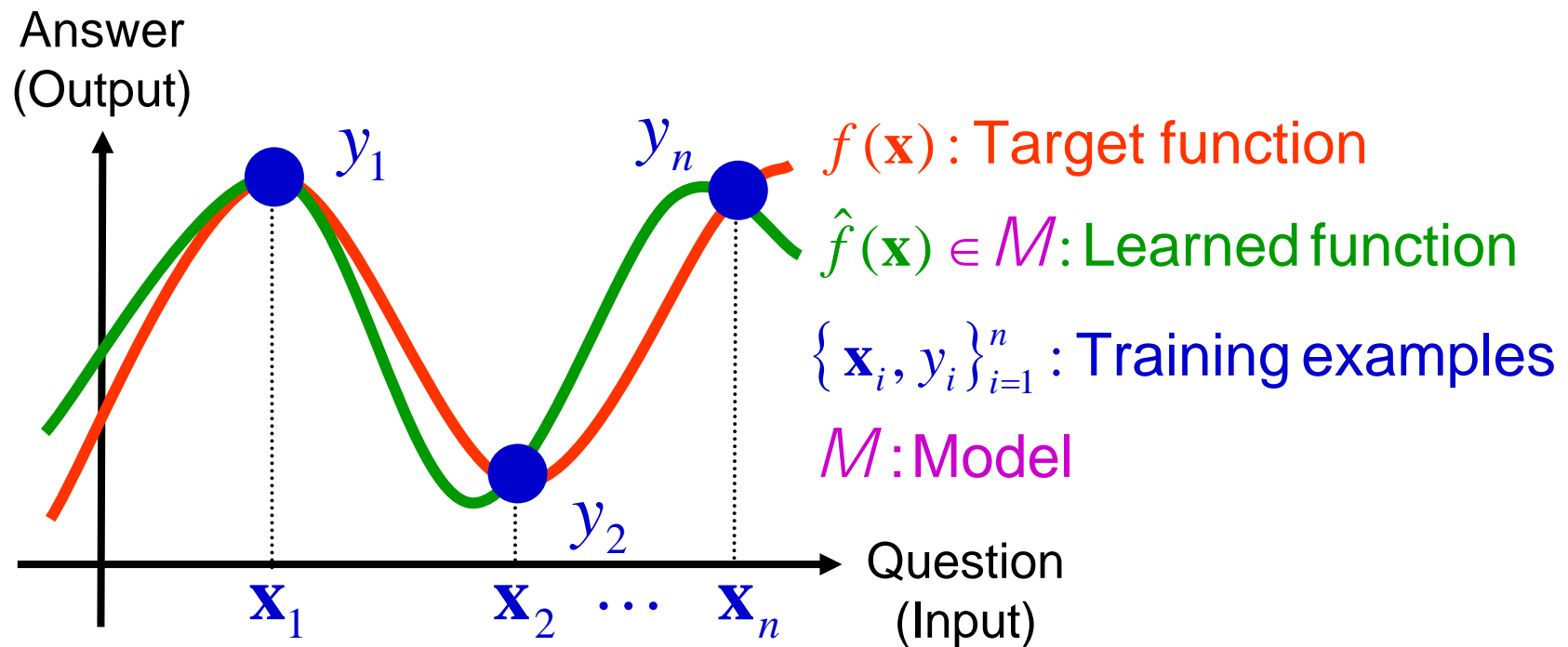http://sugiyama-www.cs.titech.ac.jp/~sugi/

Focus of This Course

- There are 3 topics in learning research.
  - Understanding human brains
  - Developing learning machines
  - Mathematically clarifying mechanism of learning
- There are 3 types of learning.
  - Supervised learning
  - Unsupervised learning
  - Reinforcement learning
- Topics of supervised learning:
  - Active learning
  - Model selection
  - Learning methods
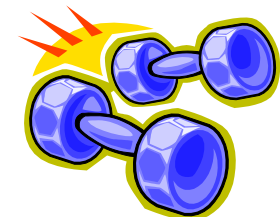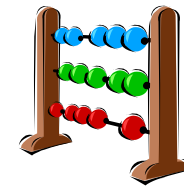
Supervised Learning
As Function Approximation

$f(\mathbf{x})$: Target function

$\hat{f}(\mathbf{x}) \in M$: Learned function

$\{\mathbf{x}_i, y_i\}_{i=1}^{n}$: Training examples

M : Model

Using training examples $\{\mathbf{x}_i, y_i\}_{i=1}^{n}$,
find a function $\hat{f}(\mathbf{x})$ from a model M
that well approximates the target function $f(\mathbf{x})$.

Formal Notation and Assumptions

- $\mathcal{D} \subset \mathbb{R}^d$: Input domain
- $f(\boldsymbol{x})$:Learning target function ($\mathcal{D} \to \mathbb{R}$)
- $\boldsymbol{x}_i \in \mathcal{D}$:Training input point
- $y_i = f(\boldsymbol{x}_i) + \epsilon_i$:Training output value
- ϵ_i :mean zero, independent and identically distributed ("i.i.d.")

$$\mathbb{E}_{\boldsymbol{\epsilon}}[\epsilon_i] = 0 \qquad \mathbb{E}_{\boldsymbol{\epsilon}}[\epsilon_i \epsilon_j] = \begin{cases} \sigma^2 & (i = j) \\ 0 & (i \neq j) \end{cases}$$

- $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$:Training examples
- $\hat{f}(\boldsymbol{x})$:Learned function
- $\mathcal{M}$:Model

Generalization Error

- We want to obtain $\hat{f}(\boldsymbol{x})$ such that output values at unlearned test input points $\boldsymbol{t}$ can be accurately estimated.

- Suppose $\boldsymbol{t}$ follows a probability distribution with density $q(\boldsymbol{x})$.

- Expected test error (generalization error):

$$G = \int_{\mathcal{D}} \left(\hat{f}(\boldsymbol{t}) - f(\boldsymbol{t}) \right)^2 q(\boldsymbol{t}) d\boldsymbol{t}$$

- Goal: Obtain $\hat{f}(\boldsymbol{x})$ such that G is minimized.

Formal Description of Problems

$$G = \int_{\mathcal{D}} \left(\hat{f}(\boldsymbol{t}) - f(\boldsymbol{t}) \right)^2 q(\boldsymbol{t}) d\boldsymbol{t}$$

- **Active learning:** $\displaystyle \min_{\{\boldsymbol{x}_i\}_{i=1}^n} G$

- **Model selection:** $\displaystyle \min_{\mathcal{M}} G$

- **Learning methods:** $\displaystyle \min_{\hat{f} \in \mathcal{M}} G$

Today's Plan

■ Models

- Linear models
- Kernel models

■ Learning methods

- Least-squares learning

Linear/Non-Linear Models

- Model is a set of functions from which learning result functions are searched.
- We use a family of functions $\hat{f}(x)$ parameterized by

$$\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_b)^\top$$

- Linear model: $\hat{f}(x)$ is linear with respect to $\boldsymbol{\alpha}$
  (Note: not necessarily linear with respect to x)
- Non-linear model: Otherwise

Linear Models

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{b} \alpha_i \varphi_i(\boldsymbol{x})$$

- $\{\varphi_i(\boldsymbol{x})\}_{i=1}^{b}$:Linearly independent functions
- For example, when $d = 1$
  - Polynomial
    $$1, x, x^2, \ldots, x^{b-1}$$
  - Trigonometric polynomial
    $$1, \sin x, \cos x, \ldots, \sin kx, \cos kx$$
    $$b = 2k + 1$$

Multi-Dimensional Linear Models

- For multidimensional input $(d > 1)$, a product model could be used.

$$\hat{f}(\boldsymbol{x}) = \sum_{i_1=1}^{c} \sum_{i_2=1}^{c} \cdots \sum_{i_d=1}^{c}$$

$$\alpha_{i_1, i_2, \ldots, i_d} \varphi_{i_1}(x^{(1)}) \varphi_{i_2}(x^{(2)}) \cdots \varphi_{i_d}(x^{(d)})$$

$$\boldsymbol{x} = (x^{(1)}, x^{(2)}, \ldots, x^{(d)})^{\top}$$

- The number of parameters is $b = c^d$, which increases exponentially w.r.t. d.
- Infeasible for large d !

Additive Models

- For large d, we have to reduce the number of parameters.

- Additive model:

$$\hat{f}(\boldsymbol{x}) = \sum_{j=1}^{d} \sum_{i=1}^{c} \alpha_{i,j} \varphi_i(x^{(j)})$$

- The number of parameters is only $b = cd$.

- However, additive model is too simple so its representation capability may not be rich enough in some application.

Kernel Models

- **Linear model**:

  $\{\varphi_i(\boldsymbol{x})\}_{i=1}^{b}$ do not depend on $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$

- **Kernel model**:

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{n} \alpha_i K(\boldsymbol{x}, \boldsymbol{x}_i)$$

- $K(\boldsymbol{x}, \boldsymbol{x}')$: **Kernel function**

  - Suppose kernel is symmetric:

$$K(\boldsymbol{x}, \boldsymbol{x}') = K(\boldsymbol{x}', \boldsymbol{x})$$

  - e.g., Gaussian kernel

$$K(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|^2}{2h^2}\right)$$

Kernel Models (cont.)

■ Put kernel functions at training input points.
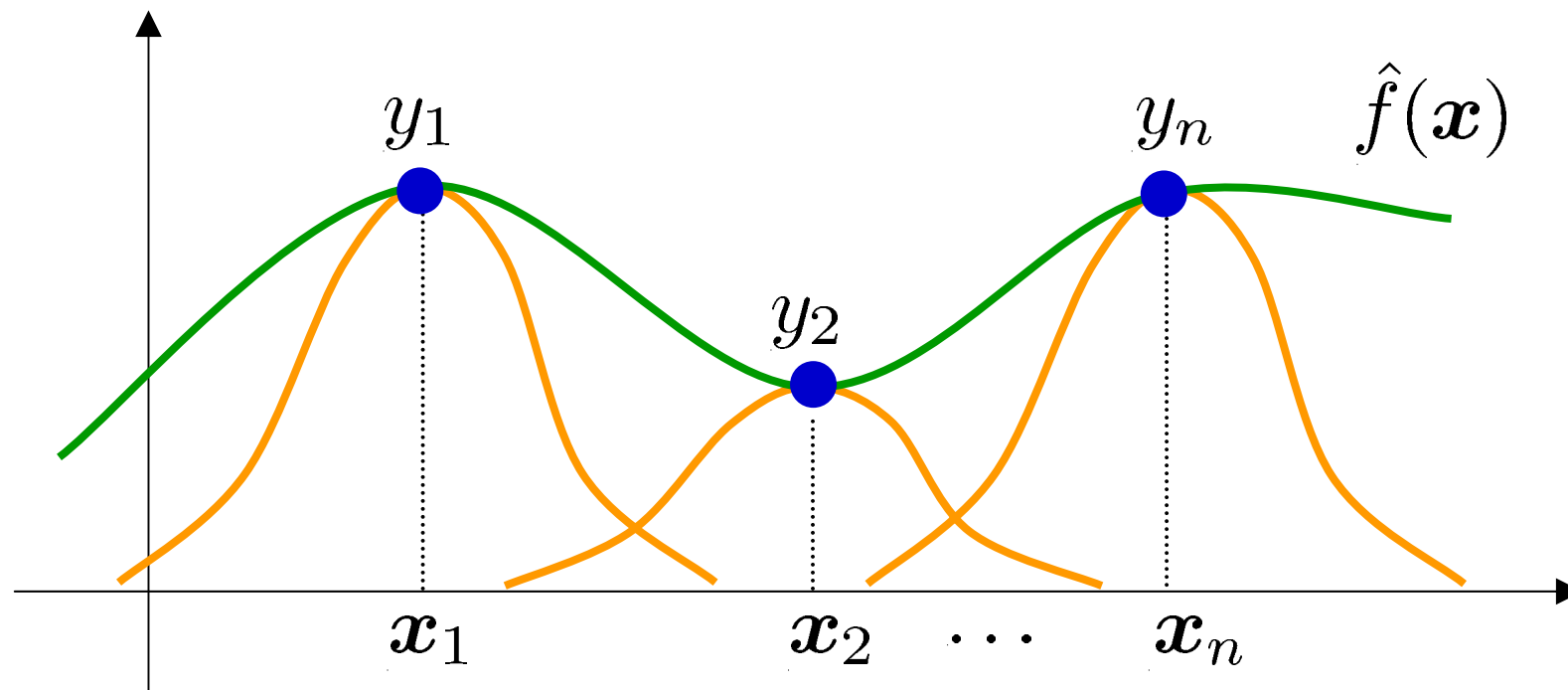
Kernel Models (cont.)

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{n} \alpha_i K(\boldsymbol{x}, \boldsymbol{x}_i)$$

- The number of parameters is n, which is independent of the input dimensionality d.

- Although kernel model is linear w.r.t. $\boldsymbol{\alpha}$, the number of parameters grows as the number of training samples increases.

- Mathematical treatment could be different from ordinary linear models (called "non-parametric models" in statistics).

Summary of Linear Models

■ **Linear model (product)**:
High flexibility, high complexity

■ **Linear model (additive)**:
Low flexibility, low complexity

■ **Kernel model**:
Moderate flexibility, moderate complexity

■ Good model depends on applications.

■ Later in model selection, we discuss how to choose appropriate models.

Learning Methods

■**Linear learning methods**:

Parameter vector $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_b)^\top$ is estimated linearly w.r.t.

$$\boldsymbol{y} = (y_1, y_2, \ldots, y_n)^\top$$

■**Non-linear learning methods**: Otherwise

Linear Learning for Linear Models / Kernel Models

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{b} \alpha_i \varphi_i(\boldsymbol{x})$$

■ In linear learning methods, a learned parameter vector is given by

$$\hat{\boldsymbol{\alpha}} = \boldsymbol{L}\boldsymbol{y} \qquad \boldsymbol{L} : \text{Learning matrix}$$

Least-Squares Learning

- Learn $\boldsymbol{\alpha}$ such that the squared error at training input points is minimized:

$$\hat{\boldsymbol{\alpha}}_{LS} = \underset{\boldsymbol{\alpha} \in \mathbb{R}^b}{\operatorname{argmin}} J_{LS}(\boldsymbol{\alpha})$$

$$J_{LS}(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i) - y_i \right)^2$$

$$= \|\boldsymbol{X}\boldsymbol{\alpha} - \boldsymbol{y}\|^2$$

$\boldsymbol{X}_{i,j} = \varphi_j(\boldsymbol{x}_i)$:Design matrix $(n \times b)$

- In the following, we assume $\operatorname{rank}(\boldsymbol{X}) = b$

How to Obtain Solutions

■ Extreme-value condition:

$$\nabla J_{LS}(\hat{\boldsymbol{\alpha}}_{LS}) = 2\boldsymbol{X}^{\top}(\boldsymbol{X}\hat{\boldsymbol{\alpha}}_{LS} - \boldsymbol{y}) = 0$$

$$\Longrightarrow \quad \hat{\boldsymbol{\alpha}}_{LS} = (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}^{\top}\boldsymbol{y}$$

■ Therefore, LS is linear learning.

$$\hat{\boldsymbol{\alpha}}_{LS} = \boldsymbol{L}_{LS}\boldsymbol{y}$$

$$\boldsymbol{L}_{LS} = (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}^{\top}$$

If you are not familiar with vector-derivatives, see e.g,
"Matrix Cookbook" (http://matrixcookbook.com)

Example of LS

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{b} \alpha_i \varphi_i(\boldsymbol{x})$$

■ Trigonometric polynomial model

$$1, \sin x, \cos x, \ldots, \sin 15x, \cos 15x \quad (b = 31)$$
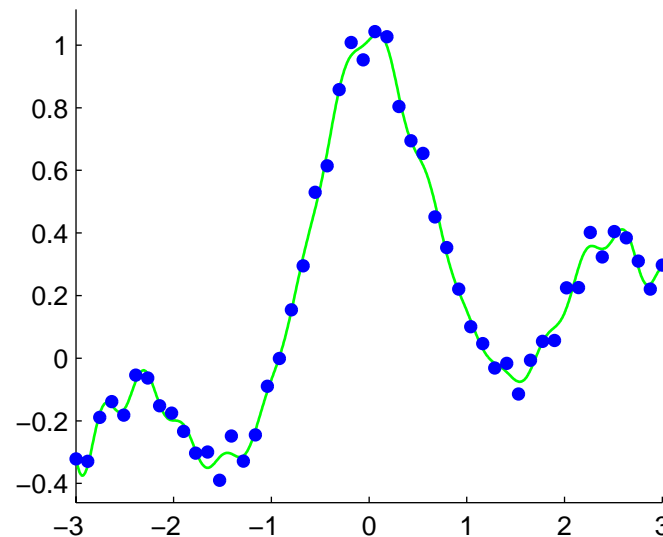
Homework

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{n} \alpha_i K(\boldsymbol{x}, \boldsymbol{x}_i)$$

1. Prove that the LS solution in kernel models is given by

$$\hat{\boldsymbol{\alpha}}_{LS} = \boldsymbol{L}_{LS} \boldsymbol{y}$$

$$\boldsymbol{L}_{LS} = \boldsymbol{K}^{-1}$$

$$\boldsymbol{K}_{i,j} = K(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

(Kernel matrix)

Homework (cont.)

2. For your own toy 1-dimensional data, perform simulations using

- Gaussian kernel models
- Least-squares learning

and analyze the results when, e.g.,

- Target functions
- Number of samples
- Noise level
- Width of Gaussian kernel

are changed.

■ Deadline: beginning of next class