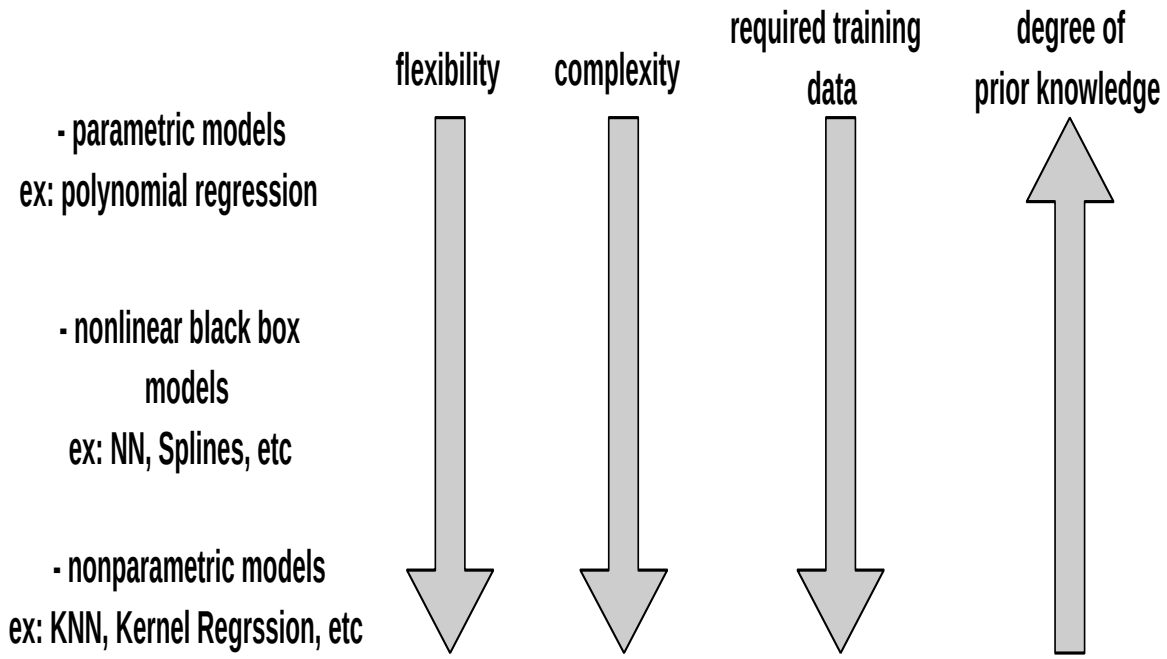
Model Selection: Balancing training data and prior knowledge



One example

- Let's suppose that we want to approximate the following function:

$$y = 1 * x^2 + 2 * x + 1.$$

- The following models are considered:
  - Polynomial regression: $y = a * x^2 + b * x + c$;
  - Radial Basis Function network:

$$y = \sum_{q=1}^{Q} w_q \phi_q(x),$$

$$\phi_q(x) = \exp\left(-\frac{(x - \widehat{x})^2}{\sigma^2}\right)$$

  - k nearest neighbours:

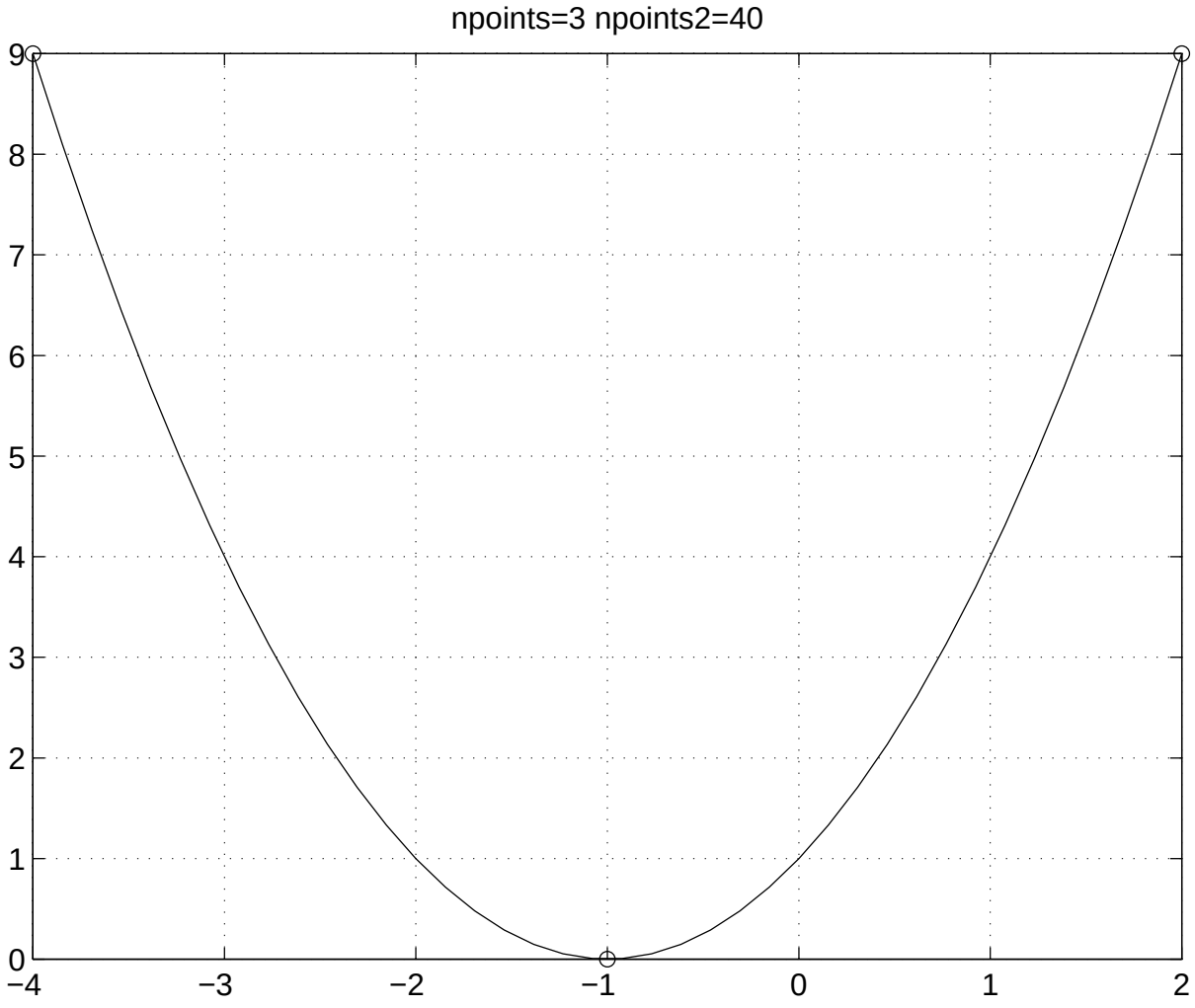
$$y = \frac{\sum_{i=1}^{k} y_i}{k},$$

$$\{y_i \mid \min_{k \ points} |x - x_i|\}$$

polynomial regression

Characteristics:

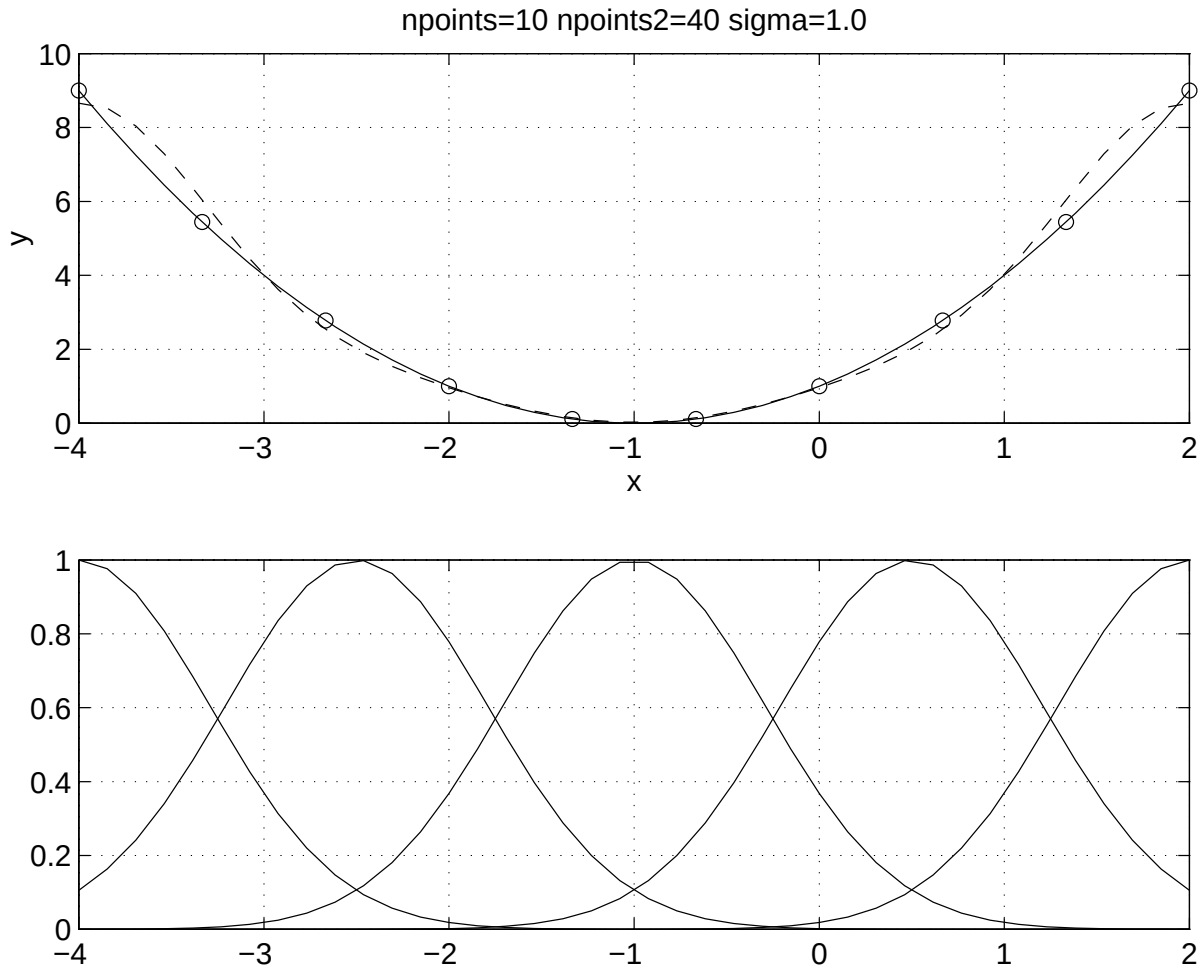
- Estimated parameters: a=1.0, b=2.0, c=1.0;
- Number of training data points: 3;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 0.0$



RBF network - example 1

Characteristics:

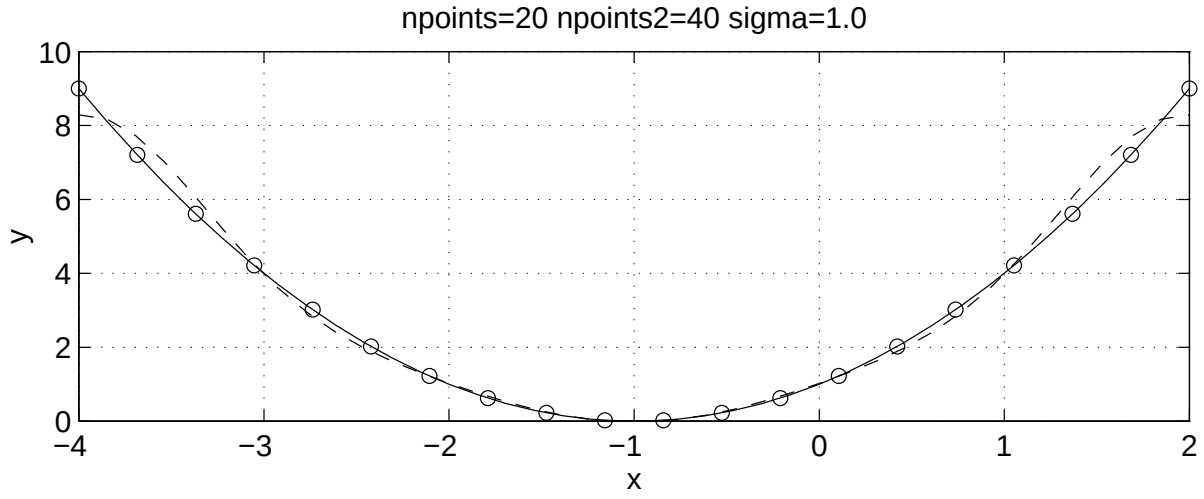
- Number of basis functions: 5;
- $\sigma = 1$;
- Number of training data points: 20;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 0.0742$

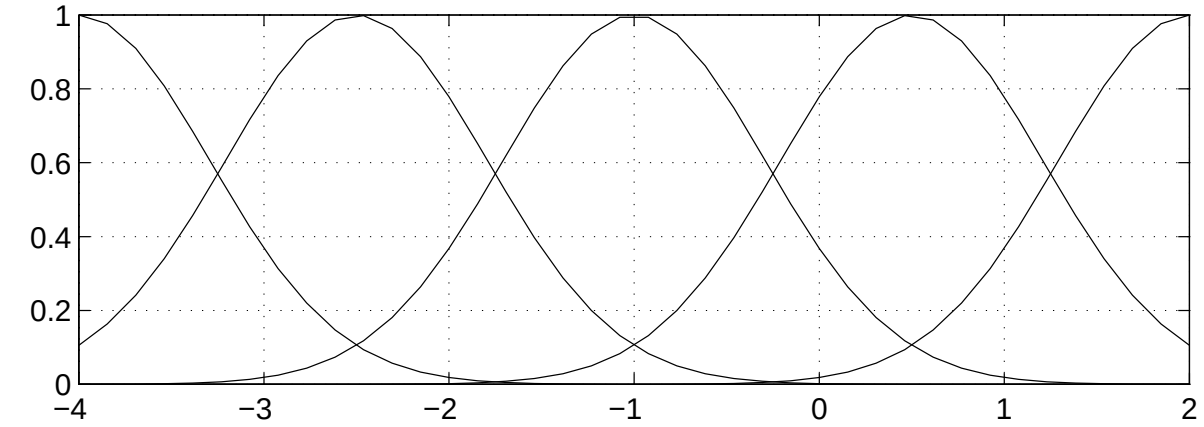


RBF network - example 2

Characteristics:

- Number of basis functions: 5;
- $\sigma = 1.0$;
- Number of training data points: 10;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 0.1250$

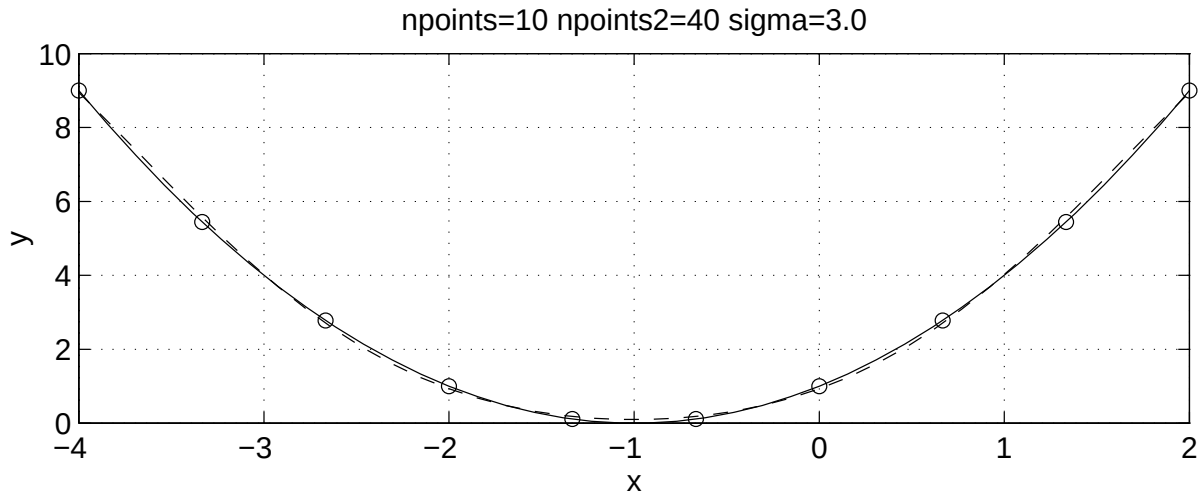


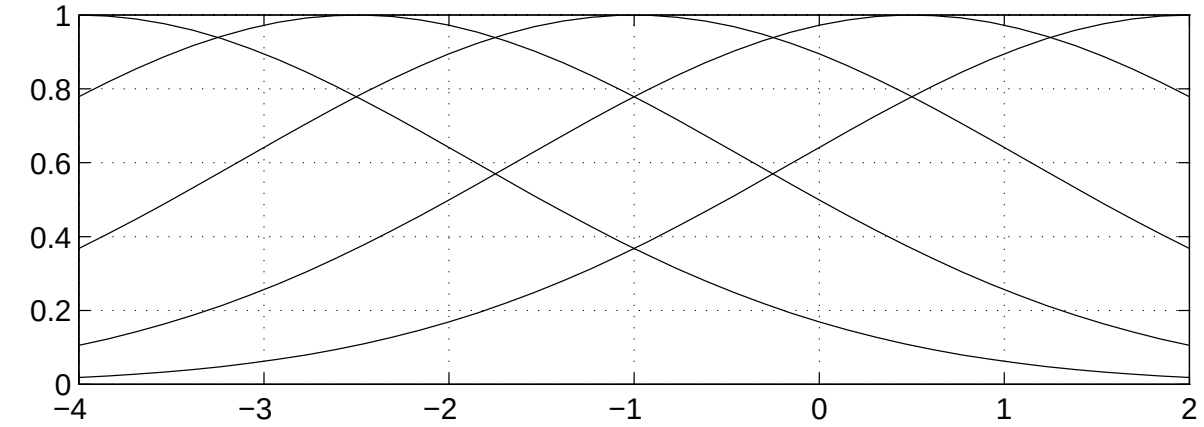


RBF network - example 3

Characteristics:

- Number of basis functions: 5;
- $\sigma = 3.0$;
- Number of training data points: 10;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 0.075$

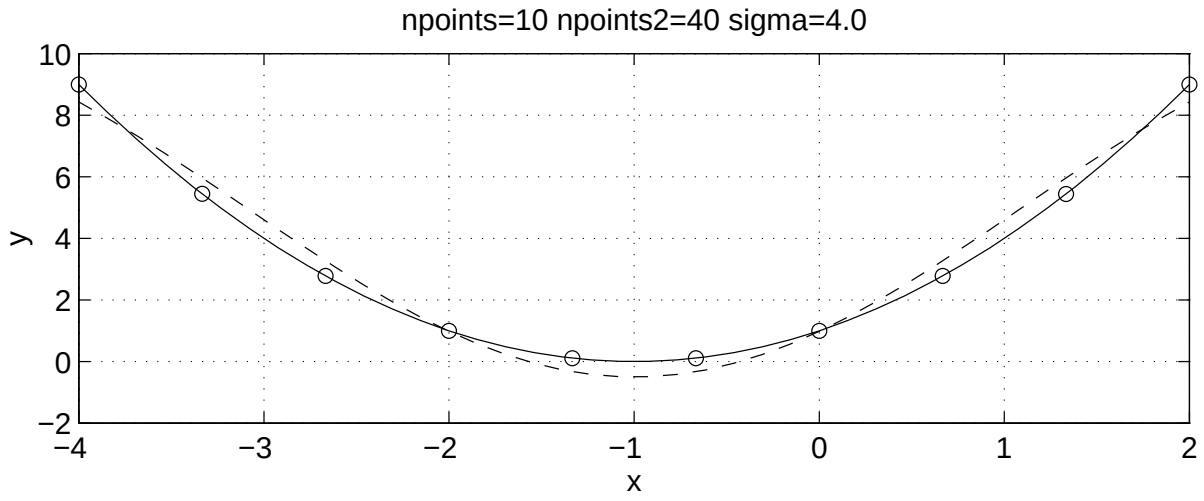


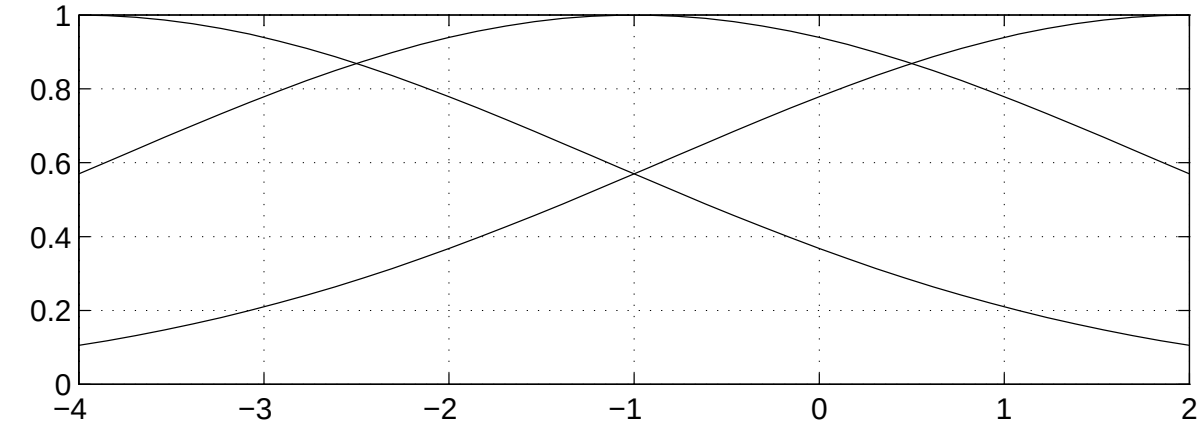


RBF network - example 4

Characteristics:

- Number of basis functions: 3;
- $\sigma = 5$;
- Number of training data points: 10;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 0.1660$

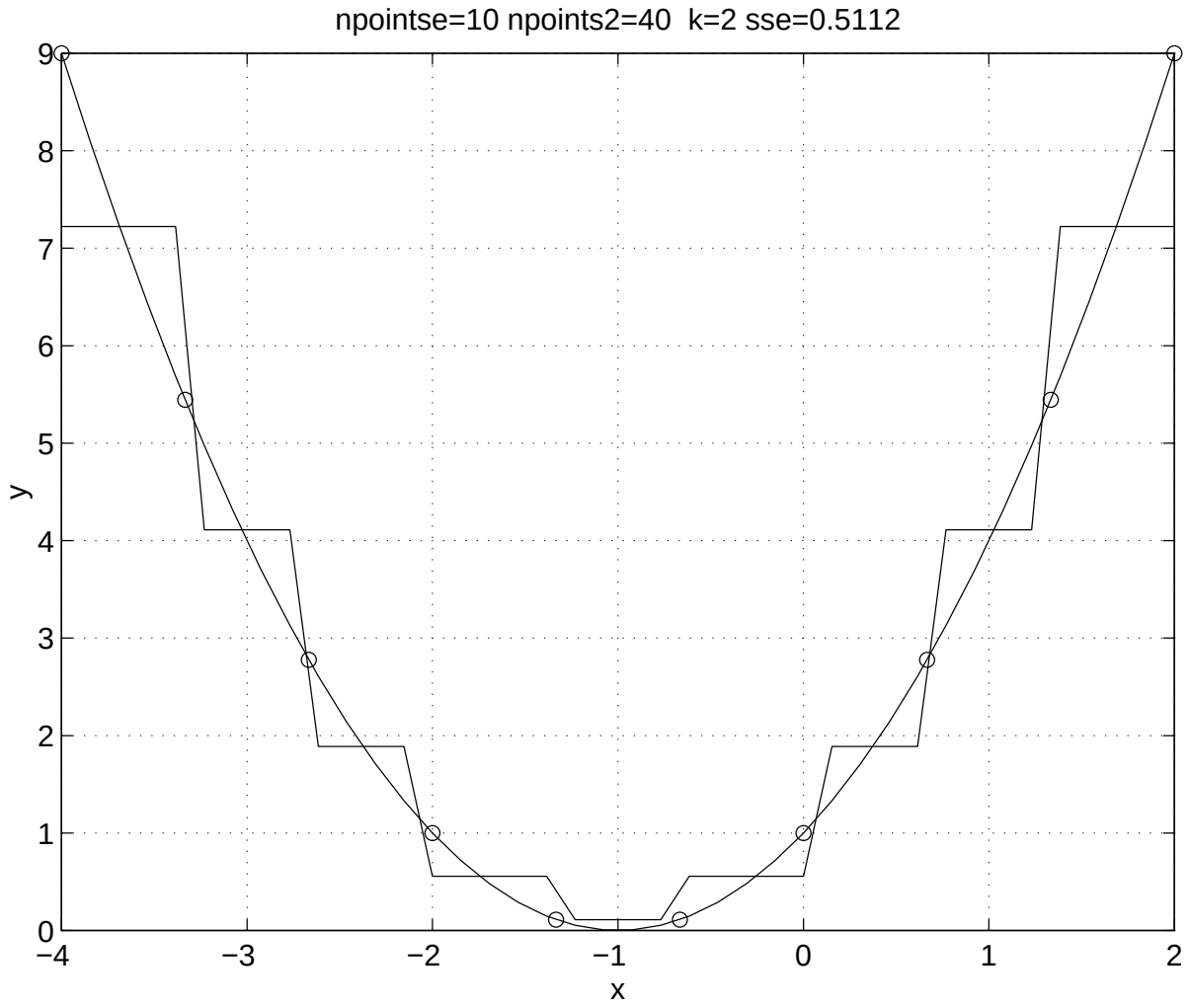




K-nn - example 1

Characteristics:

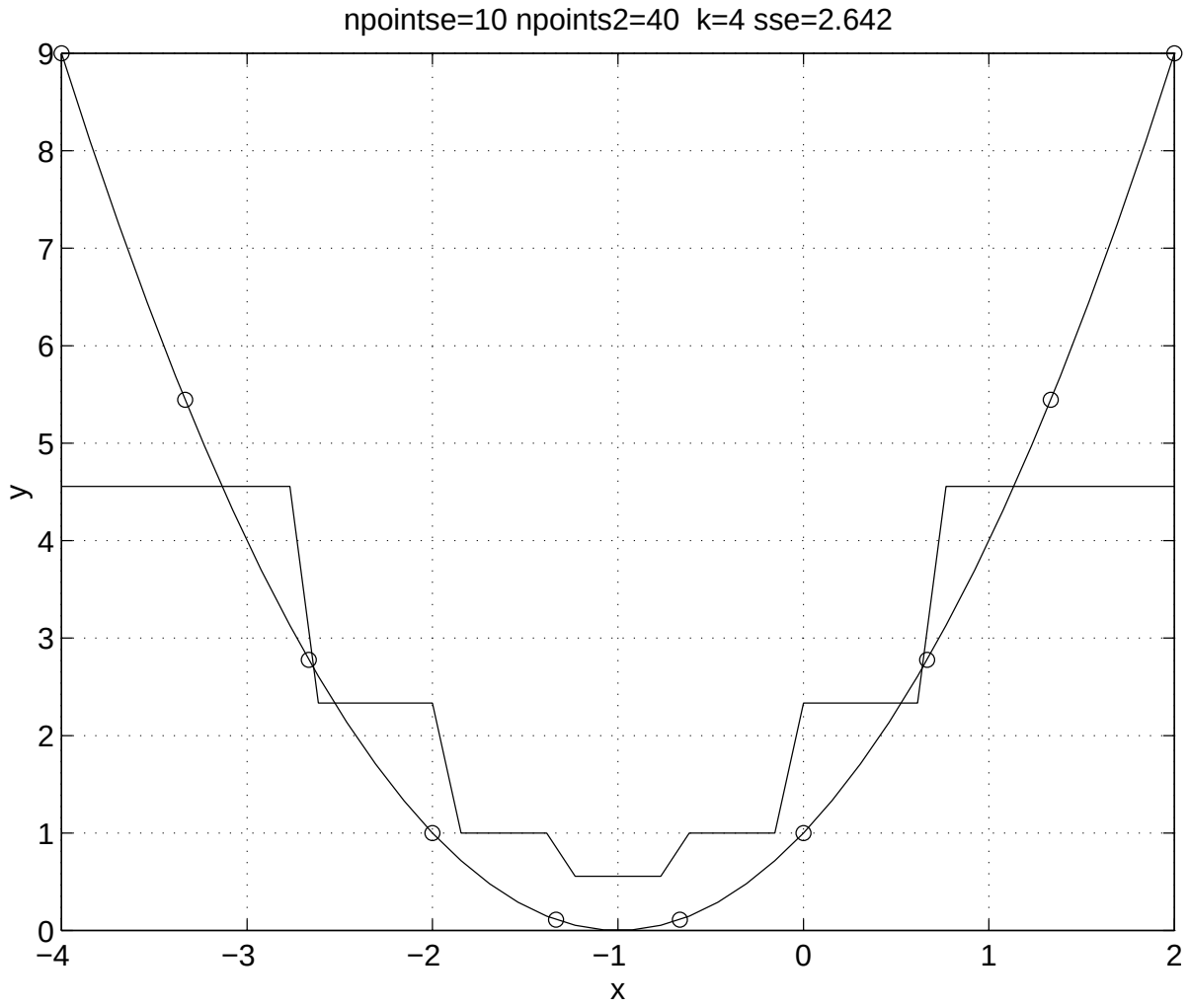
- $k = 2$
- Number of training data points: 10;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 0.5112$



K-nn - example 2

Characteristics:

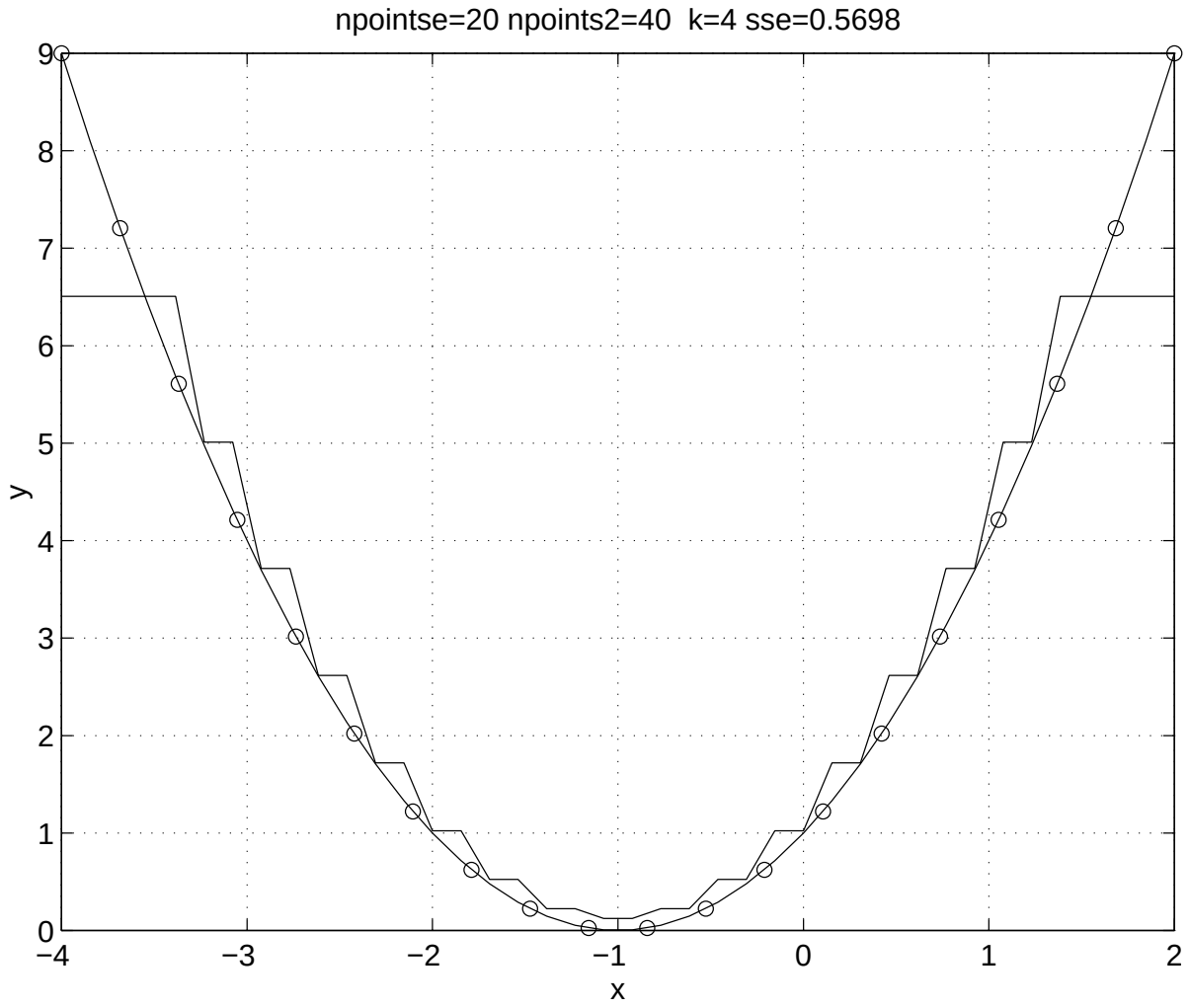
- $k = 4$
- Number of training data points: 10;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 2.642$



K-nn - example 3

Characteristics:

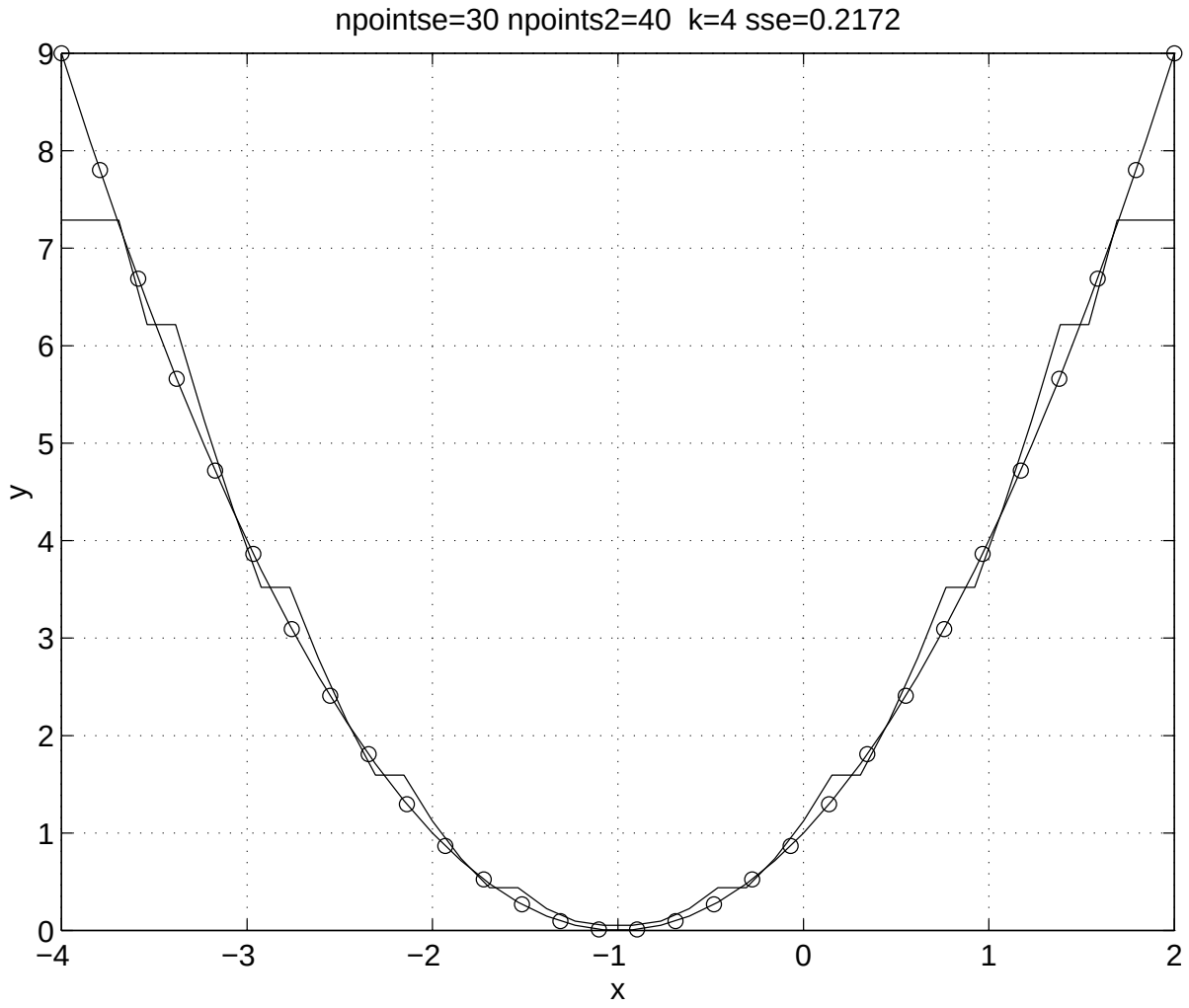
- $k = 4$
- Number of training data points: 20;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 0.5698$



K-nn - example 4

Characteristics:

- $k = 4$
- Number of training data points: 30;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 0.2172$



K-nn - example 5

Characteristics:

- $k = 4$
- Number of training data points: 40;
- Number of test data points: 40;
- Resulting $MSE = \sum_{i=1}^{N} \frac{|e_i|^2}{N} = 0.1475$