Least Squares

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Schedule

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2. 04/15 Regression 1
3. 04/22 Regression 2
- 04/30 Cancelled
4. 05/13 Classification 1
5. 05/20 Classification 2
6. 05/27 Deep learning 1
- 06/03 No lecture
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11. 07/08 Representation learning 1
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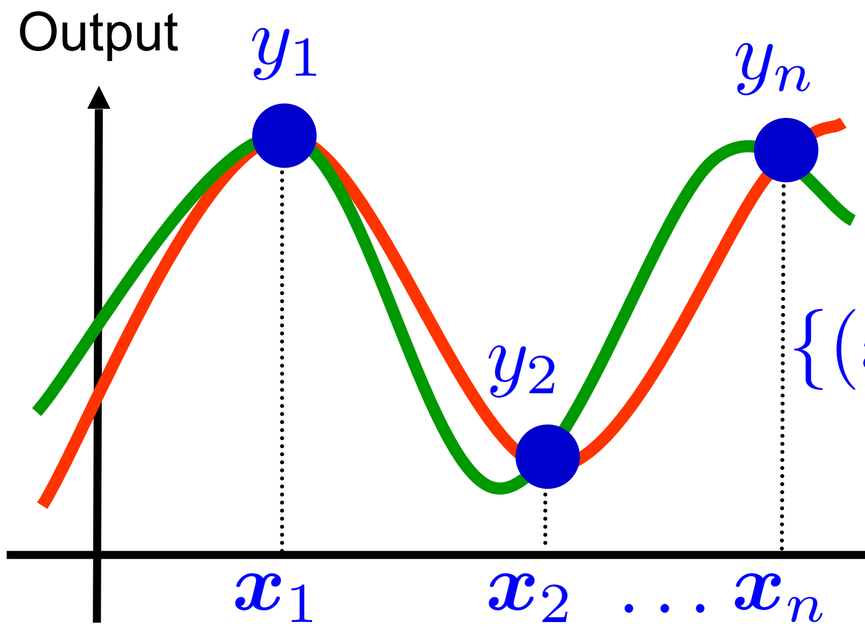
Regression = Function Approximation



$f(\boldsymbol{x})$: function to be learned

$\hat{f}(\boldsymbol{x})$: learned function

$\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$: training samples

$$y_i = f(\boldsymbol{x}_i)\ (+\text{noise})$$

Learn a function that is close to the underlying function by using training samples

Contents

Linear/non-linear model

- Model: candidate set to search for a learned function
  - A model is specified when we choose parameter $\boldsymbol{\theta}$

$$\{f_{\boldsymbol{\theta}}(\boldsymbol{x}) \mid \boldsymbol{\theta} = (\theta_1, \ldots, \theta_b)^\top\}$$

- Linear model: $f_{\boldsymbol{\theta}}(\boldsymbol{x})$ is linear w.r.t. $\boldsymbol{\theta}$

  (note: does not mean linear w.r.t. the input $\boldsymbol{x}$)
- Non-linear model: other models

Contents

Linear model

b functions

- Usual form: $$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{b} \theta_j \phi_j(\boldsymbol{x})$$ $\boldsymbol{x} \in \mathbb{R}^d$

  θ_j is j-th element of $\boldsymbol{\theta}$

- $\{\boldsymbol{\phi}_j(\boldsymbol{x})\}_{j=1}^{b}$: known basis functions that are linearly independent

- Examples of basis functions when $d = 1$:
  - Identity: $\phi(x) = x$ (model becomes linear in input)
  - Polynomial functions: $(1,\ x,\ x^2,\ \ \ldots,\ x^{b-1})$
  - Sinusoidal functions: $(1, \sin x, \cos x, \ldots, \sin kx, \cos kx)$

$b = 2k + 1$

Multi-dimensional linear model

- Additive model:

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

T : transpose

$d \geq 2$

Ref: $\boldsymbol{x}_i$ is i-th sample

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{k=1}^{d} \sum_{j=1}^{b'} \theta_{k,j} \phi_j(x^{(k)})$$

- Number of parameters: $b = b'd$
  - Increases linearly w.r.t. input dimension d.
  - Note: Multiplicative model (in the next slide) grows exponentially w.r.t. d.
- Since it only considers the sum of one-dimensional basis functions, it cannot represent complex functions with interactions.

Multi-dimensional linear model

- Multiplicative model for multi-dimensional inputs:

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j_1=1}^{b'} \cdots \sum_{j_d=1}^{b'} \theta_{j_1,\ldots,j_d} \phi_{j_1}(x^{(1)}) \cdots \phi_{j_d}(x^{(d)})$$

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

- # of Params: $b = (b')^d$
  - Exponentially grows w.r.t. input dim d
  - $b = 10^{100}$ when $b' = 10, \quad d = 100$
  - Not practical from a computational/statistical perspective
- Can only be used when d is small (We will discuss about sparsity in the sparse learning lecture!)

Contents

Kernel model

- Linear model (that we discussed so far):
  - Basis functions $\{\phi_j(\boldsymbol{x})\}_{j=1}^{b}$ do not depend on the training samples $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$
- Kernel model:
  - We use training input samples $\{\boldsymbol{x}_i\}_{i=1}^{n}$ to design the basis functions

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{n} \theta_j K(\boldsymbol{x}, \boldsymbol{x}_j)$$

  - Ex: Gaussian kernel

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

$\|\boldsymbol{a}\|^2 = \boldsymbol{a}^\top \boldsymbol{a}$

$h(>0)$: bandwidth

Kernel model

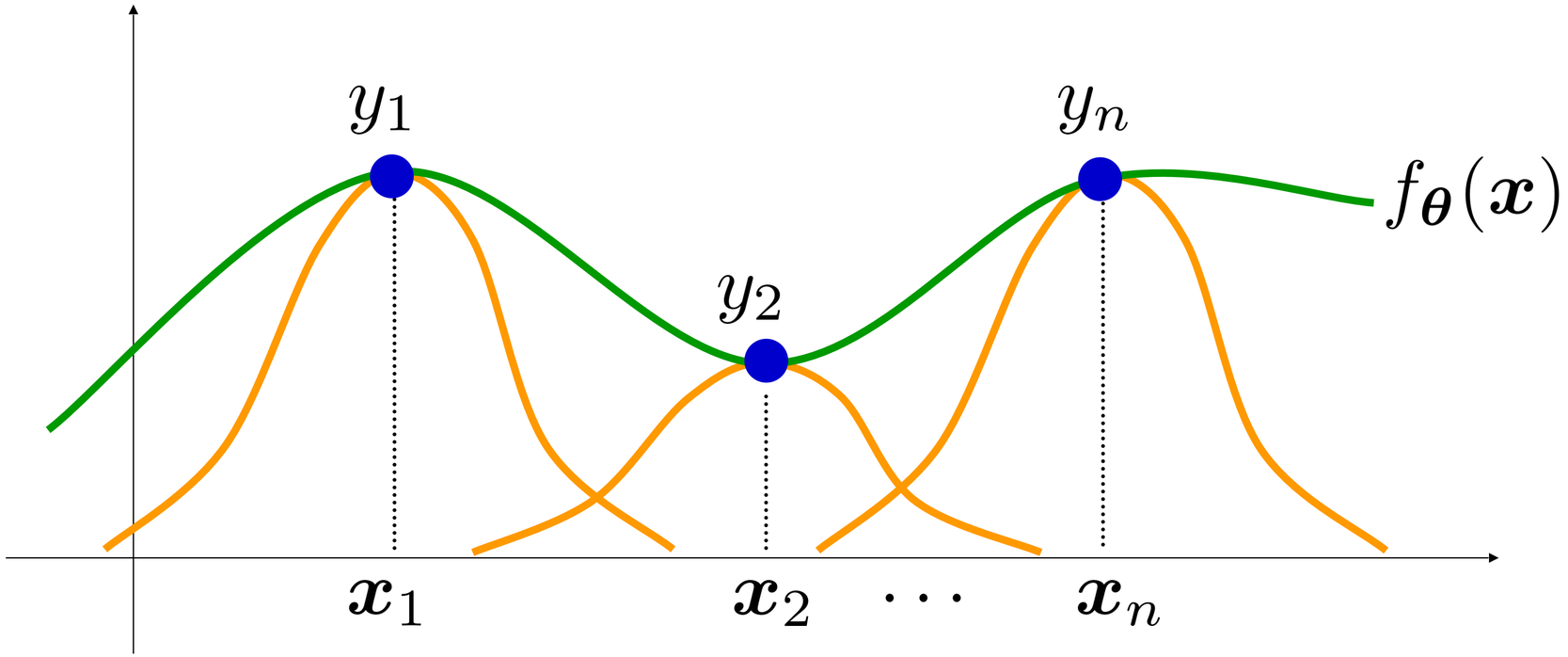
$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{n} \theta_j K(\boldsymbol{x}, \boldsymbol{x}_j)$$

- The # of params is n and does not depend on input dim d
- Linear in parameter:
  - kernel models is a type of linear model
- However, the # of params depend on the # of training samples, so have different statistical properties. Sometimes called nonparametric models due to this reason.
- In the scope of this course, you can treat kernel models as linear models.

Gaussian kernel model

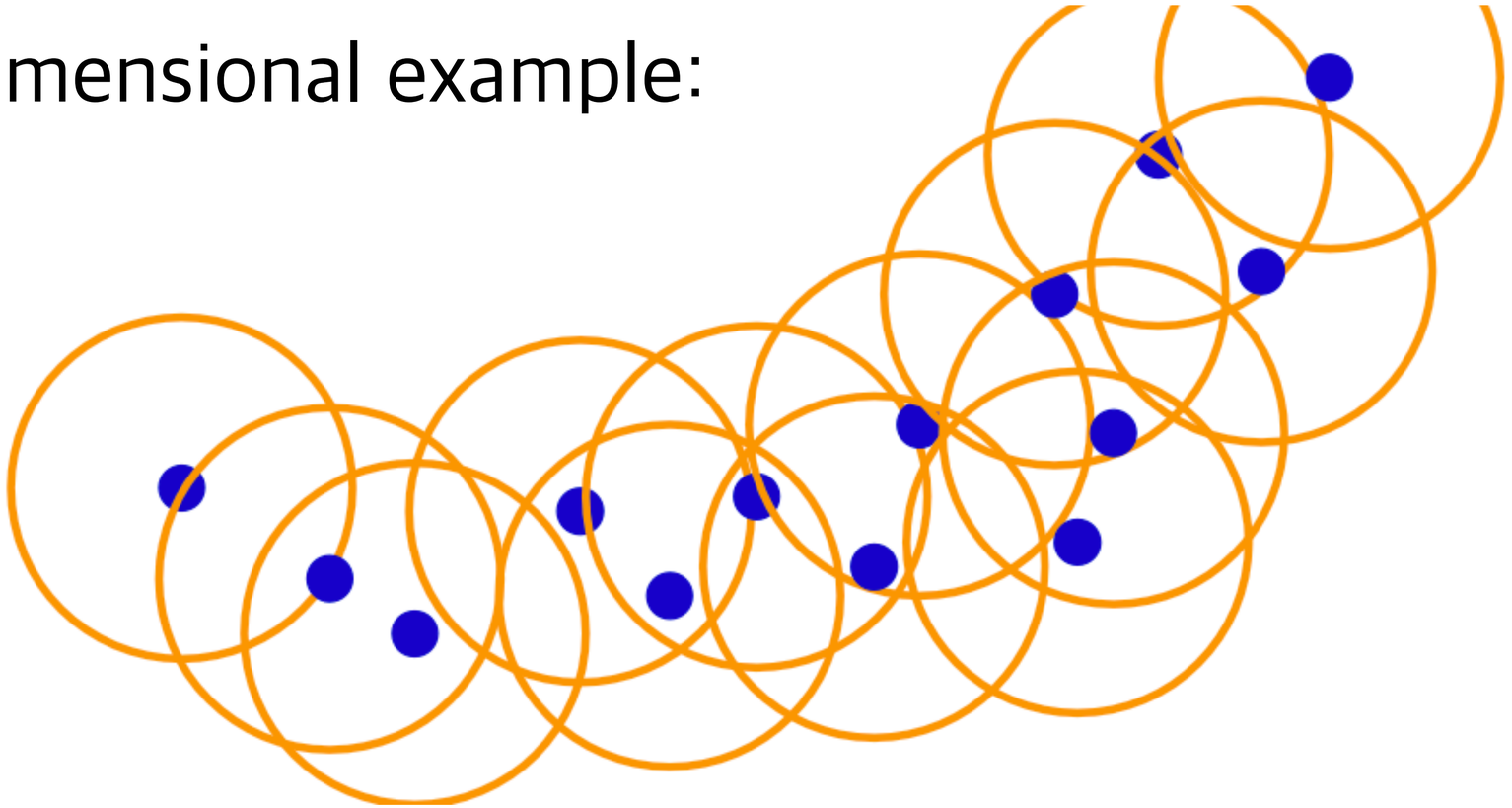
$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{n} \theta_j \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}_j\|^2}{2h^2}\right)$$

- Place Gaussian functions on each training input samples.



Gaussian kernel model

- When the n training samples are biased in their distribution across the input space, the Gaussian kernel model automatically ignores regions where there are no training input samples.
- A 2-dimensional example:



Contents

Non-linear model

- Models that are not linear w.r.t. the parameters
  - An example: a linear model with the basis functions including the parameter.

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{b} \alpha_j \phi(\boldsymbol{x}; \boldsymbol{\beta}_j)$$

$$\boldsymbol{\theta} = (\boldsymbol{\alpha}^\top, \boldsymbol{\beta}_1^\top, \ldots, \boldsymbol{\beta}_b^\top)^\top$$

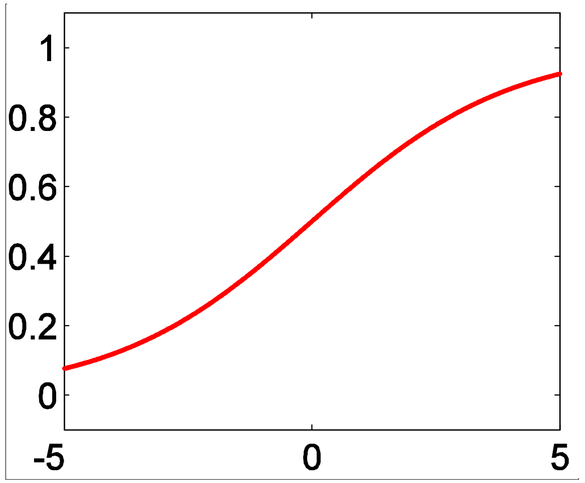
$\boldsymbol{\phi}(\boldsymbol{x}; \boldsymbol{\beta})$: non-linear w.r.t. $\boldsymbol{\beta}$

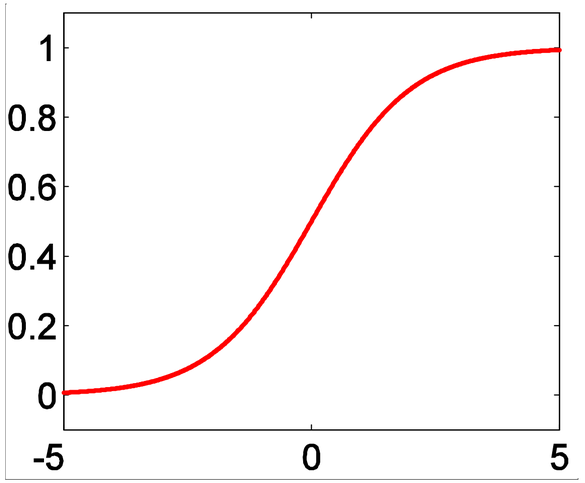
Ex 1: basis function that includes param

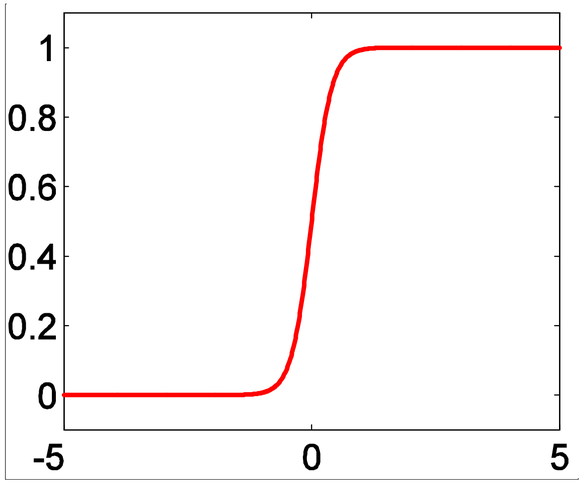
- Sigmoid function:

$$\phi(\boldsymbol{x};\boldsymbol{\beta}) = \frac{1}{1+\exp\left(-\boldsymbol{x}^\top \boldsymbol{w} - \gamma\right)} \qquad \boldsymbol{\beta} = (\boldsymbol{w}^\top, \gamma)^\top$$

For $d = 1$ and $\gamma = 0$:







w: small

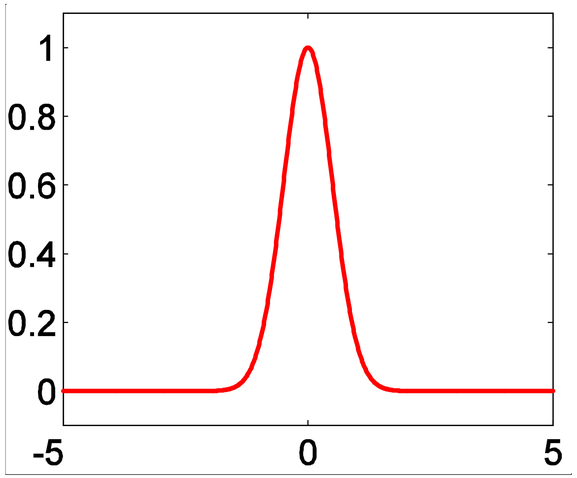
w: medium

w: large

Ex 2: basis function that includes param

- Gaussian kernel: In contrast to linear Gaussian kernel models, we can learn the center and bandwidth of the Gaussian function

$$\phi(\boldsymbol{x};\boldsymbol{\beta}) = \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{c}\|^2}{2h^2}\right) \qquad \boldsymbol{\beta} = (\boldsymbol{c}^\top, h)^\top$$



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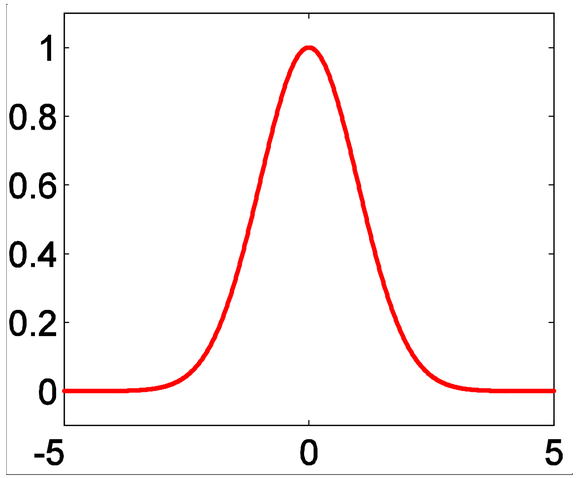

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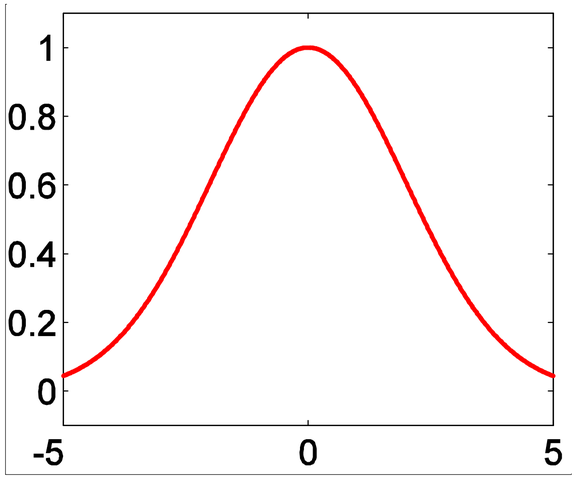


h: large

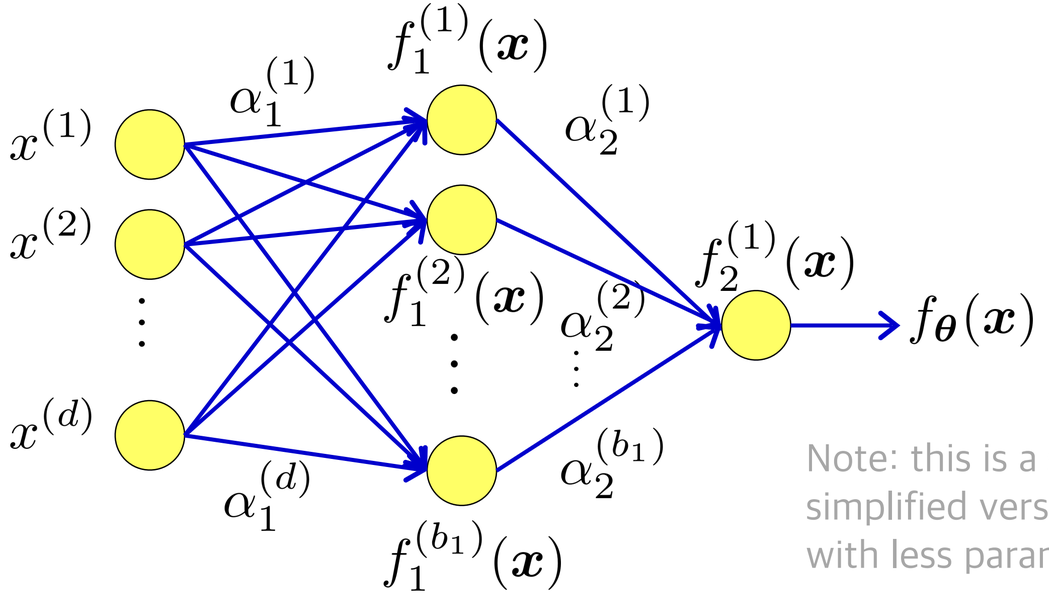
Non-linear model

- Model that is non-linear w.r.t. the parameters
  - Hierarchical model

$$f_k^{(i)}(\boldsymbol{x}) = \sum_{j=1}^{b_{k-1}} \alpha_k^{(j)} \phi(f_{k-1}^{(j)}(\boldsymbol{x})), \quad f_0^{(i)}(\boldsymbol{x}) = x^{(i)}$$

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = f_K^{(1)}(\boldsymbol{x})$$

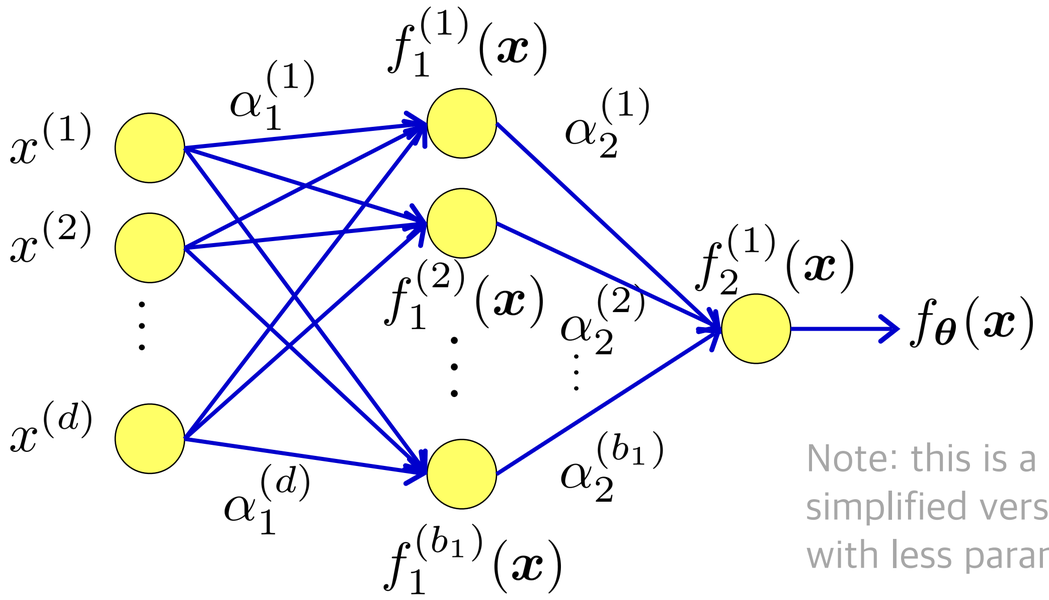
$$\boldsymbol{\theta} = (\boldsymbol{\alpha}_1^\top, \ldots, \boldsymbol{\alpha}_K^\top)^\top$$



Note: this is a slightly simplified version of an MLP with less parameters.

Some history on perceptrons

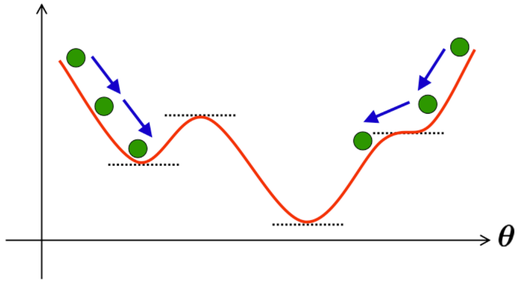
- The human brain consists of countless nerve cells connected in a network-like pattern.
- Sigmoid function behaves similarly to the nerve cells.
- Artificial neural networks are also called perceptrons.
- Mathematically, a 3-layer perceptron can approximate any function.



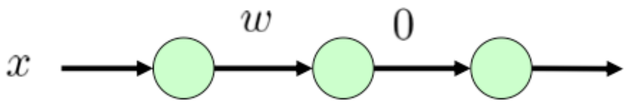
Note: this is a slightly simplified version of an MLP with less parameters.

Difficulty of training hierarchical models

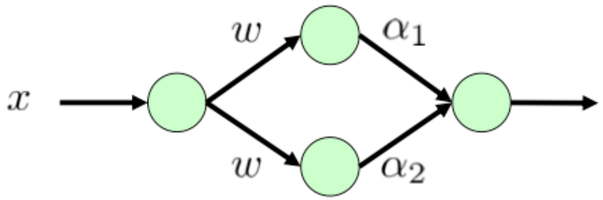
Historically, hierarchical models were **difficult to train**!



- Due to the existence of numerous local optima, finding the global optimum is difficult.
- Parameters and functions do not have a one-to-one correspondence.
  - When the weights of the second layer are zero, changing the weights of the first layer does not affect the function.



  - When the weights of the first layer are equal, if the sum of the weights of the second layer $\alpha_1 + \alpha_2$ is a constant, the function remains the same.



Modern deep learning largely mitigate these training difficulties, and we will discuss this in later lectures.

Summary of learning models

- Linear model: linear w.r.t. the parameters
  - Additive model: small number of params, low flexibility
  - Multiplicative model: High flexibility but too many params
  - kernel model: moderate flexibility and number of params
- Non-linear model: Non-linear w.r.t. to parameters
  - Hierarchical model: we will discuss this in the future
- We need to perform “model selection” since the decision will depend on the application.
- In this course: mainly use kernel models, occasionally hierarchical models such as neural network models.

Contents

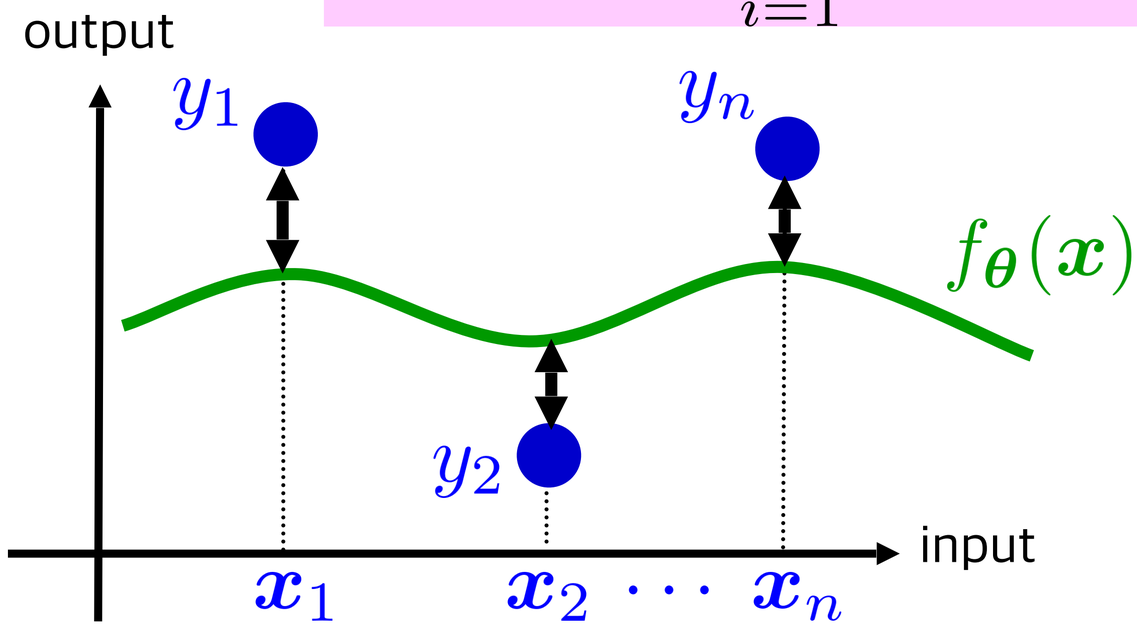
1. Learning model (Chap.2)
2. Least squares regression (Chap.3)
3. Regularized regression (Chap. 4)

Least squares regression

- Objective: minimize the squared error between the training outputs

$$\widehat{\boldsymbol{\theta}}_{\mathrm{LS}} = \operatorname*{argmin}_{\boldsymbol{\theta}} J_{\mathrm{LS}}(\boldsymbol{\theta})$$

$$J_{\mathrm{LS}}(\boldsymbol{\theta}) = \frac{1}{2}\sum_{i=1}^{n}\Big(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i\Big)^2$$



Deriving the solution

- Rewrite the objective for model $f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{b} \theta_j \phi_j(\boldsymbol{x})$

$$J_{\mathrm{LS}}(\boldsymbol{\theta}) = \frac{1}{2} \sum_{i=1}^{n} \left(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i \right)^2$$

$$= \frac{1}{2} \|\boldsymbol{\Phi}\boldsymbol{\theta} - \boldsymbol{y}\|^2 = \frac{1}{2} (\boldsymbol{\Phi}\boldsymbol{\theta} - \boldsymbol{y})^\top (\boldsymbol{\Phi}\boldsymbol{\theta} - \boldsymbol{y})$$

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

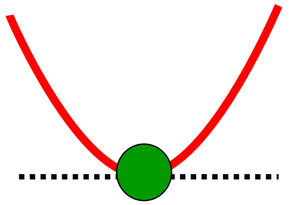
$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_1(\boldsymbol{x}_1) & \cdots & \phi_b(\boldsymbol{x}_1) \\ \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{x}_n) & \cdots & \phi_b(\boldsymbol{x}_n) \end{pmatrix} : \text{Design matrix}$$

Deriving the solution (2)

- Partial derivative is zero:

$$\nabla_{\boldsymbol{\theta}} J_{\mathrm{LS}} = \left(\frac{\partial J_{\mathrm{LS}}}{\partial \theta_1}, \ldots, \frac{\partial J_{\mathrm{LS}}}{\partial \theta_b} \right)^\top = \boldsymbol{\Phi}^\top \boldsymbol{\Phi} \boldsymbol{\theta} - \boldsymbol{\Phi}^\top \boldsymbol{y} = \boldsymbol{0}$$

$$\frac{\partial}{\partial \boldsymbol{\theta}} \boldsymbol{\theta}^\top \boldsymbol{A} \boldsymbol{\theta} = 2 \boldsymbol{A} \boldsymbol{\theta} \qquad \frac{\partial}{\partial \boldsymbol{\theta}} \boldsymbol{b}^\top \boldsymbol{\theta} = \boldsymbol{b}$$



- Equation satisfied by the solution:

$$\boldsymbol{\Phi}^\top \boldsymbol{\Phi} \boldsymbol{\theta} = \boldsymbol{\Phi}^\top \boldsymbol{y} \quad \Rightarrow \quad \widehat{\boldsymbol{\theta}}_{\mathrm{LS}} = (\boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^\top \boldsymbol{y}$$

Note: assume $\left(\boldsymbol{\Phi}^\top \boldsymbol{\Phi}\right)^{-1}$ exists

- We analytically obtained the solution!

Why is $\boldsymbol{\Phi}^\top\boldsymbol{\Phi}$ non-singular?

- Recall that $\{\phi_j(\boldsymbol{x})\}_{j=1}^b$ are known basis functions that are linearly independent. So the rank of $\boldsymbol{\Phi}$ is b.
- We first derive that $\boldsymbol{\Phi}^\top\boldsymbol{\Phi}$ is positive definite:
  - If $\boldsymbol{a} \equiv \boldsymbol{\Phi}\boldsymbol{c}$, then $\boldsymbol{c}^\top\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\boldsymbol{c} = \boldsymbol{a}^\top\boldsymbol{a} = \sum_{i=1}^n a_i^2 \geq 0$.
  - Since $\boldsymbol{\Phi}$ is full column rank, $\boldsymbol{a} \neq \boldsymbol{0}$ for any $\boldsymbol{c} \neq \boldsymbol{0}$.
  - Therefore we have $\boldsymbol{c}^\top\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\boldsymbol{c} > 0$.
- Since $\boldsymbol{\Phi}^\top\boldsymbol{\Phi}$ is positive definite, it is non-singular.
  - Proof by contradiction: If $\boldsymbol{\Phi}^\top\boldsymbol{\Phi}$ is singular, it means there exists a $\boldsymbol{c} \neq \boldsymbol{0}$ such that $\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\boldsymbol{c} = 0$. Then $\boldsymbol{c}^\top\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\boldsymbol{c} = \boldsymbol{c}^\top\boldsymbol{0} = 0$.

Second-order condition

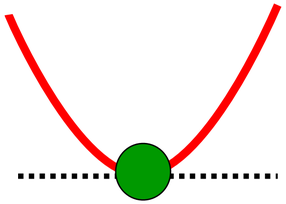
- To make sure the solution achieves a minimum instead of the maximum, we can check the second-order condition.
- We already derived:

$$\nabla_{\boldsymbol{\theta}} J_{\mathrm{LS}} = \boldsymbol{\Phi}^{\top}\boldsymbol{\Phi}\boldsymbol{\theta} - \boldsymbol{\Phi}^{\top}\boldsymbol{y}$$

- We can further derive the Hessian:

$$\nabla^2_{\boldsymbol{\theta}} J_{\mathrm{LS}} = \boldsymbol{\Phi}^{\top}\boldsymbol{\Phi}$$

- From the previous slide, we know the Hessian is positive definite.

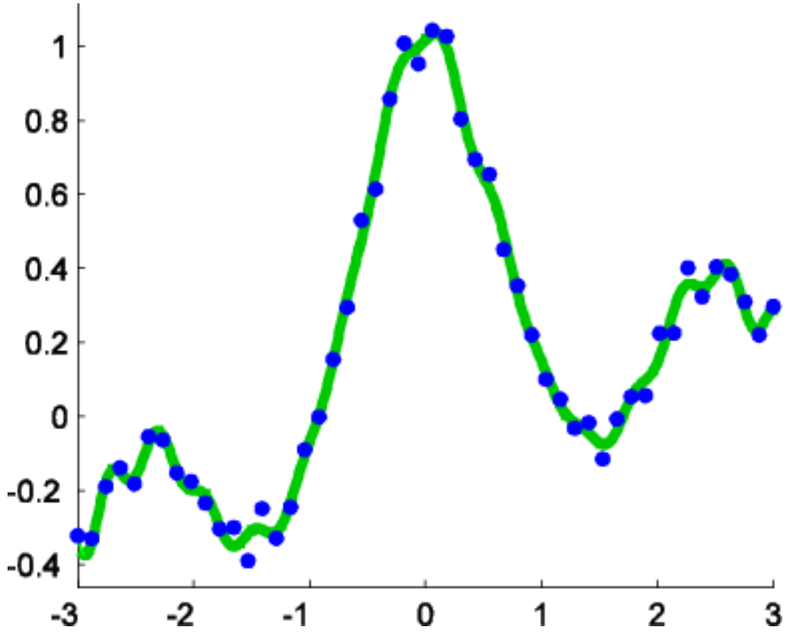


Example

- An example of least squares regression with a sinusoidal model $f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{b} \theta_j \phi_j(\boldsymbol{x})$

$$\phi_i(\boldsymbol{x}) = 1, \sin(x/2), \cos(x/2), \ldots, \sin(15x/2), \cos(15x/2)$$

true function: $f(x) = \sin(\pi x)/(\pi x) + 0.1x$



Example with Python


```
import numpy as np; import matplotlib; matplotlib.use('TkAgg'); import
matplotlib.pyplot as plt; np.random.seed(0)  # set seed for reproducibility

def generate_sample(xmin, xmax, sample_size):
    x = np.linspace(start=xmin, stop=xmax, num=sample_size)
    pix = np.pi * x
    target = np.sin(pix) / pix + 0.1 * x
    noise = 0.05 * np.random.normal(loc=0., scale=1., size=sample_size)
    return x, target + noise

def calc_design_matrix(x):
    sample_size = len(x)
    phi = np.empty(shape=(sample_size, 31))  # design matrix
    phi[:, 0] = 1.
    phi[:, 1::2] = np.sin(x[:, None] * np.arange(1, 16)[None] / 2)
    phi[:, 2::2] = np.cos(x[:, None] * np.arange(1, 16)[None] / 2)
    return phi

# create sample
sample_size = 50; xmin, xmax = -3, 3
x, y = generate_sample(xmin=xmin, xmax=xmax, sample_size=sample_size)

phi = calc_design_matrix(x) # calculate design matrix

theta = np.linalg.solve(phi.T.dot(phi), phi.T.dot(y[:, None])) # solve LS

# create data to visualize the prediction
X = np.linspace(start=xmin, stop=xmax, num=5000)
Phi = calc_design_matrix(X)
prediction = Phi.dot(theta)

# visualization
plt.clf(); plt.scatter(x, y, c='green', marker='o')
plt.plot(X, prediction); plt.show()
```

Exercise

- Prove that when the noise in the training output follows a normal distribution independently, the least squares regression is consistent with the maximum likelihood estimation of the Gaussian model.

$$\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \quad y_i = f(\boldsymbol{x}_i) + \epsilon_i \quad \epsilon_i \overset{\text{i.i.d.}}{\sim} N(0, \sigma^2)$$

- Probabilistic model: $p_{\boldsymbol{\theta}}(y|\boldsymbol{x}) = \dfrac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\dfrac{(y - f_{\boldsymbol{\theta}}(\boldsymbol{x}))^2}{2\sigma^2}\right)$
- Log-likelihood: $L(\boldsymbol{\theta}) = \sum_{i=1}^n \log p_{\boldsymbol{\theta}}(y_i|\boldsymbol{x}_i)$
- Likelihood estimation: $\max_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$

$$J_{\mathrm{LS}}(\boldsymbol{\theta}) = \frac{1}{2}\sum_{i=1}^n \left(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i\right)^2$$

Justification of least squares regression

- When the noise in the output follows a normal distribution independently:
  - Consistency: the least squares solution converges in probability to the optimal solution.
    - If there are an infinite number of samples, the optimal parameters can be obtained.
  - Asymptotic efficiency: has the smallest asymptotic variance among asymptotically normal estimators.
    - When there are a sufficiently large number of samples, the estimation results are stable.

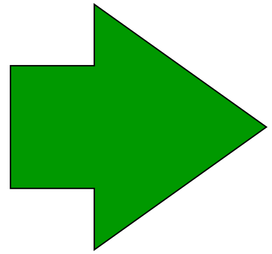
Least squares regression w/ kernel models

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{n} \theta_j K(\boldsymbol{x}, \boldsymbol{x}_j)$$

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

- Least squares objective:

$$J_{\mathrm{LS}}(\boldsymbol{\theta}) = \frac{1}{2}\|\boldsymbol{K}\boldsymbol{\theta} - \boldsymbol{y}\|^2$$



$$\widehat{\boldsymbol{\theta}}_{\mathrm{LS}} = \boldsymbol{K}^{-1}\boldsymbol{y}$$

Kernel matrix:

$$\boldsymbol{K} = \begin{pmatrix} K(\boldsymbol{x}_1, \boldsymbol{x}_1) & \cdots & K(\boldsymbol{x}_1, \boldsymbol{x}_n) \\ \vdots & \ddots & \vdots \\ K(\boldsymbol{x}_n, \boldsymbol{x}_1) & \cdots & K(\boldsymbol{x}_n, \boldsymbol{x}_n) \end{pmatrix}$$

Details of derivation

- Objective and solution:

$$J_{\mathrm{LS}}(\boldsymbol{\theta}) = \frac{1}{2}\|\boldsymbol{K}\boldsymbol{\theta} - \boldsymbol{y}\|^2 \quad \Longrightarrow \quad \widehat{\boldsymbol{\theta}}_{\mathrm{LS}} = \boldsymbol{K}^{-1}\boldsymbol{y}$$

- Since partial derivative is zero, we can derive:

$$\widehat{\boldsymbol{\theta}}_{\mathrm{LS}} = (\boldsymbol{K}^\top \boldsymbol{K})^{-1}\boldsymbol{K}^\top \boldsymbol{y}$$

- A property of Kernel matrix: $\boldsymbol{K}^\top = \boldsymbol{K}$
- Hence,

$$\widehat{\boldsymbol{\theta}}_{\mathrm{LS}} = (\boldsymbol{K}^2)^{-1}\boldsymbol{K}\boldsymbol{y} = \boldsymbol{K}^{-1}\boldsymbol{y}$$

$$\boldsymbol{K} = \begin{pmatrix} K(\boldsymbol{x}_1, \boldsymbol{x}_1) & \cdots & K(\boldsymbol{x}_1, \boldsymbol{x}_n) \\ \vdots & \ddots & \vdots \\ K(\boldsymbol{x}_n, \boldsymbol{x}_1) & \cdots & K(\boldsymbol{x}_n, \boldsymbol{x}_n) \end{pmatrix} \qquad K(\boldsymbol{x}, \boldsymbol{c}) = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{c}\|^2}{2h^2}\right)$$

Summary of least squares regression

- **Main objective**: minimize the squared error between the training output and the predictions.
- **Regression**: basic technique for modeling the relationship between input and output variables.
- **When noise in the output is Gaussian**: the method can be interpreted as maximum likelihood estimation.
- **Analytical solutions**: for linear models and kernel models, we can find the optimal parameters analytically.

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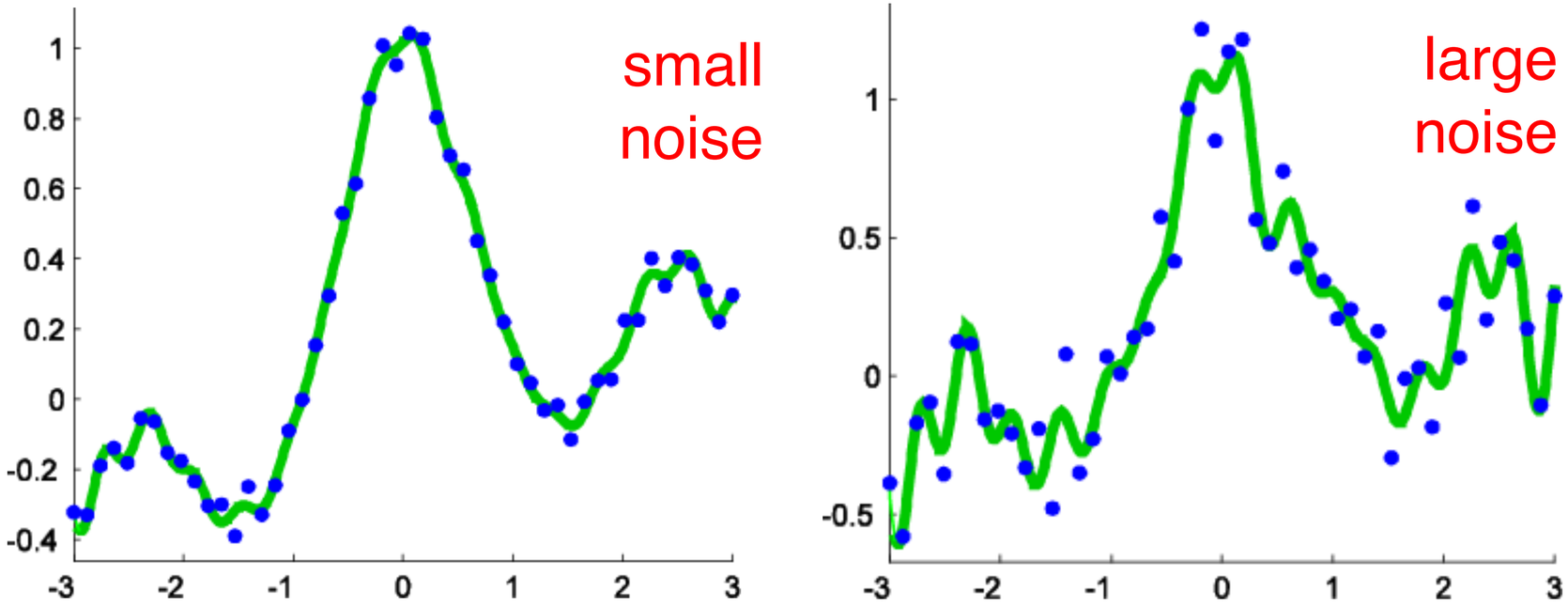
1. Learning model (Chap.2)
2. Least squares regression (Chap.3)
3. Regularized regression (Chap. 4)
   A) Constrained least squares regression
   B) Model selection

Issue of least squares regression

- Overfitting: occurs when a model adapts too much to the noise in the training samples.



$$\phi_i(\boldsymbol{x}) = 1, \sin x/2, \cos x/2, \ldots, \sin 15x/2, \cos 15x/2$$

➡ properly constrain the model to prevent this

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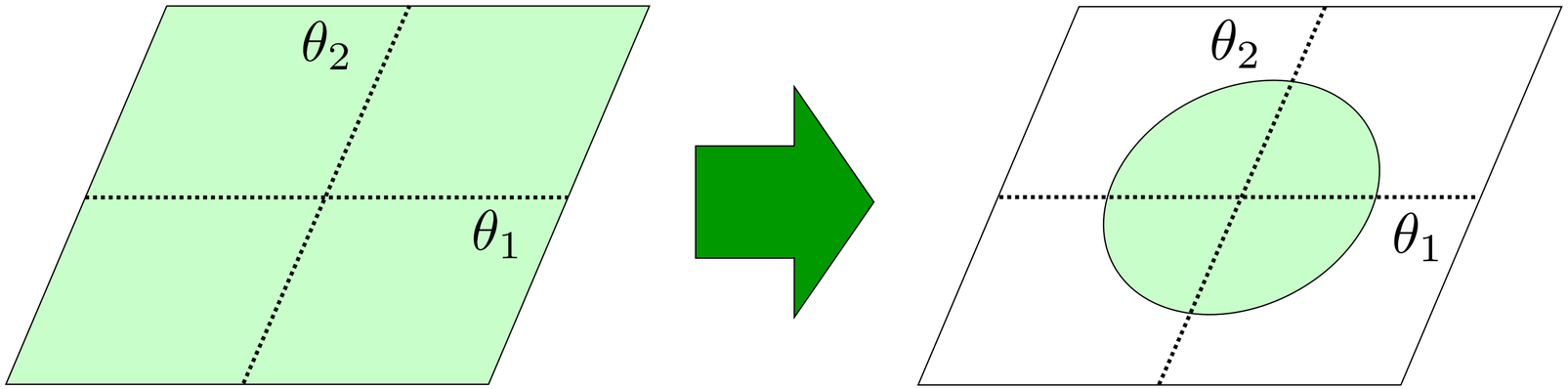
ℓ_2 –restricted least squares regression

- Avoid overfitting by restricting the model to be within a hyper-cube.
  (Because we want the absolute values of each elements of $\boldsymbol{\theta}$ to be small!)

$$\min_{\boldsymbol{\theta}} \frac{1}{2} \sum_{i=1}^{n} \Big(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i \Big)^2 \quad \text{subject to } \|\boldsymbol{\theta}\|^2 \leq R$$

$R \geq 0$ $\quad f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{b} \theta_j \phi_j(\boldsymbol{x})$



Ordinary least squares regression

ℓ_2 -restricted least squares regression

Deriving the solution

$$\min_{\boldsymbol{\theta}} \frac{1}{2} \sum_{i=1}^{n} \Big(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i \Big)^2 \quad \text{subject to } \|\boldsymbol{\theta}\|^2 \leq R$$

- Equivalent expression:

$$\min_{\boldsymbol{\theta}} \left[\frac{1}{2} \sum_{i=1}^{n} \Big(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i \Big)^2 + \frac{\lambda}{2} \|\boldsymbol{\theta}\|^2 \right]$$

  - $\lambda (> 0)$: constant that is specified by R
- We can use λ instead of R in practice.

Interpretation

$$\min_{\boldsymbol{\theta}} \left[\frac{1}{2} \sum_{i=1}^{n} \left(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i \right)^2 + \frac{\lambda}{2} \|\boldsymbol{\theta}\|^2 \right]$$

goodness of fit for training output

penalty term for preventing param values from becoming too large (regularization)

- The model strikes a good balance between fitting the training output well and keeping the parameter values small.
- Also called ℓ_2-regularized regression

Exercise

$$\widehat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \left[\frac{1}{2} \sum_{i=1}^{n} \left(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i \right)^2 + \frac{\lambda}{2} \|\boldsymbol{\theta}\|^2 \right]$$

- Find the solution for linear model $f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{b} \theta_j \phi_j(\boldsymbol{x})$
- Info: $\frac{1}{2} \sum_{i=1}^{n} \left(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - y_i \right)^2 = \frac{1}{2} \|\boldsymbol{\Phi}\boldsymbol{\theta} - \boldsymbol{y}\|^2$

$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_1(\boldsymbol{x}_1) & \cdots & \phi_b(\boldsymbol{x}_1) \\ \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{x}_n) & \cdots & \phi_b(\boldsymbol{x}_n) \end{pmatrix} \qquad \boldsymbol{y} = (y_1, \ldots, y_n)^\top$$

Example

- (Gaussian) kernel model

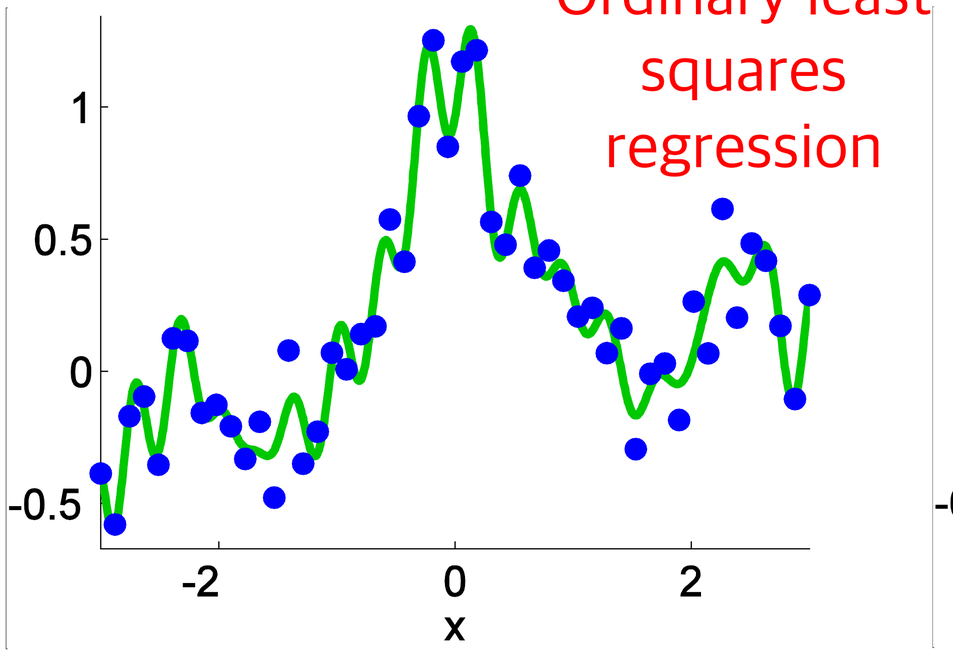
$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{n} \theta_j K(\boldsymbol{x}, \boldsymbol{x}_j)$$

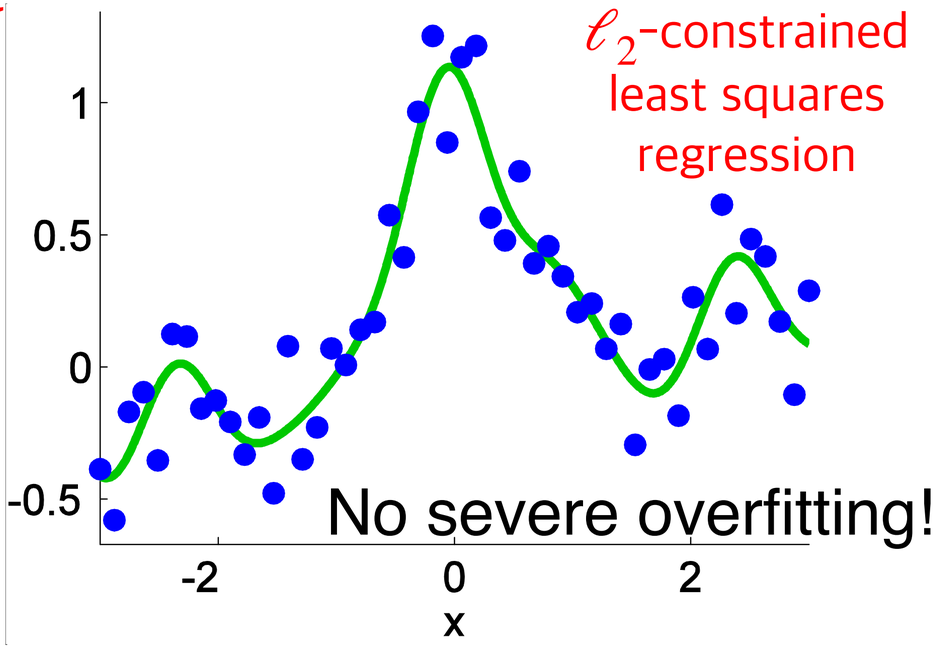
$$K(\boldsymbol{x}, \boldsymbol{c}) = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{c}\|^2}{2h^2}\right)$$

$$\widehat{\boldsymbol{\theta}} = (\boldsymbol{K}^2 + \lambda \boldsymbol{I})^{-1} \boldsymbol{K}^\top \boldsymbol{y}$$

$$\boldsymbol{K} = \begin{pmatrix} K(\boldsymbol{x}_1, \boldsymbol{x}_1) & \cdots & K(\boldsymbol{x}_1, \boldsymbol{x}_n) \\ \vdots & \ddots & \vdots \\ K(\boldsymbol{x}_n, \boldsymbol{x}_1) & \cdots & K(\boldsymbol{x}_n, \boldsymbol{x}_n) \end{pmatrix}$$

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





Example with Python

```
import numpy as np; import matplotlib; matplotlib.use('TkAgg')
import matplotlib.pyplot as plt; np.random.seed(0)  # set seed for reproducibility

def generate_sample(xmin, xmax, sample_size):
    x = np.linspace(start=xmin, stop=xmax, num=sample_size)
    pix = np.pi * x
    target = np.sin(pix) / pix + 0.1 * x
    noise = 0.05 * np.random.normal(loc=0., scale=1., size=sample_size)
    return x, target + noise

def calc_design_matrix(x, c, h):
    return np.exp(-(x[None] - c[:, None]) ** 2 / (2 * h ** 2))

# create sample
sample_size = 50
xmin, xmax = -3, 3
x, y = generate_sample(xmin=xmin, xmax=xmax, sample_size=sample_size)
# calculate design matrix
h = 0.1
k = calc_design_matrix(x, x, h)
# solve the least square problem
l = 0.3
theta = np.linalg.solve(
    k.T.dot(k) + l * np.identity(len(k)),
    k.T.dot(y[:, None]))
# create data to visualize the prediction
X = np.linspace(start=xmin, stop=xmax, num=5000)
K = calc_design_matrix(x, X, h)
prediction = K.dot(theta)
# visualization
plt.clf(); plt.scatter(x, y, c='green', marker='o')
plt.plot(X, prediction); plt.show()
```

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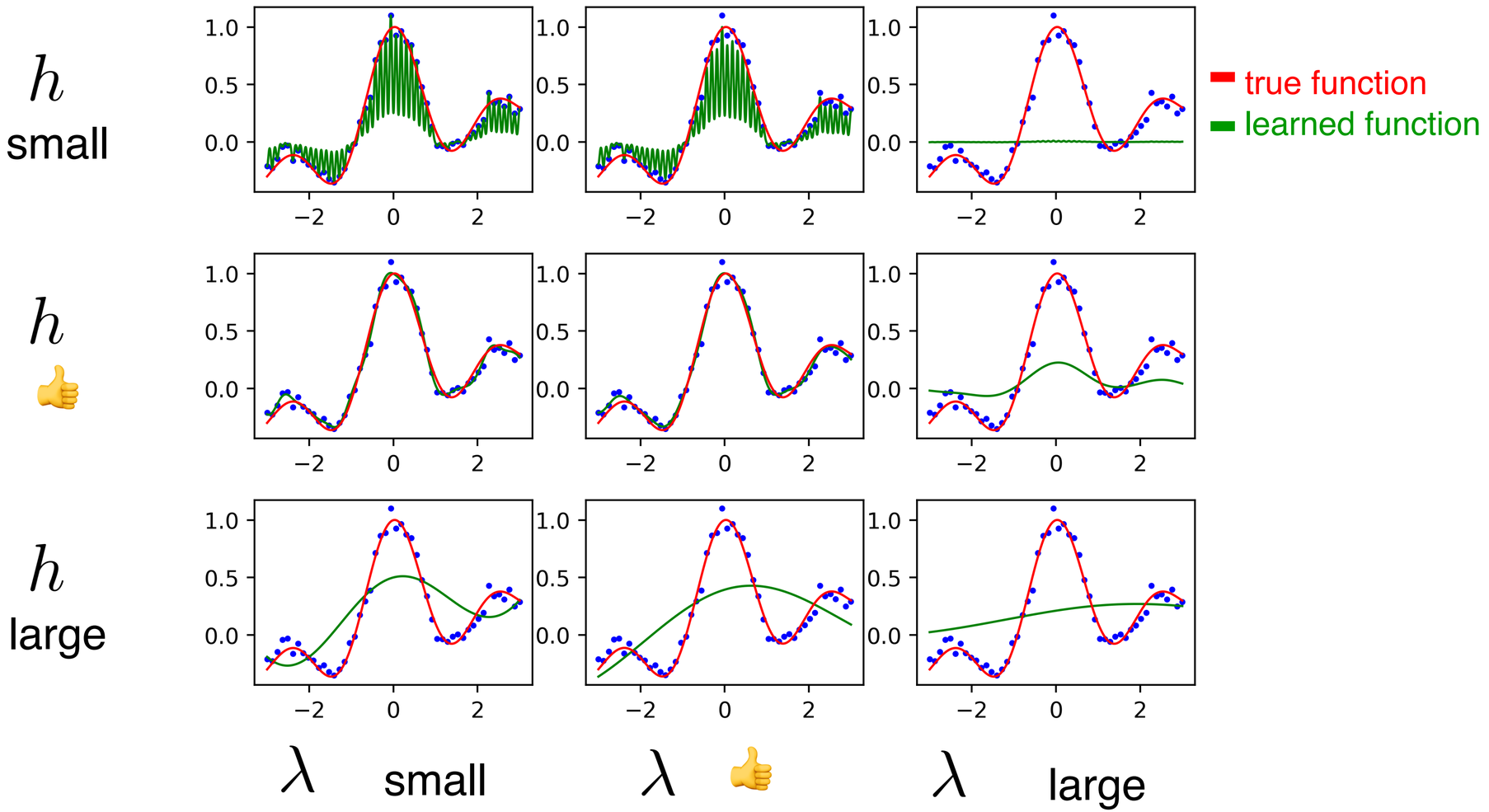
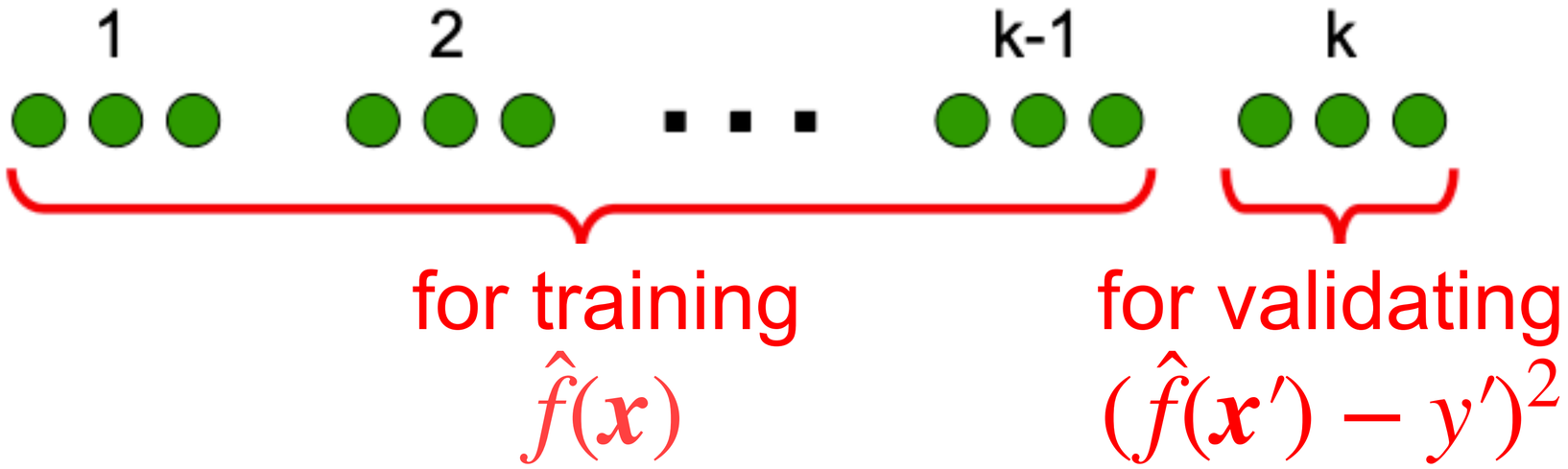
Model selection w/ regularized regression

- The results of regularized regression depends on how you choose the regularization param λ and Gaussian bandwidth h.



Cross validation

- Split **training** samples $Z = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ into k groups: $\{Z_i\}_{i=1}^k$
- Use samples from groups excluding Z_i and learn θ (fix λ, h).
- Use the remaining Z_i to check the test error.
- Repeat this for all $i \in [k]$, and return the mean of the test errors.



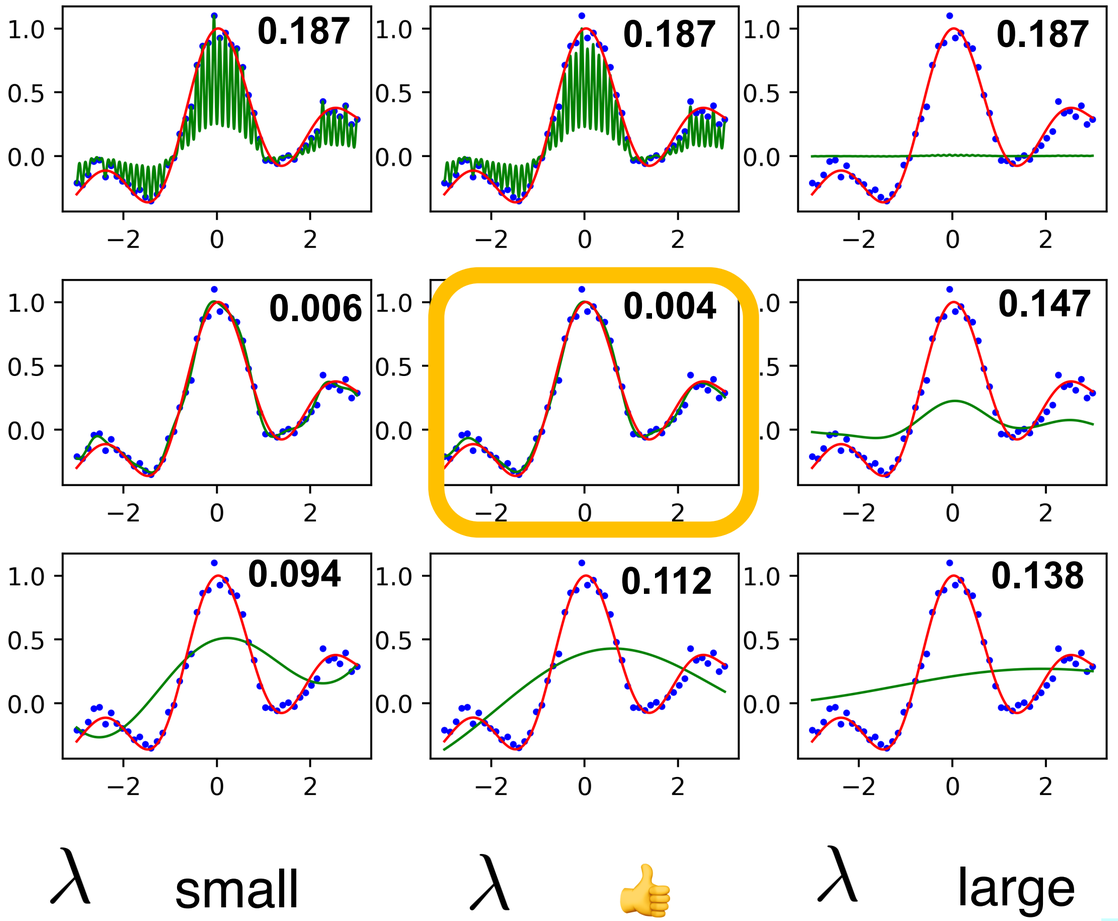
Example of CV

- Gaussian kernel model: $f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{n} \theta_j \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}_j\|^2}{2h^2}\right)$

h small

h 👍

h large



Homework for this week is implementing this.

Leave-one-out CV

- # of groups k = # of samples n

$$\frac{1}{n}\sum_{i=1}^{n}\left(\widehat{f}_i(\boldsymbol{x}_i)-y_i\right)^2$$

$\hat{f}_i(\boldsymbol{x})$: learned from data other than $(\boldsymbol{x}_i, y_i)$

  - Leave one sample out each time
- In general, regularized regression can be computationally expensive and may not be practical.
- However, for linear models, there are some regularized regression techniques that can be computed analytically.

Proving this is homework.

$$\frac{1}{n}\|\widetilde{\boldsymbol{H}}^{-1}\boldsymbol{H}\boldsymbol{y}\|^2$$

$$\boldsymbol{H}=\boldsymbol{I}-\boldsymbol{\Phi}(\boldsymbol{\Phi}^\top\boldsymbol{\Phi}+\lambda\boldsymbol{I})^{-1}\boldsymbol{\Phi}^\top$$

$\tilde{\boldsymbol{H}}$: diagonals are same as $\boldsymbol{H}$, non-diagonals are zero

Summary of regularized regression

- Least squares regression can easily overfit to noise.
- Constrain the search range of parameters using the ℓ_2-norm.
- Solution can be analytically derived.
- Model selection is important.

Contents

1. Learning model (Chap.2)
2. Least squares regression (Chap.3)
3. Regularized regression (Chap. 4)

Summary

- Models for learning a function:
  - Linear models, kernel models, non-linear models
- Least squares regression:
  - Minimizes the squared error between training samples
  - The solution can be computed analytically
- Regularized regression:
  - Reduces overfitting in least squares regression
  - The solution can be computed analytically
  - Model selection is performed using cross-validation

Schedule

1. 04/8 Introduction
2. 04/15 Regression 1
3. 04/22 Regression 2
- 04/30 Cancelled
4. 05/13 Classification 1
5. 05/20 Classification 2
6. 05/27 Deep learning 1
- 06/03 No lecture
7. 06/10 Deep learning 2
8. 06/17 Deep learning 3
9. 06/24 Semi-supervised learning
10. 07/01 Language models
11. 07/08 Representation learning 1
12. 07/15 Representation learning 2
13. 07/22 Advanced topics

Homework 1

- Implement cross-validation for ℓ_2-regularized least squares regression with a Gaussian kernel model and determine the regularization parameter and Gaussian width.

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{n} \theta_j K(\boldsymbol{x}, \boldsymbol{x}_j)$$

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

Homework 2

- Show that the mean squared error for leave-one-out cross-validation of ℓ_2-regularized regression using a linear model $f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=1}^{b} \theta_j \phi_j(\boldsymbol{x})$ can be analytically calculated as follows:

$$\frac{1}{n} \| \widetilde{\boldsymbol{H}}^{-1} \boldsymbol{H} \boldsymbol{y} \|^2$$

$$\boldsymbol{H} = \boldsymbol{I} - \boldsymbol{\Phi} (\boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \lambda \boldsymbol{I})^{-1} \boldsymbol{\Phi}^\top$$

$\tilde{\boldsymbol{H}}$: diagonals are same as $\boldsymbol{H}$, non-diagonals are zero

Homework 2 (Continued)

- Helpful information:
  - Express $\hat{\boldsymbol{\theta}}_i$ which is learned by removing $(\boldsymbol{x}_i, y_i)$ with:

$$\boldsymbol{\phi}_i = (\phi_1(\boldsymbol{x}_i), \phi_2(\boldsymbol{x}_i), \ldots, \phi_b(\boldsymbol{x}_i))^\top$$

$$\boldsymbol{\Phi} = (\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_n)^\top,$$

$$\boldsymbol{y},\ y_i,\ \boldsymbol{U} = \boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \lambda \boldsymbol{I}$$

  - A special case of Sherman-Morrison-Woodbury:

$$(\boldsymbol{U} - \boldsymbol{u}\boldsymbol{u}^\top)^{-1} = \boldsymbol{U}^{-1} + \frac{\boldsymbol{U}^{-1}\boldsymbol{u}\boldsymbol{u}^\top\boldsymbol{U}^{-1}}{1 - \boldsymbol{u}^\top\boldsymbol{U}^{-1}\boldsymbol{u}}$$

Homework 2 (Continued)

- Helpful information:
  - Express prediction for $y_{i'}$ $\boldsymbol{\phi}_i^\top \hat{\boldsymbol{\theta}}_i$ (where the parameter was learned by removing $(\boldsymbol{x}_i, y_i)$) with the following.

$$\boldsymbol{\phi}_i = (\phi_1(\boldsymbol{x}_i), \phi_2(\boldsymbol{x}_i), \ldots, \phi_b(\boldsymbol{x}_i))^\top$$

$$\boldsymbol{\Phi} = (\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \ldots, \boldsymbol{\phi}_n)^\top,$$

$$\boldsymbol{y},\ y_i,\ \boldsymbol{U} = \boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \lambda \boldsymbol{I}$$

  - Expanding on the denominator that appears in the inverse matrix formula and repeating the process of common denominator