Pattern Information Processing: Neural Networks

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Linear/Non-Linear Models

- Linear model: $\hat{f}(\boldsymbol{x})$ is linear with respect to $\boldsymbol{\alpha}$

  (Note: not necessarily linear with respect to $\boldsymbol{x}$)

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

- Non-linear model: Otherwise

Today's Plan

- Neural networks
- Least-squares in neural networks: Error back-propagation algorithm

Non-Linear Models

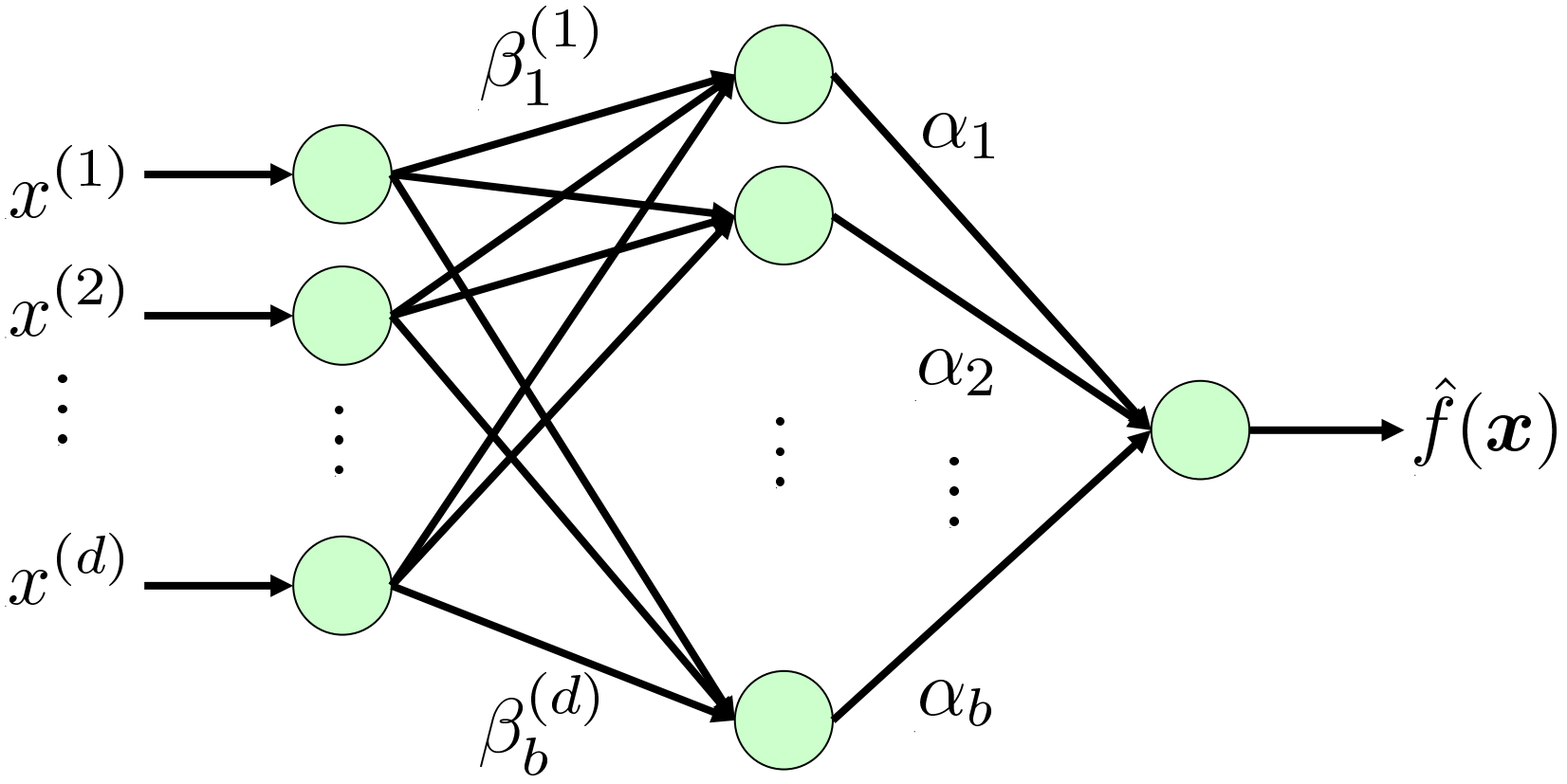
- A popular choice: Hierarchical models

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{b} \alpha_i \varphi(\boldsymbol{x}; \boldsymbol{\beta}_i)$$

- Basis function is parameterized by $\boldsymbol{\beta}_i$

Three-Layer Networks

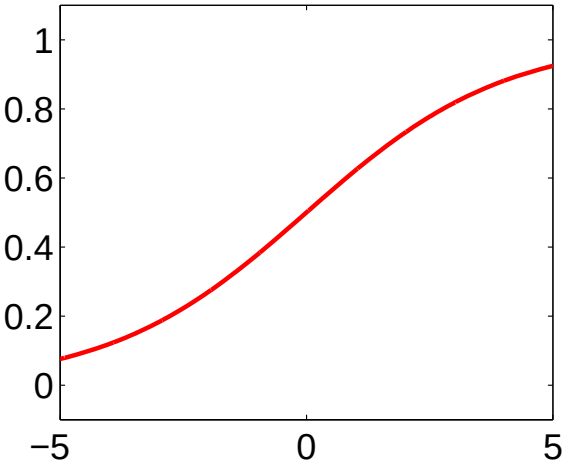
- Such a hierarchical model can be represented as a 3-layer network.



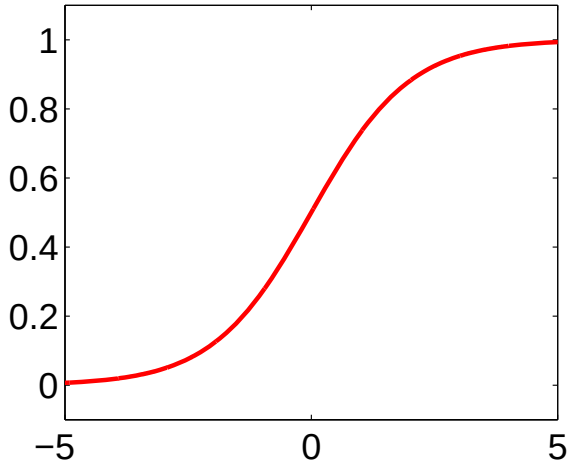
Sigmoidal Function

- A typical basis function: Sigmoidal function

$$\varphi(\boldsymbol{x};\boldsymbol{\beta},h) = \frac{1}{1+\exp\left(-\langle \boldsymbol{x},\boldsymbol{\beta}\rangle - h\right)}$$



β :Small



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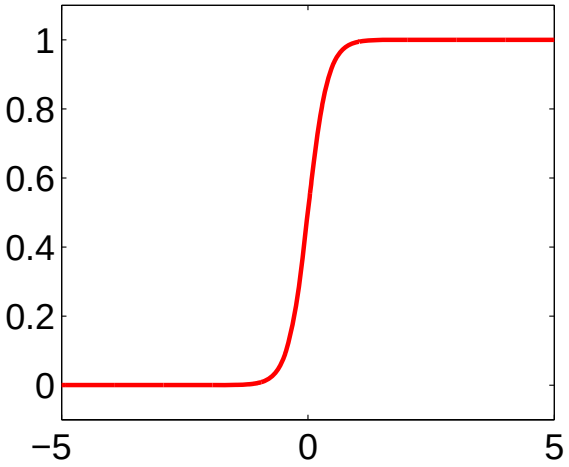


β :Large

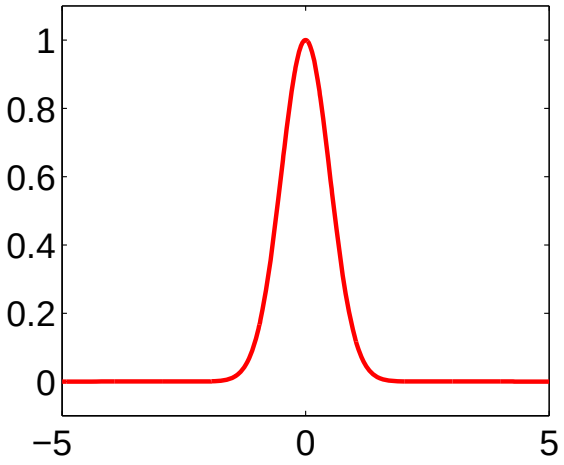
Perceptrons

- The behavior of the sigmoidal functions is similar to the neurons in the brain.
- For this reason, hierarchical models with sigmoidal functions are called artificial neural networks or perceptrons.
- Mathematically, 3-layer neural networks can approximate any continuous functions with arbitrary small error ("universal approximator").

Gaussian Radial Basis Function

- Another popular basis function:
  Gaussian radial basis function

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



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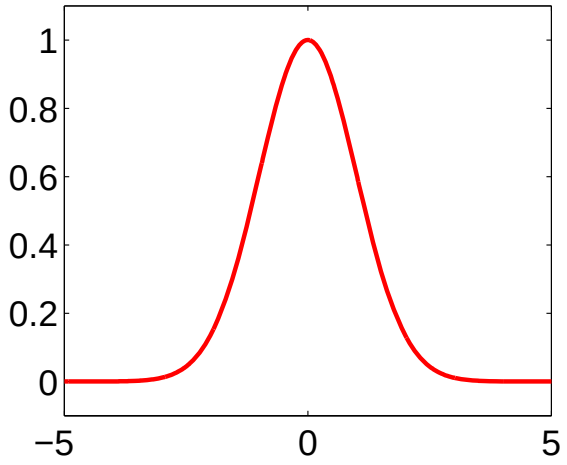

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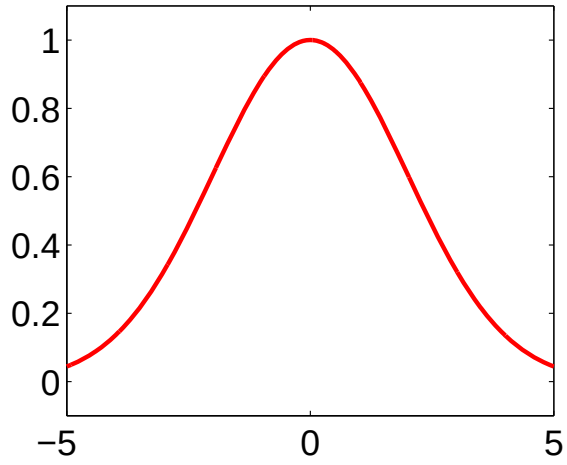

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Least-Squares Learning

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{b} \alpha_i \varphi(\boldsymbol{x}; \boldsymbol{\beta}_i)$$

$$\boldsymbol{w} = (\boldsymbol{\alpha}^\top, \boldsymbol{\beta}_1^\top, \boldsymbol{\beta}_2^\top, \ldots, \boldsymbol{\beta}_b^\top)^\top.$$

- Least-squares learning is often used for training hierarchical models.

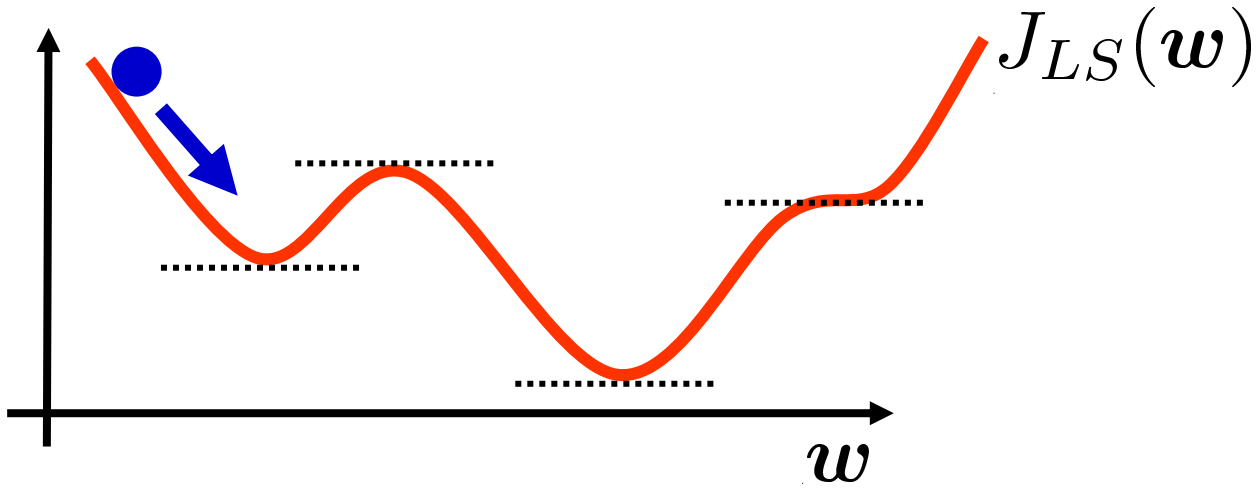
$$\min_{\boldsymbol{w}} J_{LS}(\boldsymbol{w})$$

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

How to Obtain Solutions

- No analytic solution is known.
- Simple gradient search is usually used.

$$\widehat{\boldsymbol{w}}^{new} \longleftarrow \widehat{\boldsymbol{w}}^{old} - \varepsilon \nabla J_{LS}(\widehat{\boldsymbol{w}}^{old})$$



- It converges to one of the local minima.

Error Back-Propagation

- Efficient calculation of gradient for Sigmoidal basis functions

$$\frac{\partial J_{LS}}{\partial \alpha_j} = 2 \sum_{i=1}^{n} o_{i,j} \left(\hat{f}(\boldsymbol{x}_i) - y_i \right)$$

$$\frac{\partial J_{LS}}{\partial \beta_j^{(k)}} = 2\alpha_j \sum_{i=1}^{n} o_{i,j} \left(1 - o_{i,j}\right) x_i^{(k)} \left(\hat{f}(\boldsymbol{x}_i) - y_i \right)$$

$$\frac{\partial J_{LS}}{\partial h_j} = 2\alpha_j \sum_{i=1}^{n} o_{i,j} \left(1 - o_{i,j}\right) \left(\hat{f}(\boldsymbol{x}_i) - y_i \right)$$

$$o_{i,j} = \varphi(\boldsymbol{x}_i; \boldsymbol{\beta}_j, h_j)$$

Error Back-Propagation (cont.)

- When the output values of the network are calculated, the input points are propagated following the forward path.
- On the other hand, when the gradients are calculated, the output error $(\hat{f}(\boldsymbol{x}_i) - y_i)$ is propagated backward.
- For this reason, this algorithm is called the error back-propagation.
- However, it is gradient descent so global convergence is not guaranteed.

Stochastic Gradient Descent

- In the usual gradient method, all training examples are used at the same time.
- In practice, the following stochastic method would be computationally advantageous.
  - Randomly choose one of the training examples (say, $(\boldsymbol{x}_i, y_i)$)
  - Update the parameter vector by

$$\widehat{\boldsymbol{w}}^{new} \longleftarrow \widehat{\boldsymbol{w}}^{old} - \varepsilon \nabla J_i(\widehat{\boldsymbol{w}}^{old})$$

$$J_i(\boldsymbol{w}) = (\hat{f}(\boldsymbol{x}_i) - y_i)^2$$

  - Repeat this procedure until convergence.

Avoiding Overfitting

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{b} \alpha_i \varphi(\boldsymbol{x}; \boldsymbol{\beta}_i)$$

$$\boldsymbol{w} = (\boldsymbol{\alpha}^\top, \boldsymbol{\beta}_1^\top, \boldsymbol{\beta}_2^\top, \ldots, \boldsymbol{\beta}_b^\top)^\top.$$

- LS overfits to noisy samples.
  - Regularization:

$$\min_{\boldsymbol{w}} [J_{LS}(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|^2]$$

$$J_{LS}(\boldsymbol{w}) = \sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i) - y_i \right)^2 \qquad \lambda > 0$$

  - Early stopping: Stop gradient descent before it converges

Special Structure of Neural Networks

- Parameters and functions are not one-to-one mapping.

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{b} \alpha_i \varphi(\boldsymbol{x}; \boldsymbol{\beta}_i)$$

  - If $\alpha_i = 0$, any $\boldsymbol{\beta}_i$ gives the same function.
  - Any permutation gives the same function.
- This non-identifiability causes great difficulty in the mathematical analysis of neural networks.

Homework

1. Prove that the gradients for Sigmoidal basis functions are given as

$$\frac{\partial J_{LS}}{\partial \alpha_j} = 2 \sum_{i=1}^{n} o_{i,j} \left(\hat{f}(\boldsymbol{x}_i) - y_i \right)$$

$$o_{i,j} = \varphi(\boldsymbol{x}_i; \boldsymbol{\beta}_j, h_j)$$

$$\frac{\partial J_{LS}}{\partial \beta_j^{(k)}} = 2\alpha_j \sum_{i=1}^{n} o_{i,j} \left(1 - o_{i,j}\right) x_i^{(k)} \left(\hat{f}(\boldsymbol{x}_i) - y_i \right)$$

$$\frac{\partial J_{LS}}{\partial h_j} = 2\alpha_j \sum_{i=1}^{n} o_{i,j} \left(1 - o_{i,j}\right) \left(\hat{f}(\boldsymbol{x}_i) - y_i \right)$$

Homework (cont.)

2. For your own toy 1-dimensional data, perform simulations using
   - 3-layer neural networks with sigmoid functions
   - Error back-propagation

   and analyze the results, e.g., by changing
   - Target functions
   - Number of training samples
   - Noise level
   - Number of neurons in the second layer (b)

Notification of Final Assignment

1. Apply supervised learning techniques to your data set and analyze it.
2. Write your opinion about this course

- Final report deadline: Aug 6th (Fri.)
- E-mail submission is also accepted!

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Mini-Workshop on Data Mining

- On July 20th and 27th, we have a mini-workshop on data mining, instead of regular lectures.
- We have 16 speakers in total.
- Presentation: 10 minutes per person (including Q&A).
  - Specification of your dataset
  - Employed methods
  - Outcome

Schedule

- July 13th : Preparation for workshop (no lecture)
- July 20th : Mini-workshop Day 1
- July 27th : Mini-workshop Day 2

Mini-Workshop: Program

July 20th ,2010: 10:40-12:10

- Wittawat Jitkrittum
- Nakamasa Inoue
- Yukihiro Fukunaga
- Tatsuya Shigemura
- Ahmet Cetinkaya
- Michael Hamarneh
- Yonatan Andy Fajar Nugraha
- Youhei Namiki

July 27th ,2010: 10:40-12:10

- Johan Rohdin
- Hilman F. Pardede
- Sangeeta Biswas
- Rubaiya Rahtin Khan
- Mori Syogo
- M. Rasyid Aqmar
- Nozomi Kurihara
- Yuan Liang

Talk: 9 mins. Q&A: 2 mins.