Pattern Information Processing: Neural Networks

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Today's Plan

- Sigmoidal neural networks
- Least-squares in neural networks: The error back-propagation algorithm

Non-Linear Models

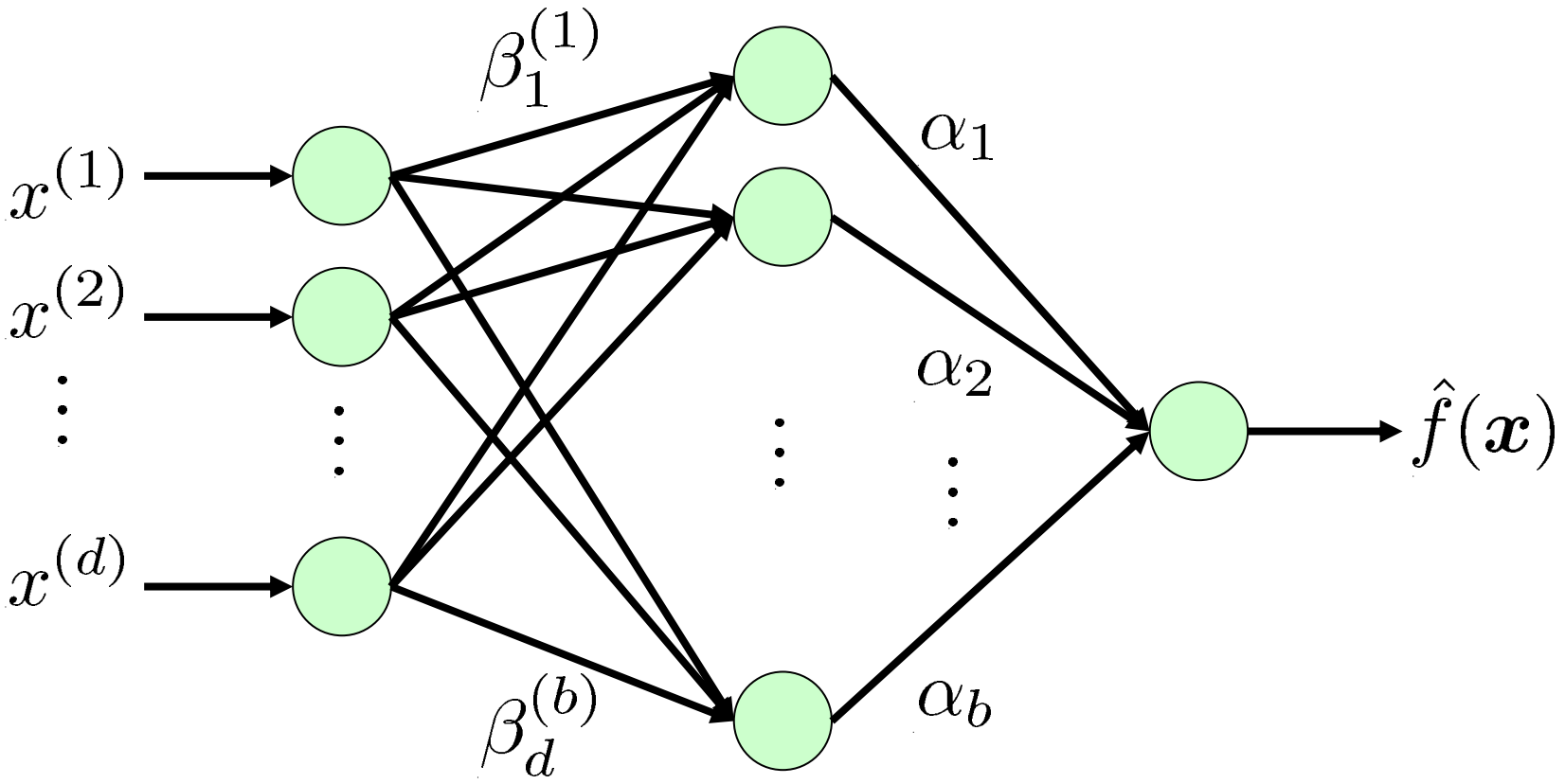
- A popular choice: Hierarchical models

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

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

Three-Layer Networks

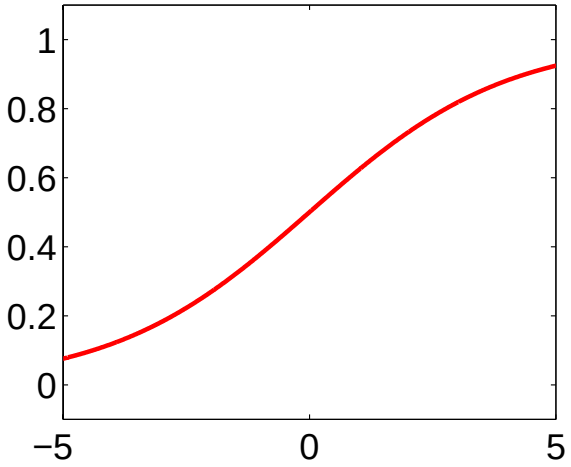
- Such a hierarchical model can be represented as a 3-layer network.



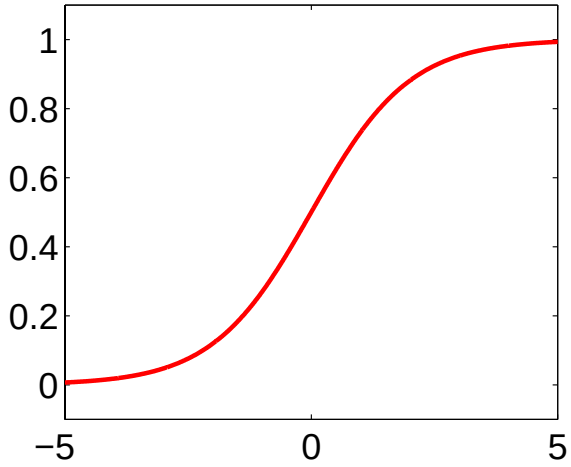
Sigmoidal Function

- 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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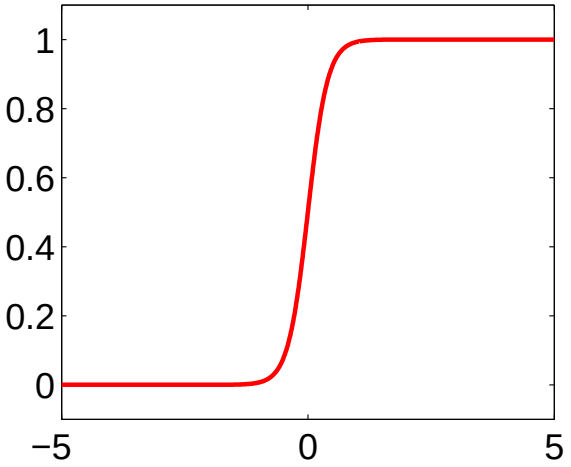

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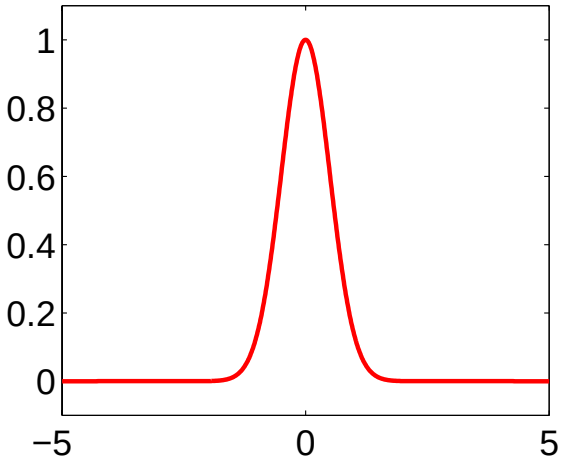
Perceptrons

- 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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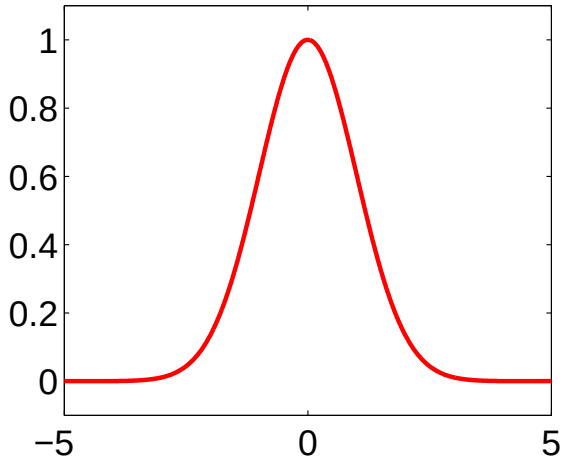

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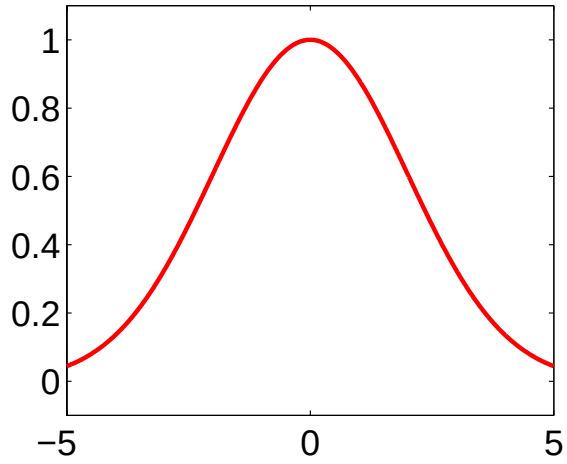

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Least-Squares Learning

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

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

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

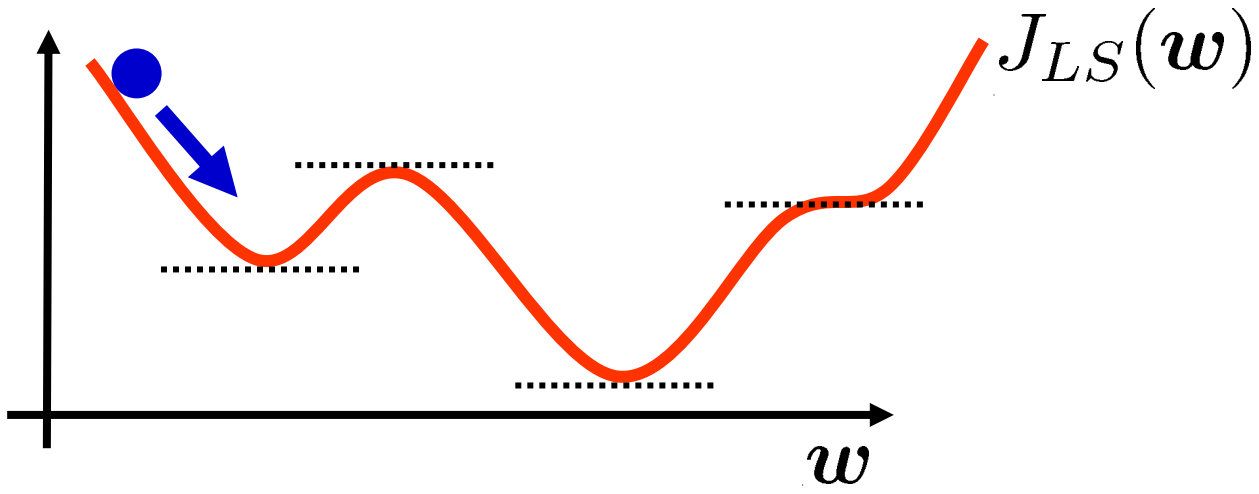
$$\min_{\boldsymbol{w}} J_{LS}(\boldsymbol{w})$$

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

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 search 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.

Homework

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

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

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

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

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 samples
   - Noise level
   - Number of hidden neurons

Supplement

- For one-dimensional input

$$\hat{f}(x) = \sum_{i=1}^{b} \alpha_i \varphi(x; \beta_i, h_i) \qquad \varphi(x; \beta, h) = \frac{1}{1 + \exp(-\beta x - h)}$$

$$\boldsymbol{w} = (\alpha_1, \alpha_2, \ldots, \alpha_b, \beta_1, \beta_2, \ldots, \beta_b, h_1, h_2, \ldots, h_b,)^\top.$$

$$\frac{\partial J_i}{\partial \alpha_j} = 2 o_{i,j} \left(\hat{f}(x_i) - y_i \right) \qquad o_{i,j} = \varphi(x_i; \beta_j, h_j)$$

$$\frac{\partial J_i}{\partial \beta_j} = 2 \alpha_j o_{i,j} \left(1 - o_{i,j}\right) x_i^{(k)} \left(\hat{f}(x_i) - y_i \right)$$

$$\frac{\partial J_i}{\partial h_j} = 2 \alpha_j o_{i,j} \left(1 - o_{i,j}\right) \left(\hat{f}(x_i) - y_i \right)$$