Multivariate classification

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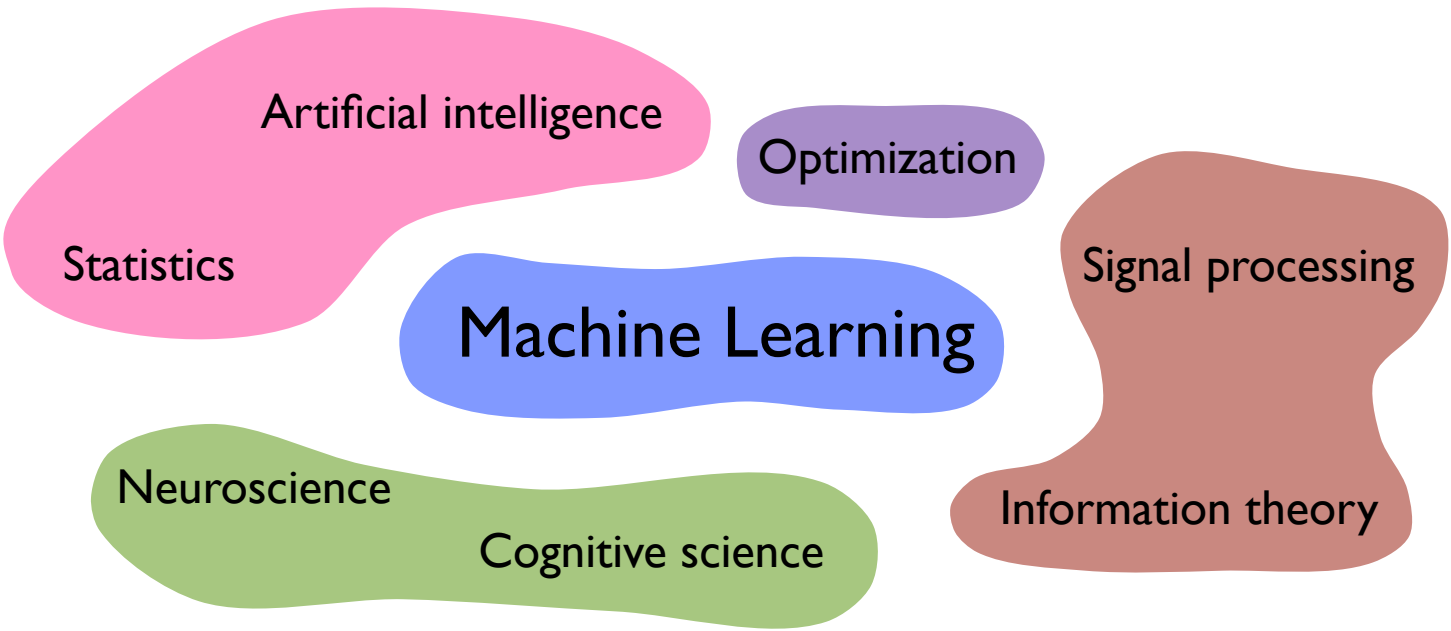
Machine learning

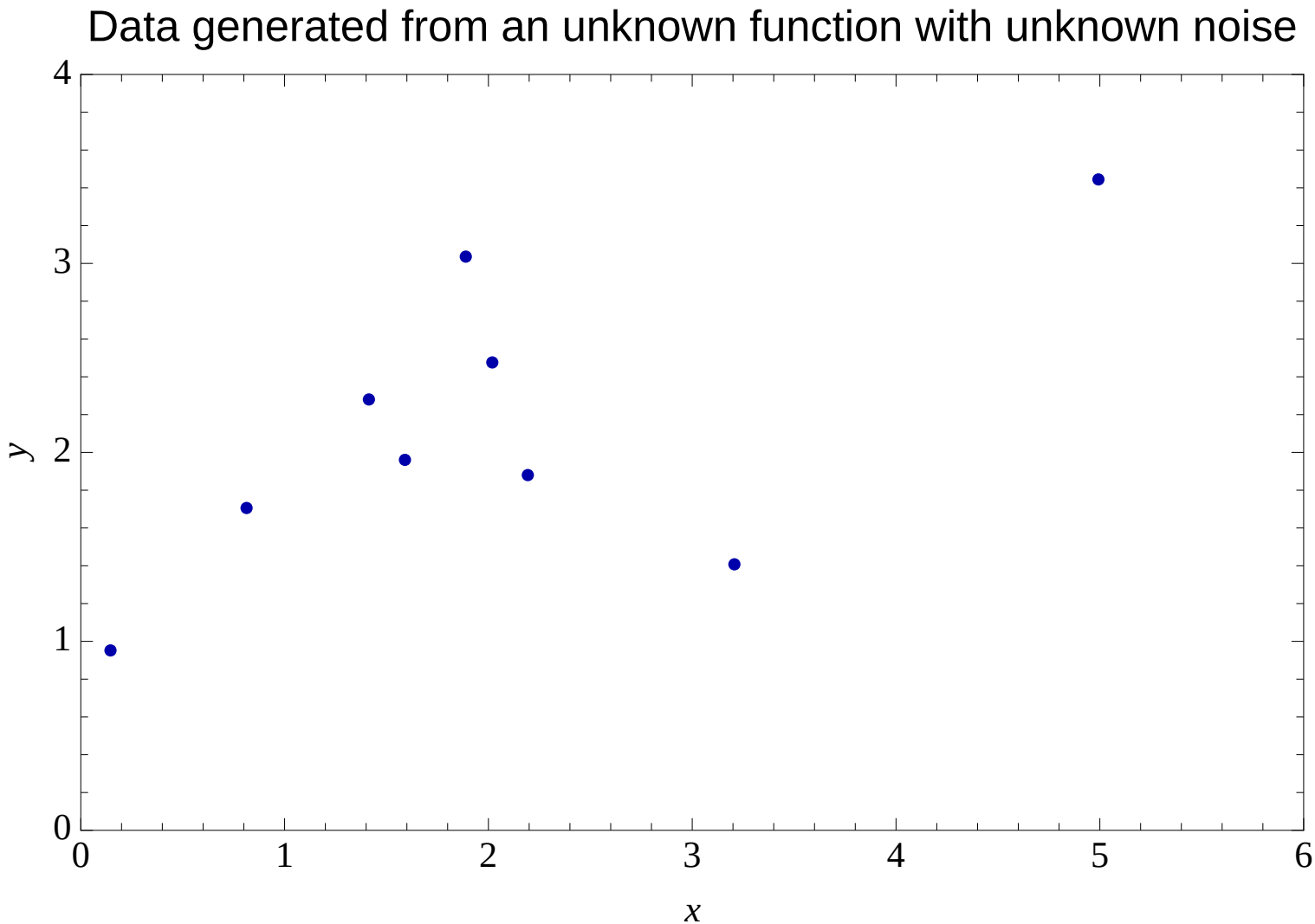
- Can be considered as a sub-domain of statistics
  - Often non-parametric, high-dimensional spaces, large data sets → computational issues (optimization) become as important as statistical issues (capacity control)
  - Most often associated to multivariate discrimination (classification)
- Best-known algorithms
  - Classification: neural network, boosting, support vector machine
  - Regression: neural network, Gaussian process
  - Density estimaton: mixture of Gaussians
  - Clustering, dimensionality reduction: PCA, k-means, spectral clustering, local linear embedding, ISOMAP, nonlinear PCA, kernel PCA

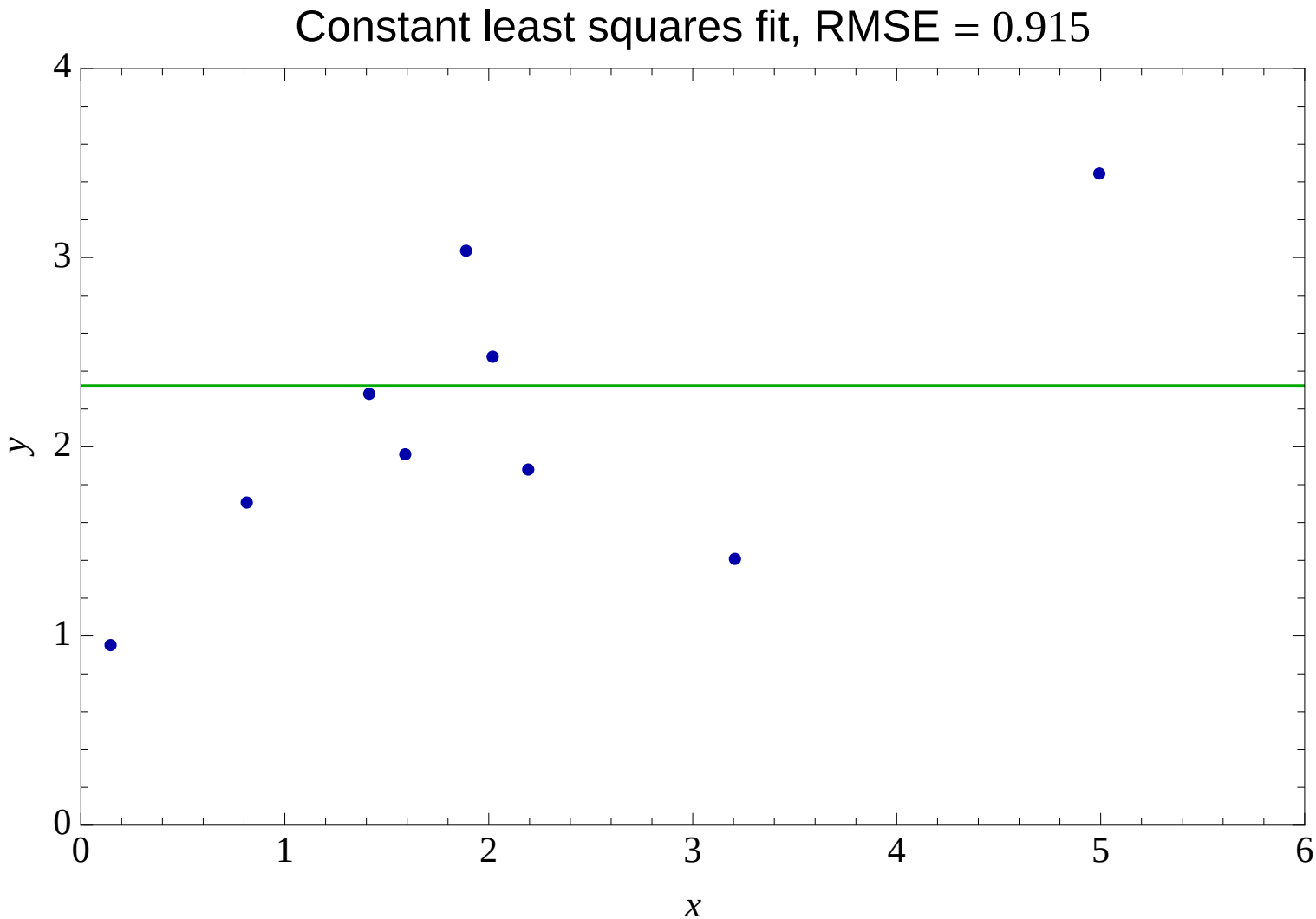
Machine learning at the crossroads

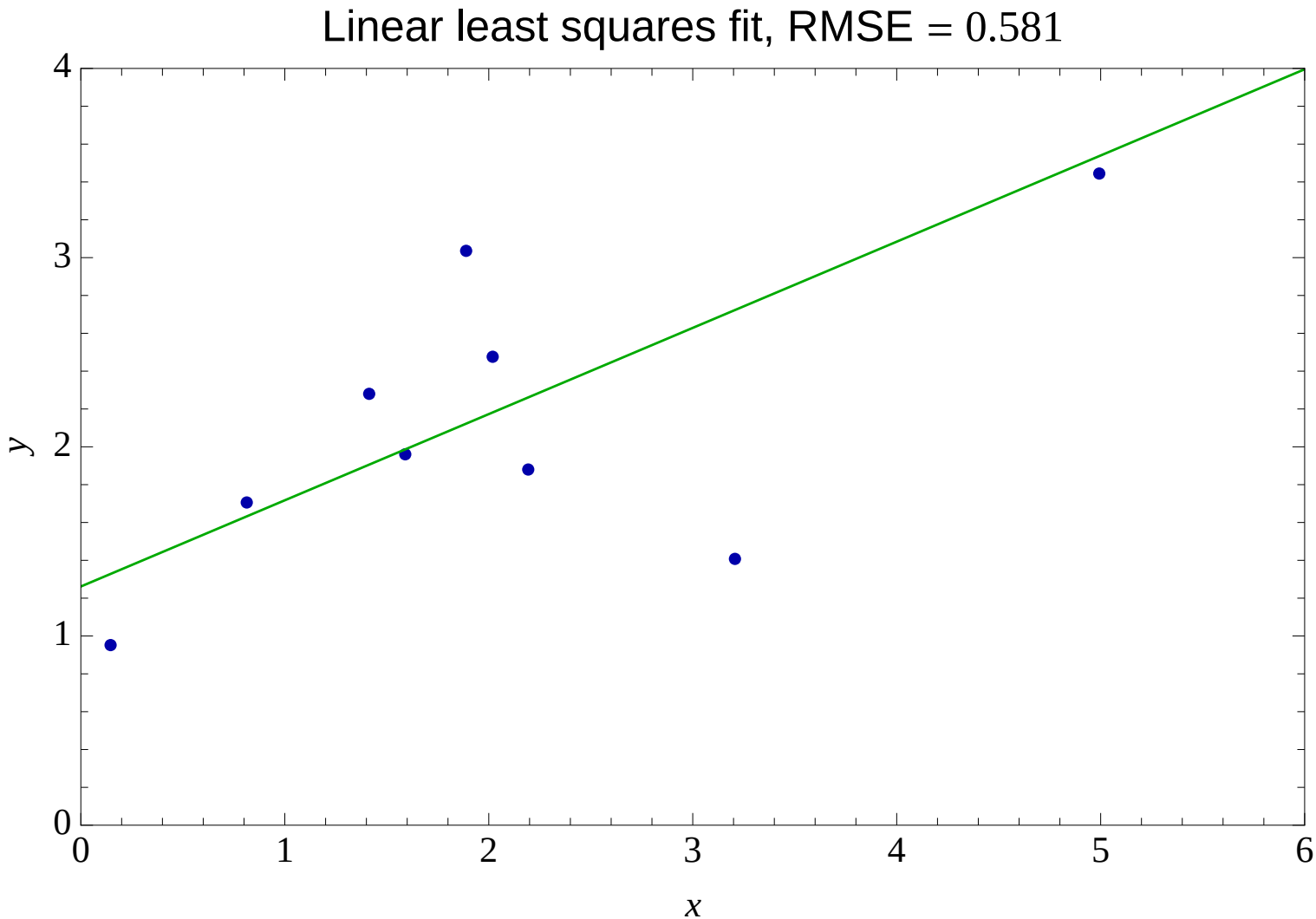


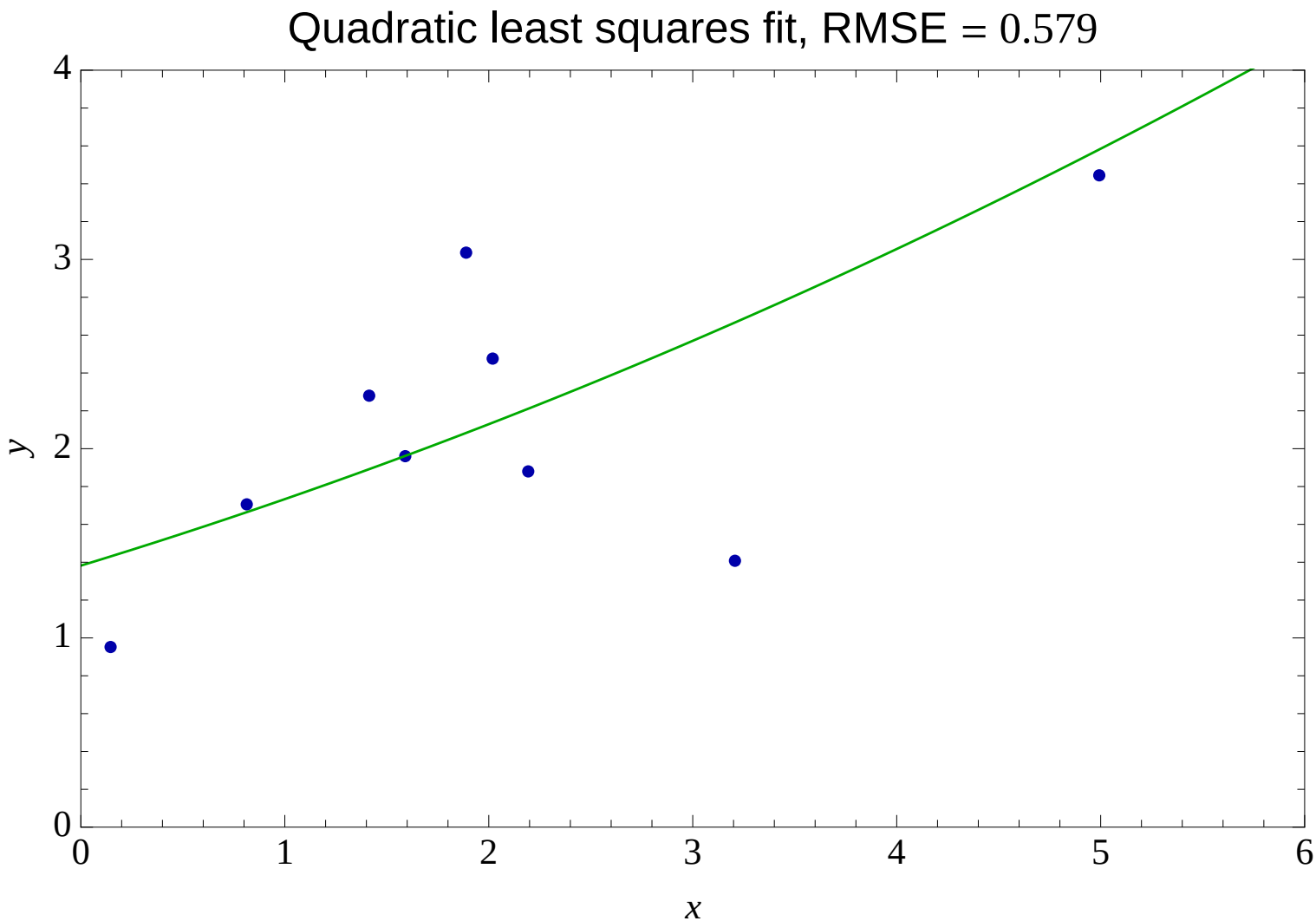
Outline

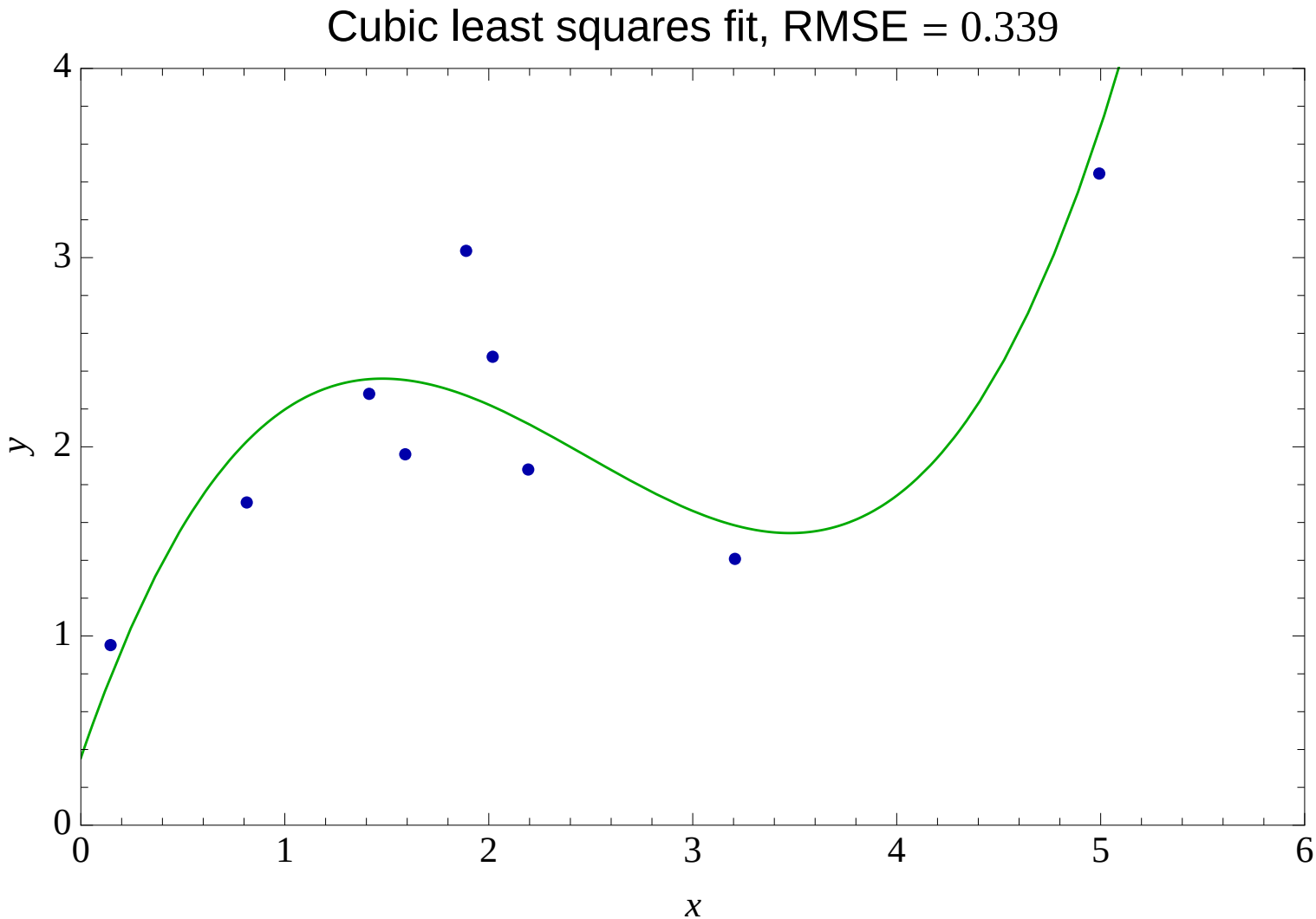
- Non-parametric fitting: two simple examples
- The formal model for classification, learning principles
- Classification algorithms (from a user's point of view)
  - perceptron, neural networks (NN)
  - AdaBoost
  - the Support Vector Machine (SVM)
- Machine learning research motivated by HEP applications

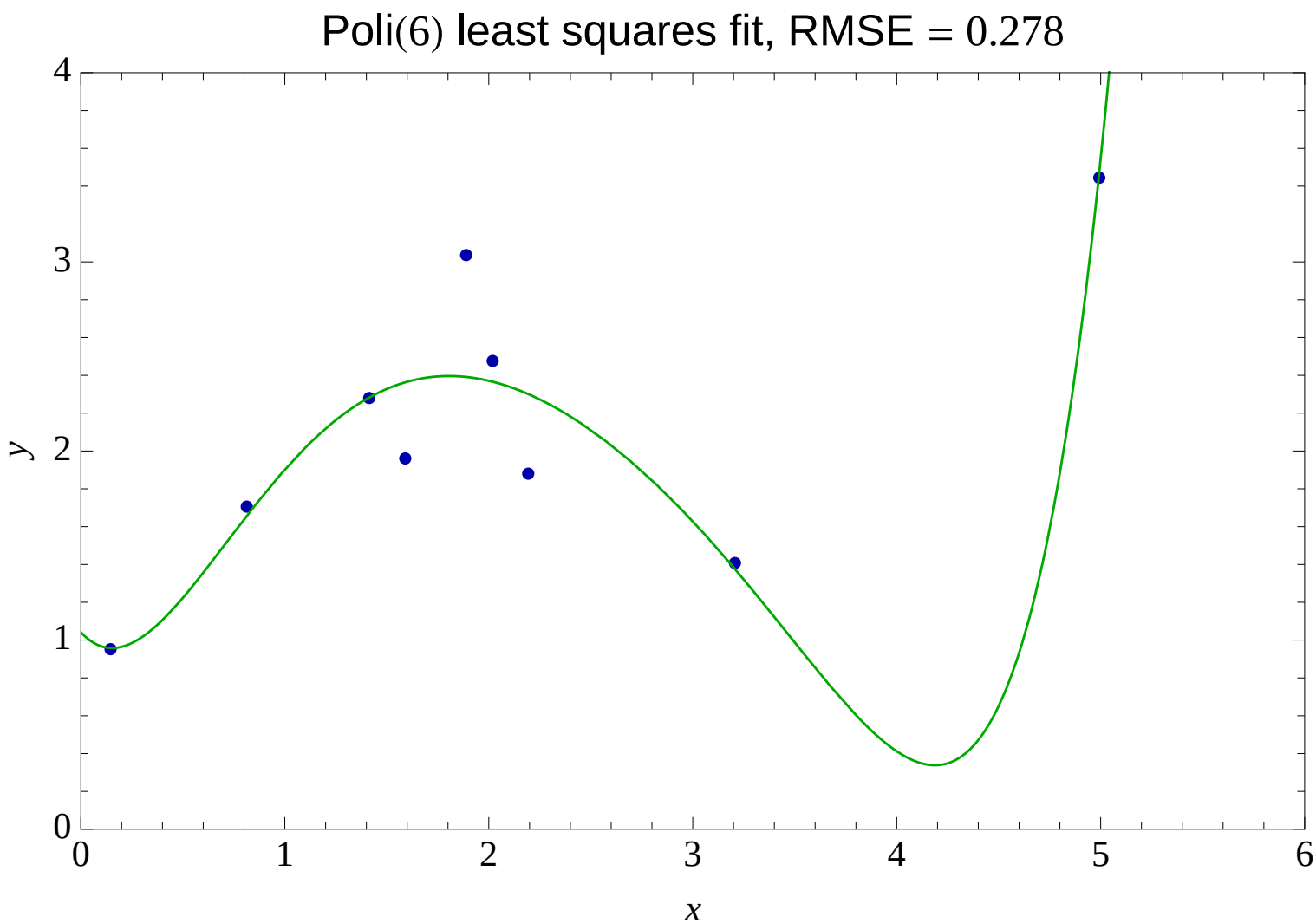

Data generated from an unknown function with unknown noise
y
x
0
1
2
3
4
5
6

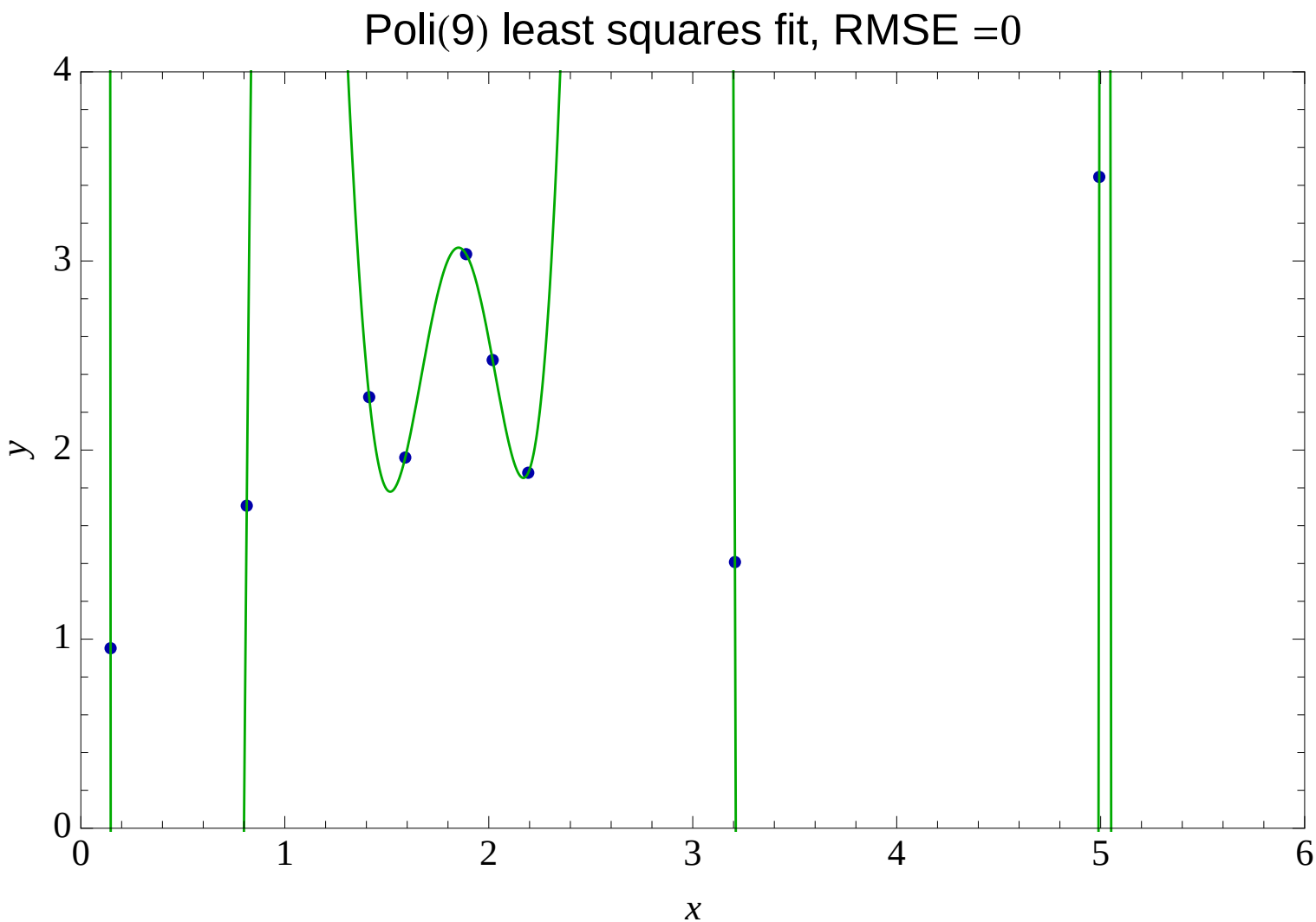

Constant least squares fit, RMSE = 0.915
y
x
0
1
2
3
4
5
6


Linear least squares fit, RMSE = 0.581
y
x
0
1
2
3
4
5
6


Quadratic least squares fit, RMSE = 0.579
y
x
0
1
2
3
4
5
6

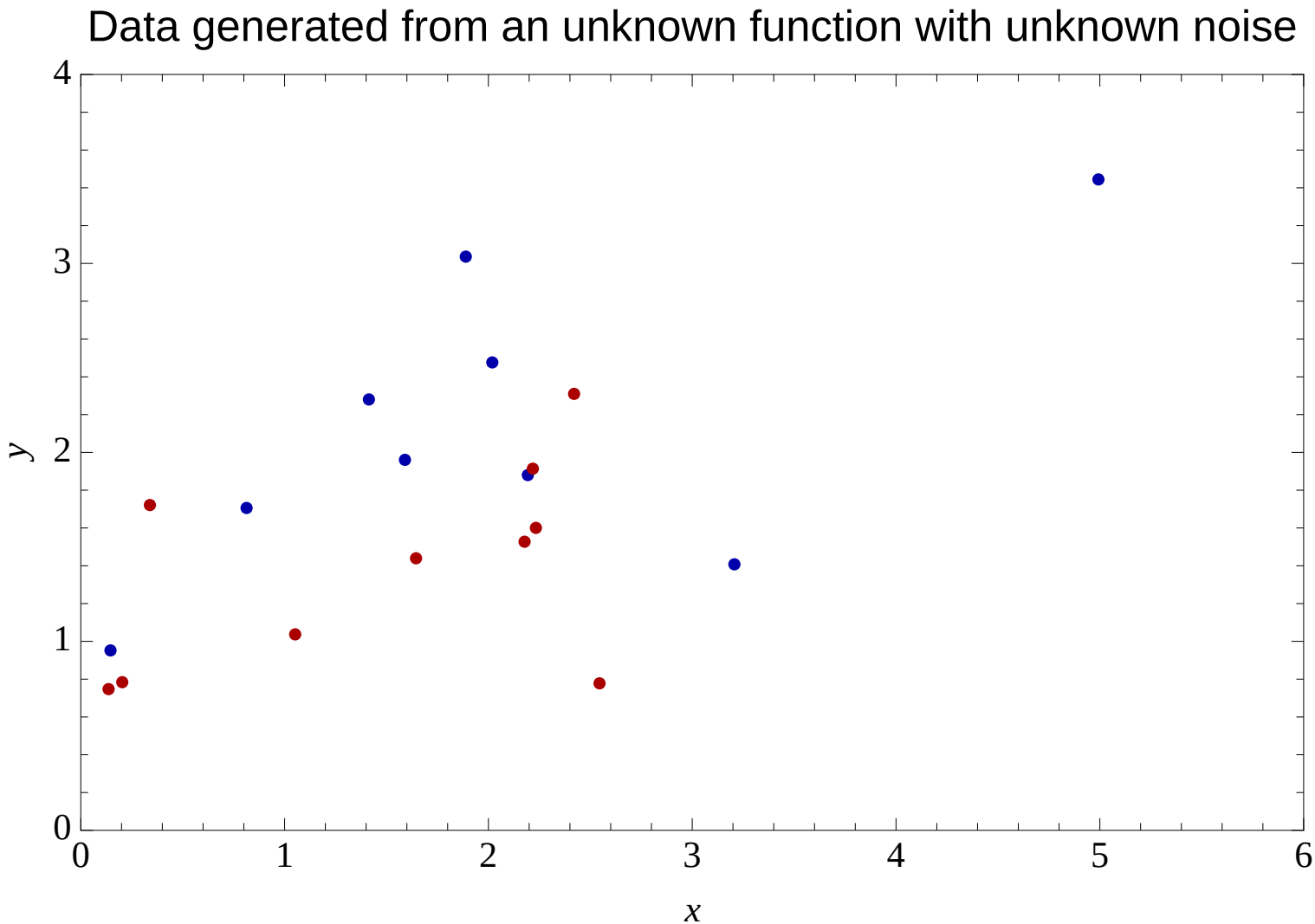

Cubic least squares fit, RMSE = 0.339
y
x
0
1
2
3
4
5
6


Poli(6) least squares fit, RMSE = 0.278
y
x
0
1
2
3
4
5
6

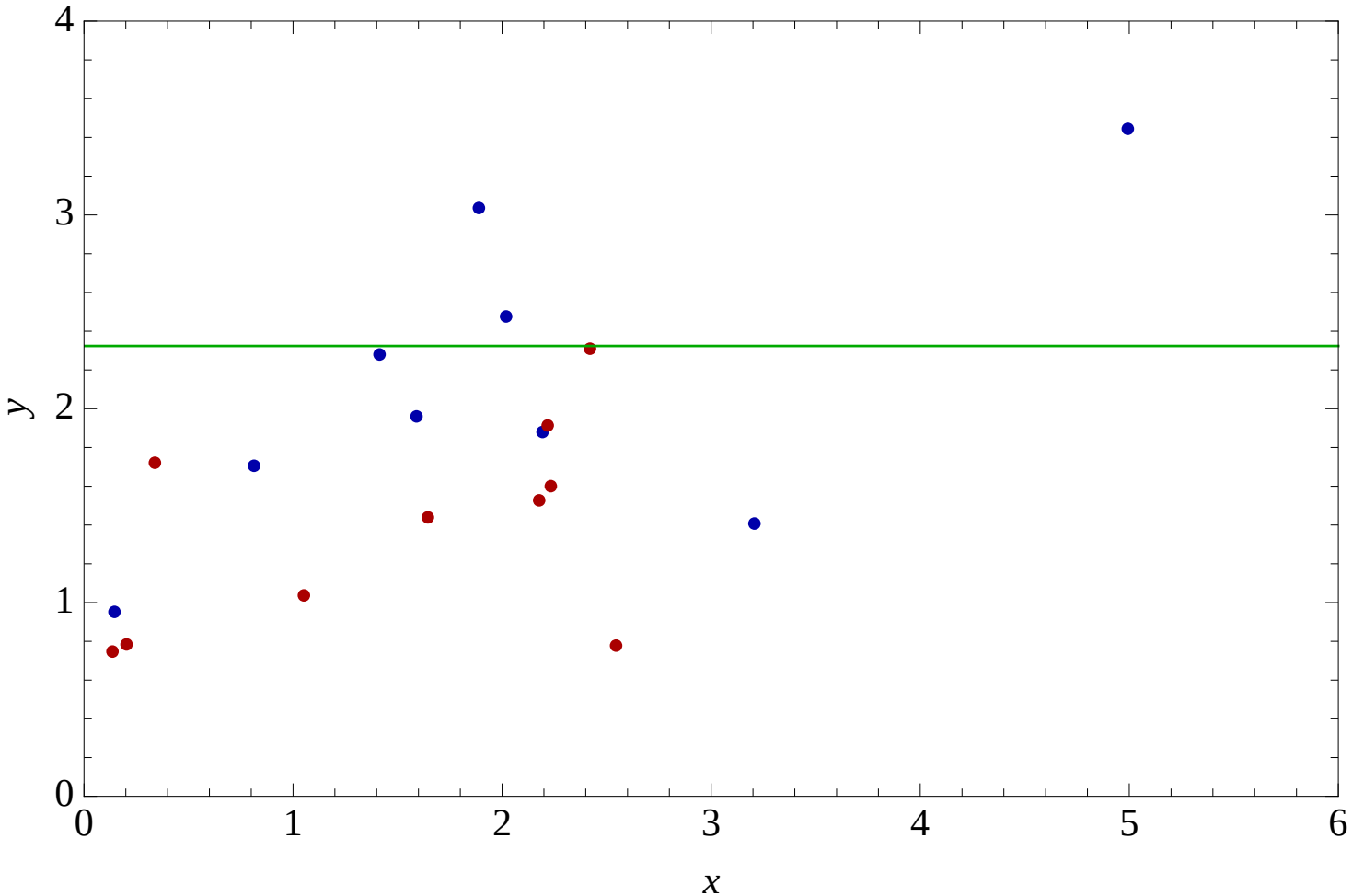

Poli(9) least squares fit, RMSE =0
y
x
0
1
2
3
4
5
6

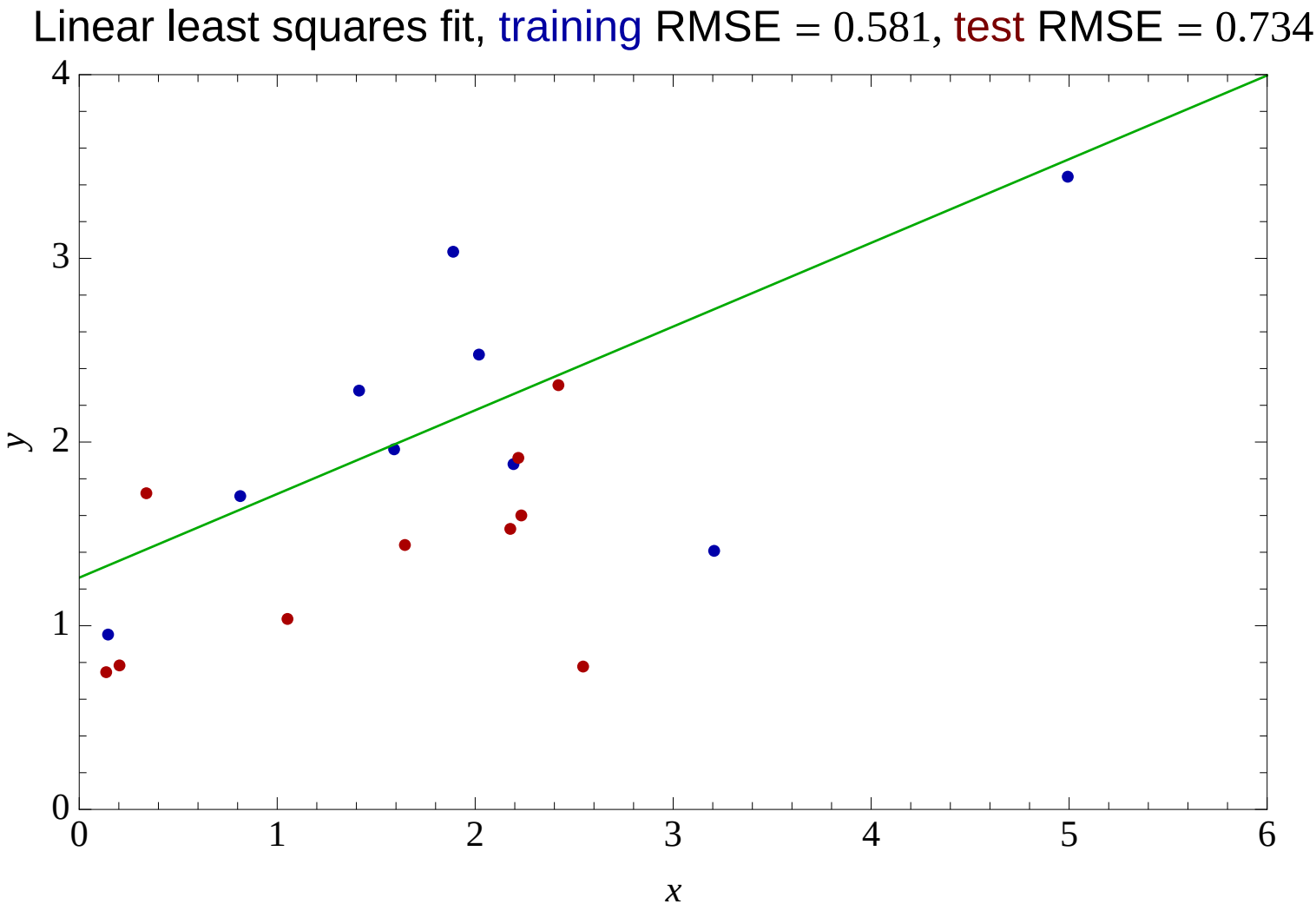
Non-parametric fitting

- Minimizing the training cost (RMSE) does not work if the function class is not fixed beforehand
- If you do not know the correct function class, you should not fix it
- Capacity control, regularization
  - theoretical results, data-independent, based on sample size and measures of complexity
  - use independent (test) set

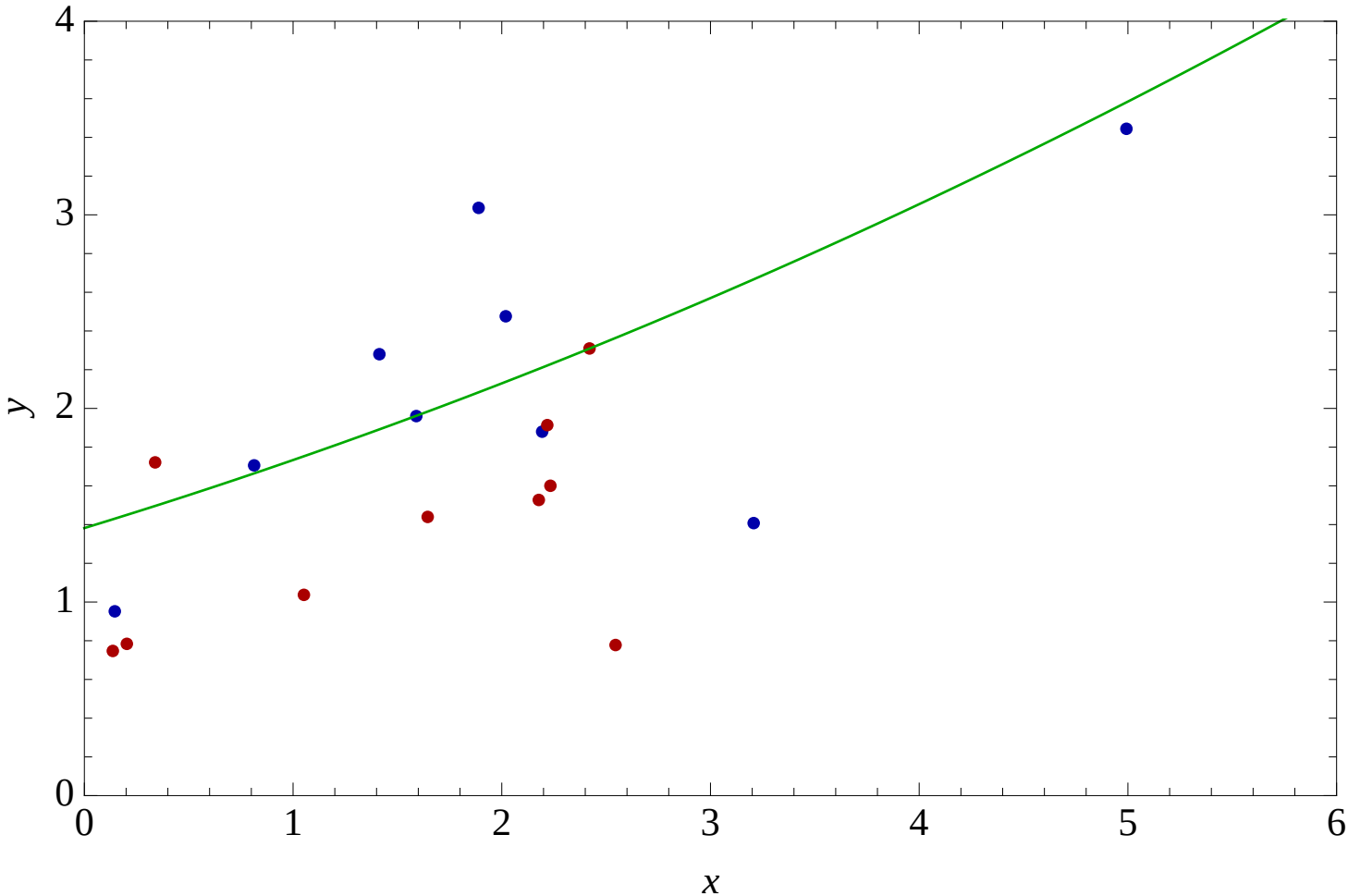

Data generated from an unknown function with unknown noise
y
x
0
1
2
3
4
5
6

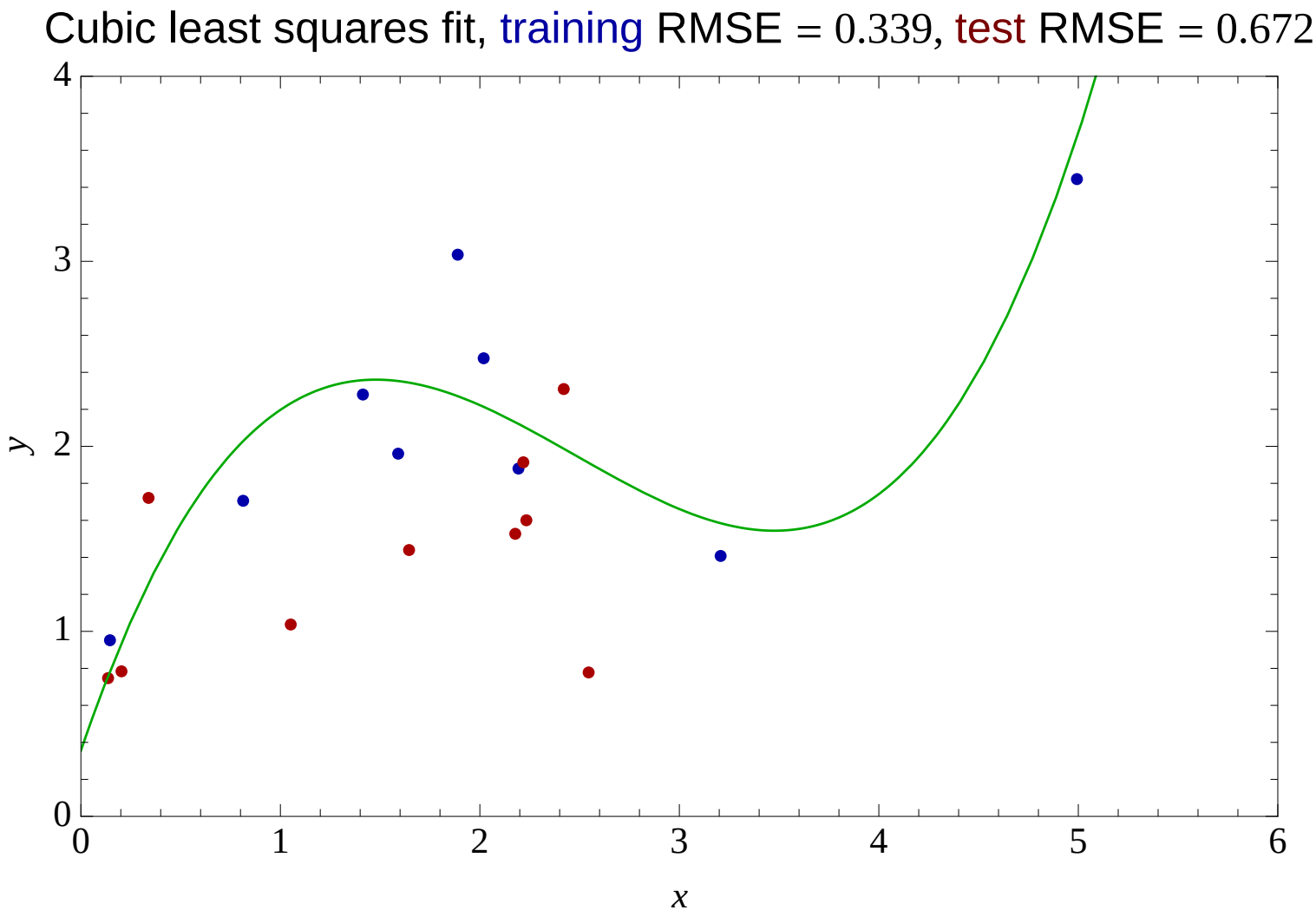
Const. least squares fit, training RMSE = 0.915, test RMSE = 1.067

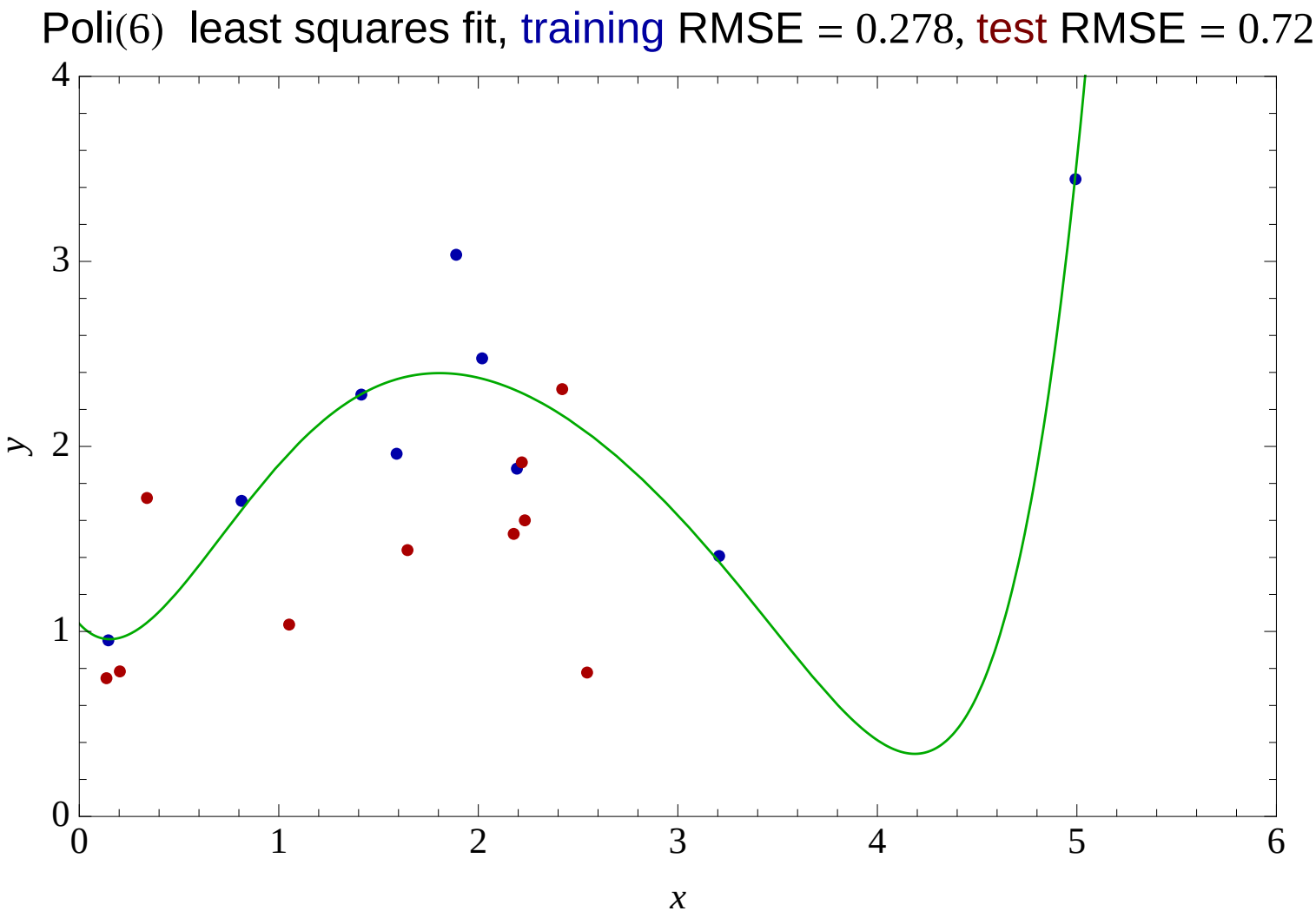


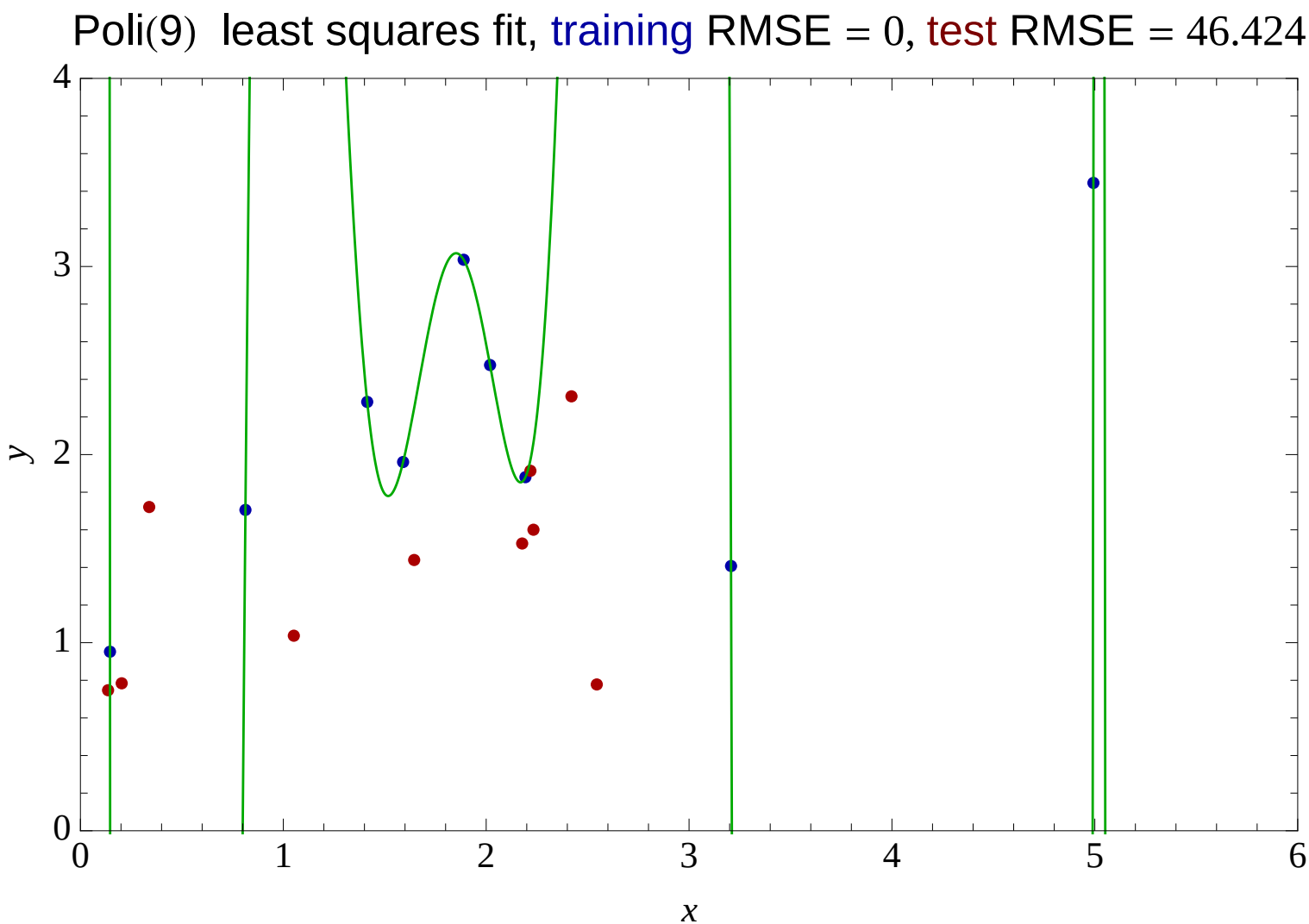

Linear least squares fit, training RMSE = 0.581, test RMSE = 0.734
y
x
0
1
2
3
4
5
6

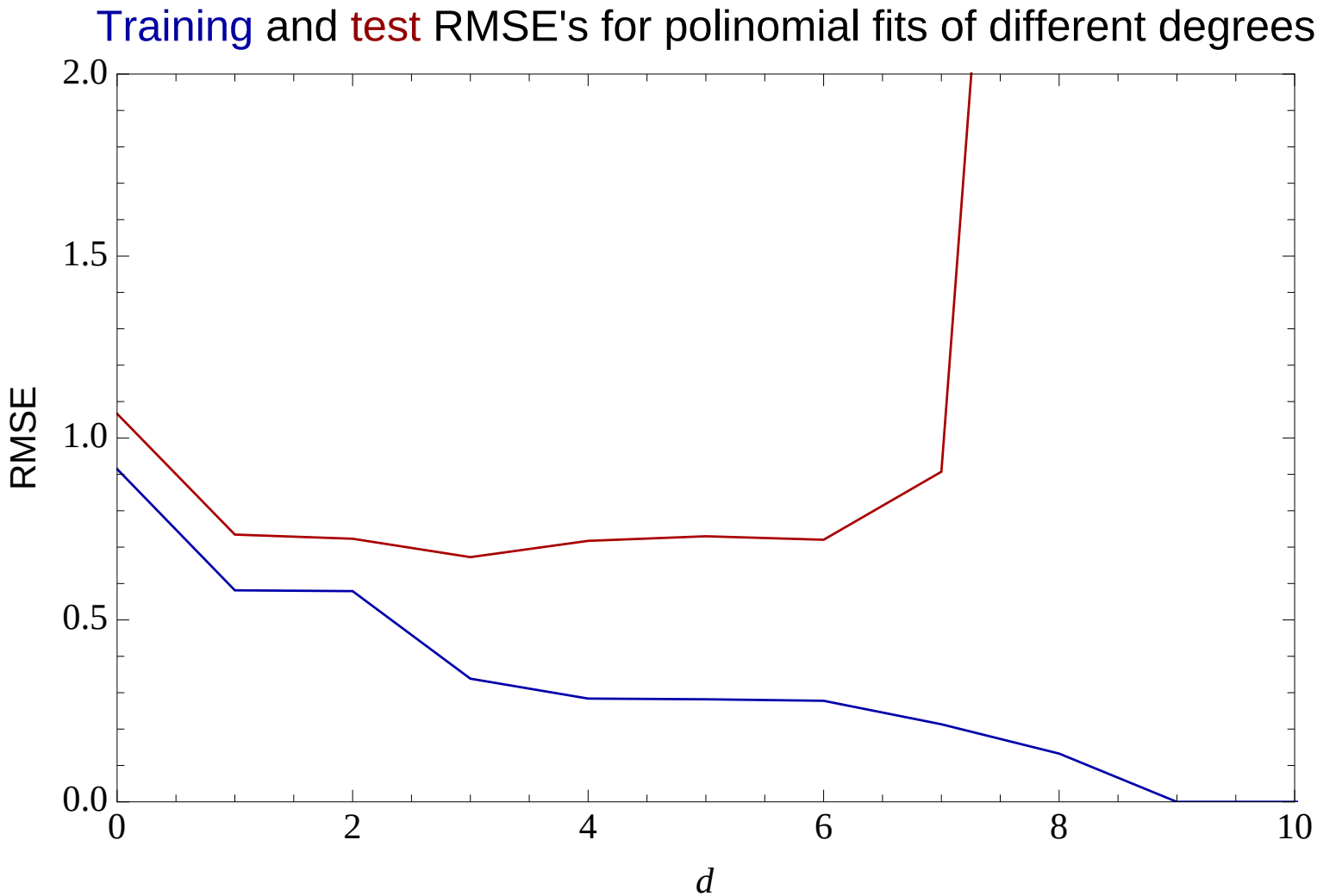
Quadr. least squares fit, training RMSE = 0.579, test RMSE = 0.723

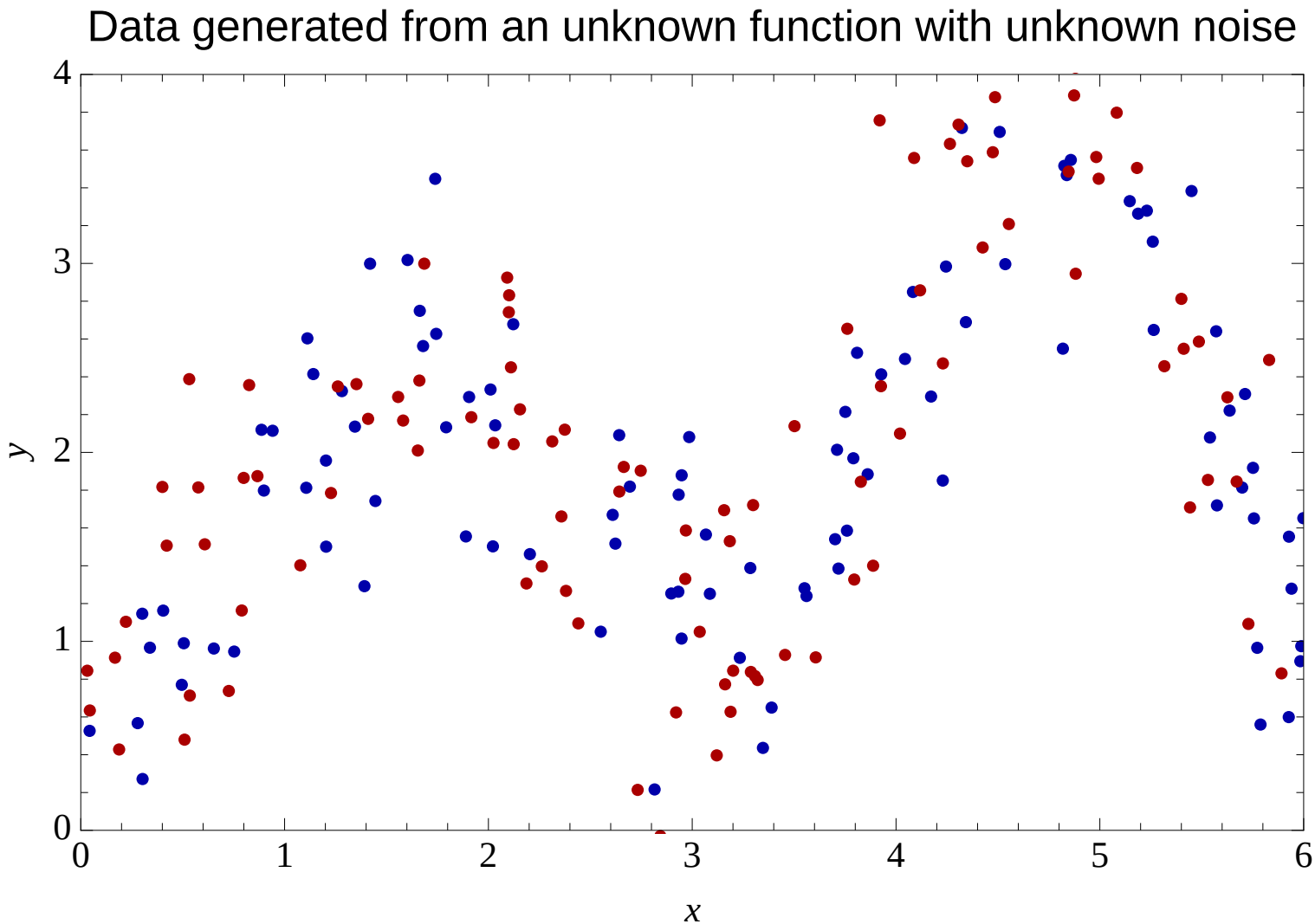


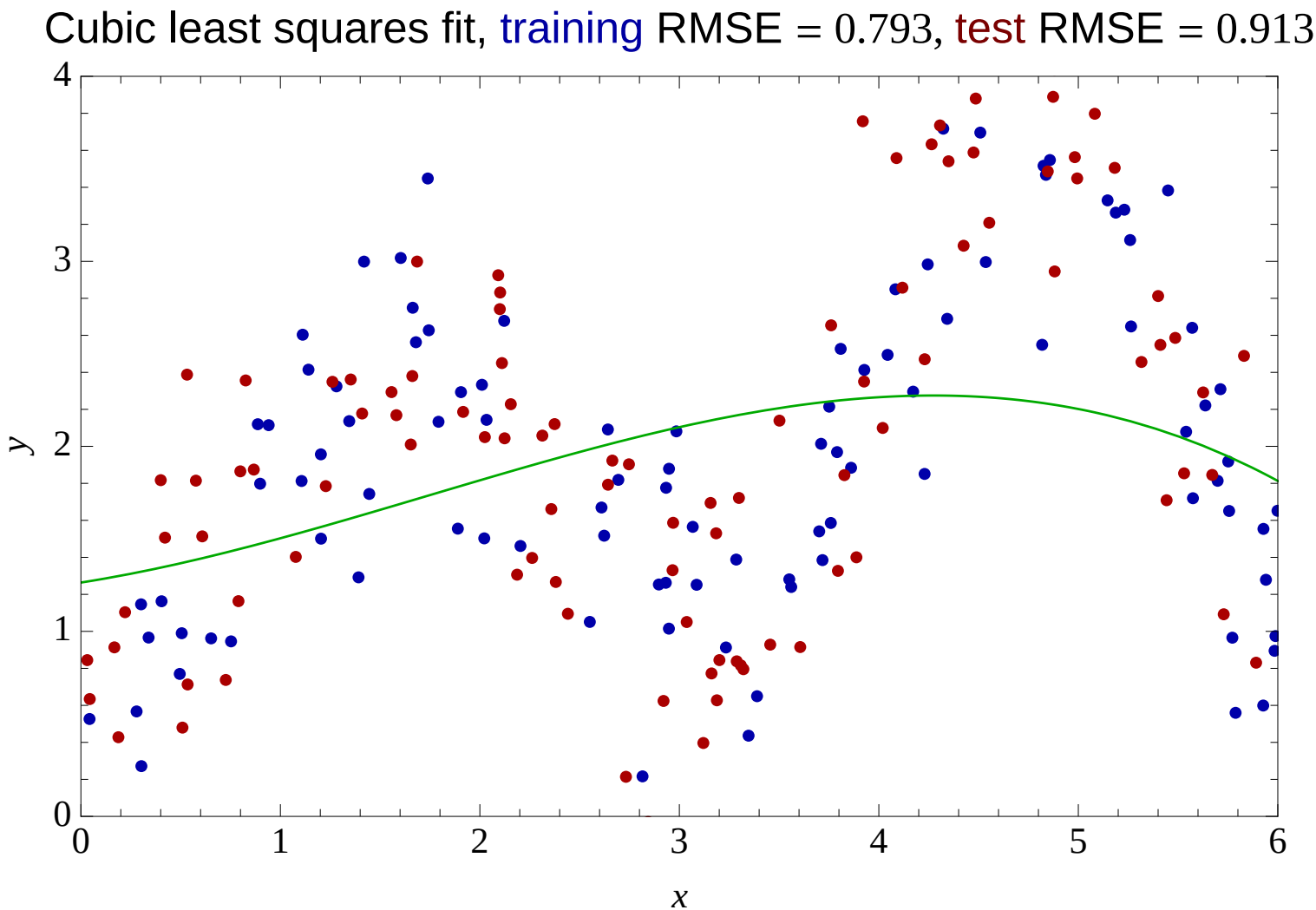

Cubic least squares fit, training RMSE = 0.339, test RMSE = 0.672
y
x
0
1
2
3
4
5
6

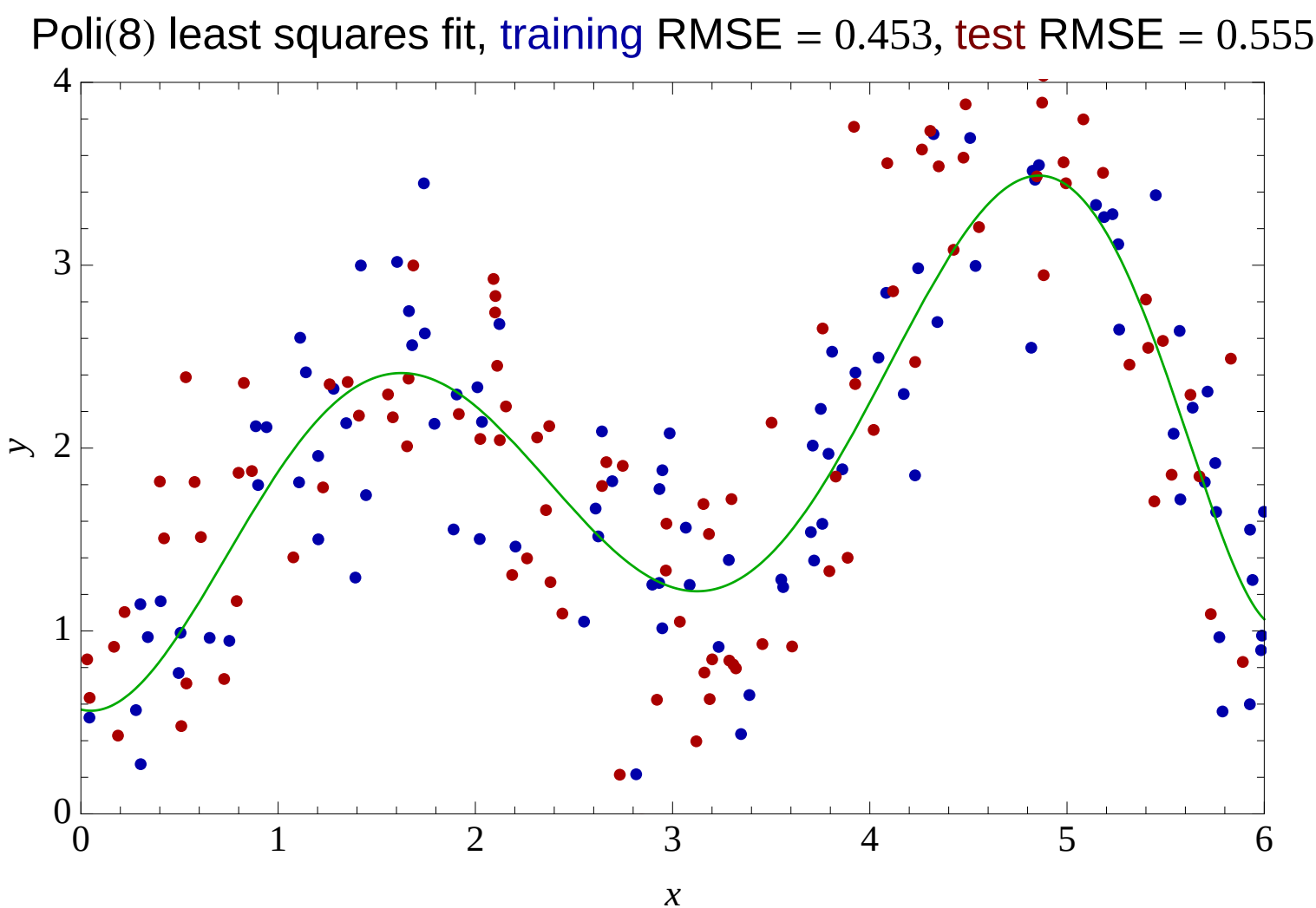

Poli(6) least squares fit, training RMSE = 0.278, test RMSE = 0.72
y
x
0
1
2
3
4
5
6

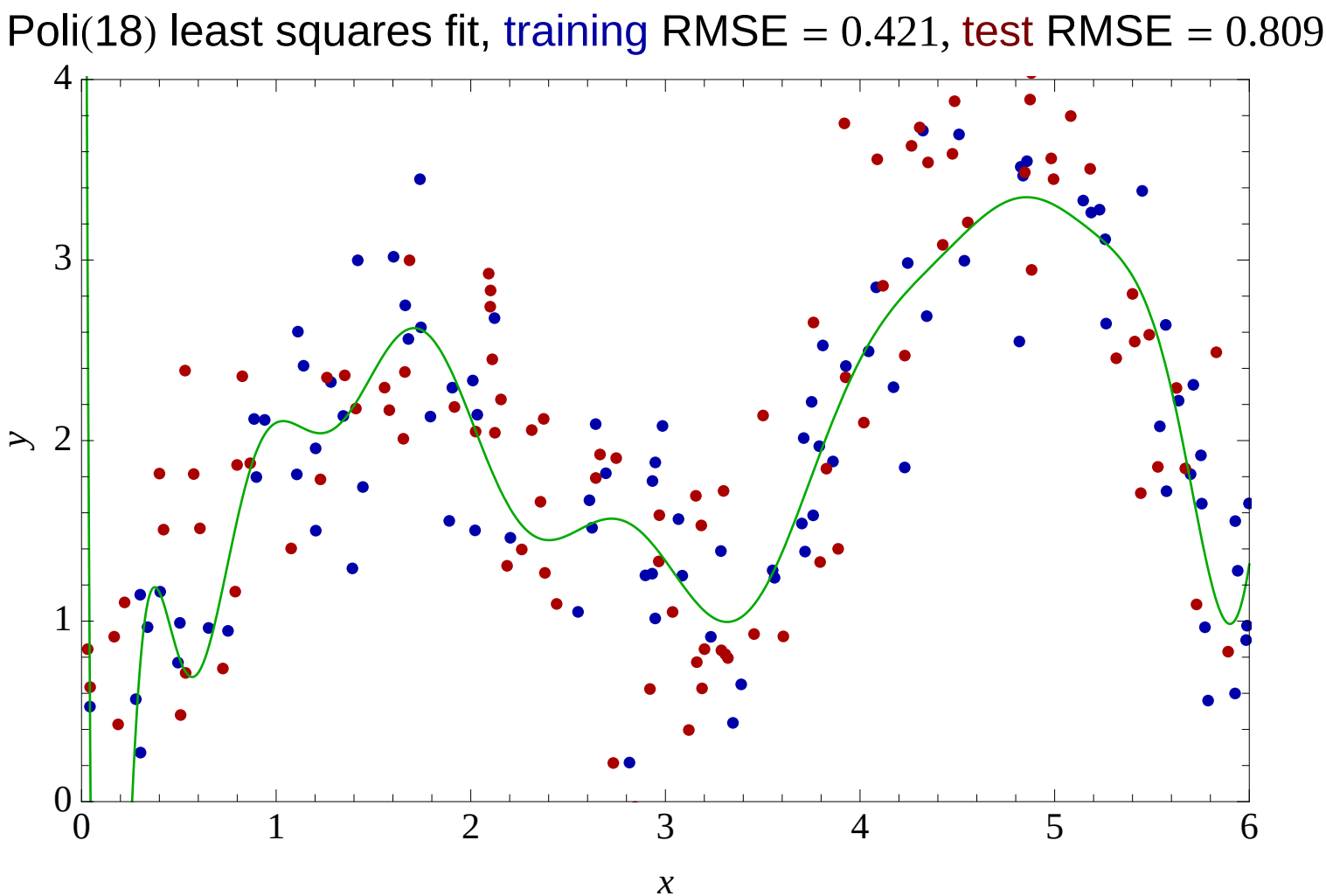

Poli(9) least squares fit, training RMSE = 0, test RMSE = 46.424
y
x
0
1
2
3
4
5
6

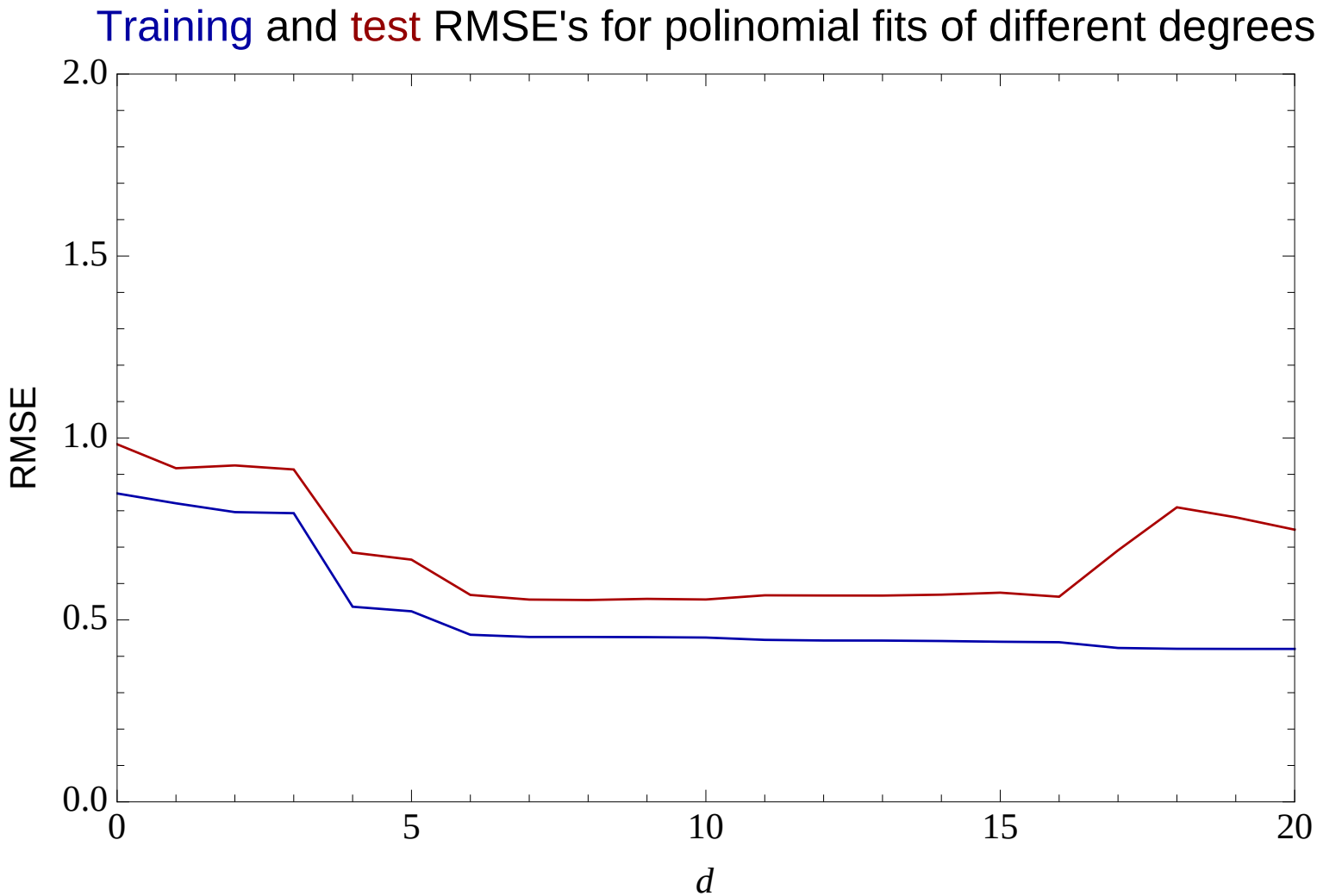

Training and test RMSE's for polinomial fits of different degrees
RMSE
2.0
1.5
1.0
0.5
0.0
0
2
4
6
8
10
d


Data generated from an unknown function with unknown noise
y
x
0
1
2
3
4
5
6


Cubic least squares fit, training RMSE = 0.793, test RMSE = 0.913
y
x
0
1
2
3
4
5
6

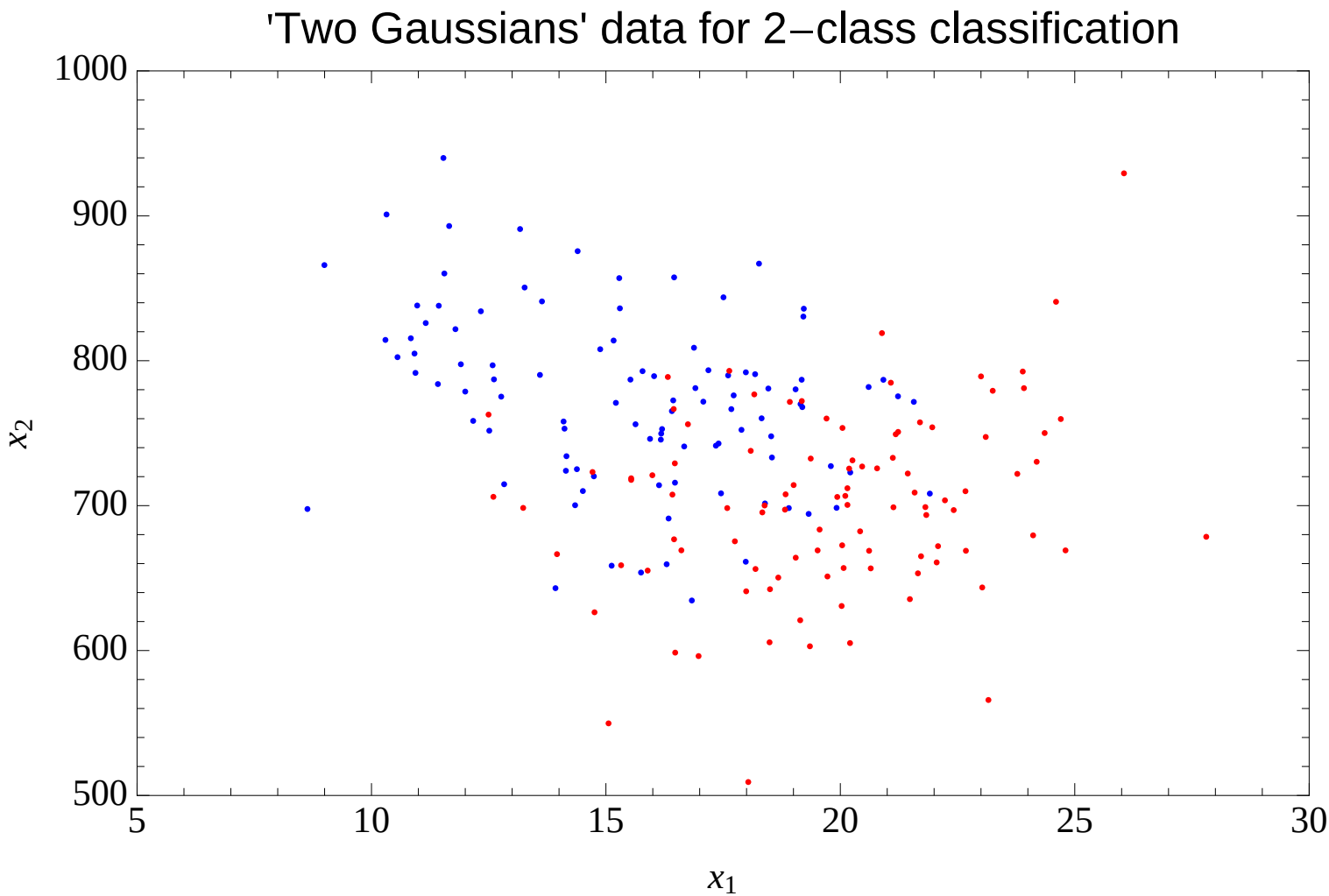

Poli(8) least squares fit, training RMSE = 0.453, test RMSE = 0.555
y
x
0
1
2
3
4
5
6

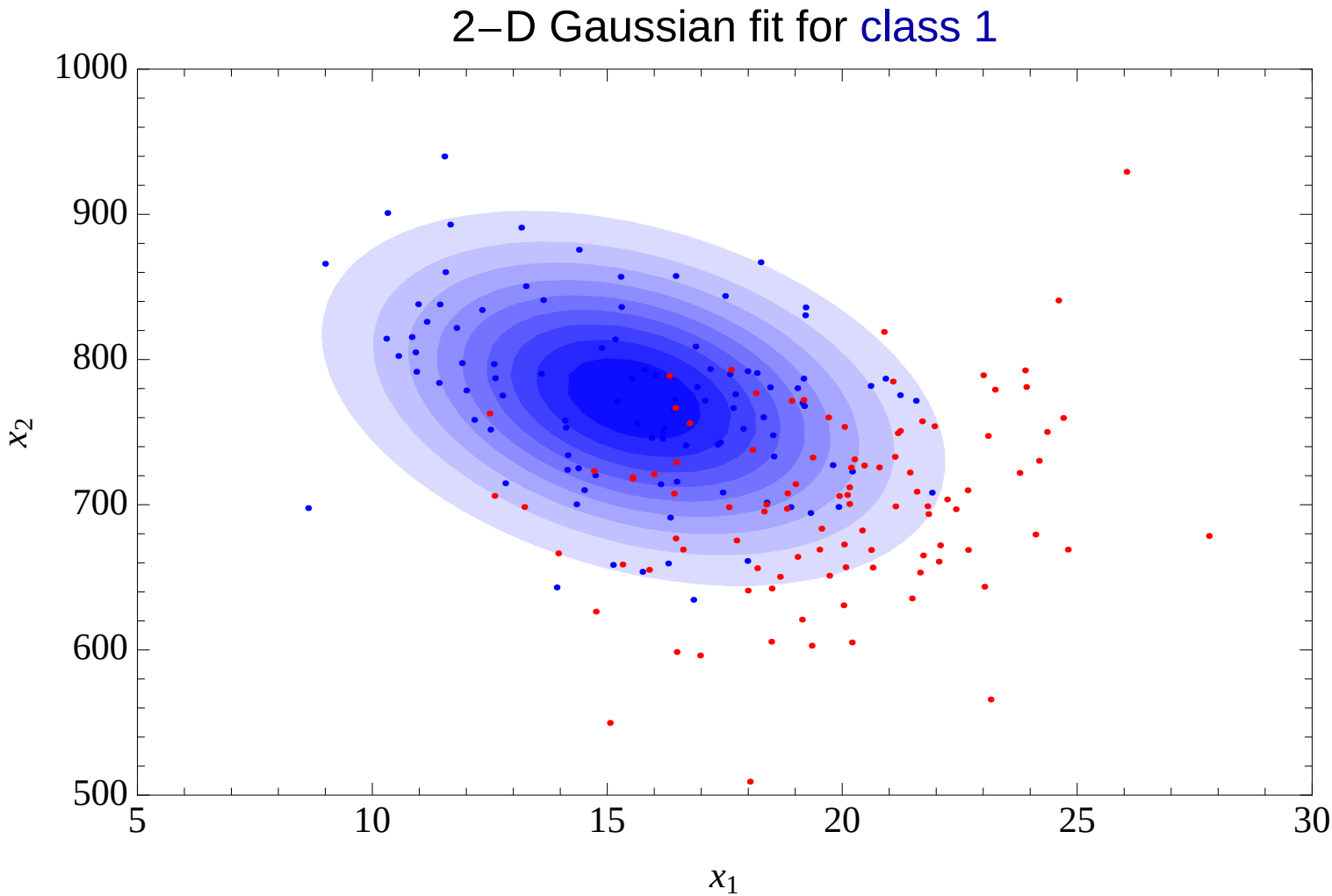

Poli(18) least squares fit, training RMSE = 0.421, test RMSE = 0.809
y
x
0
1
2
3
4
5
6

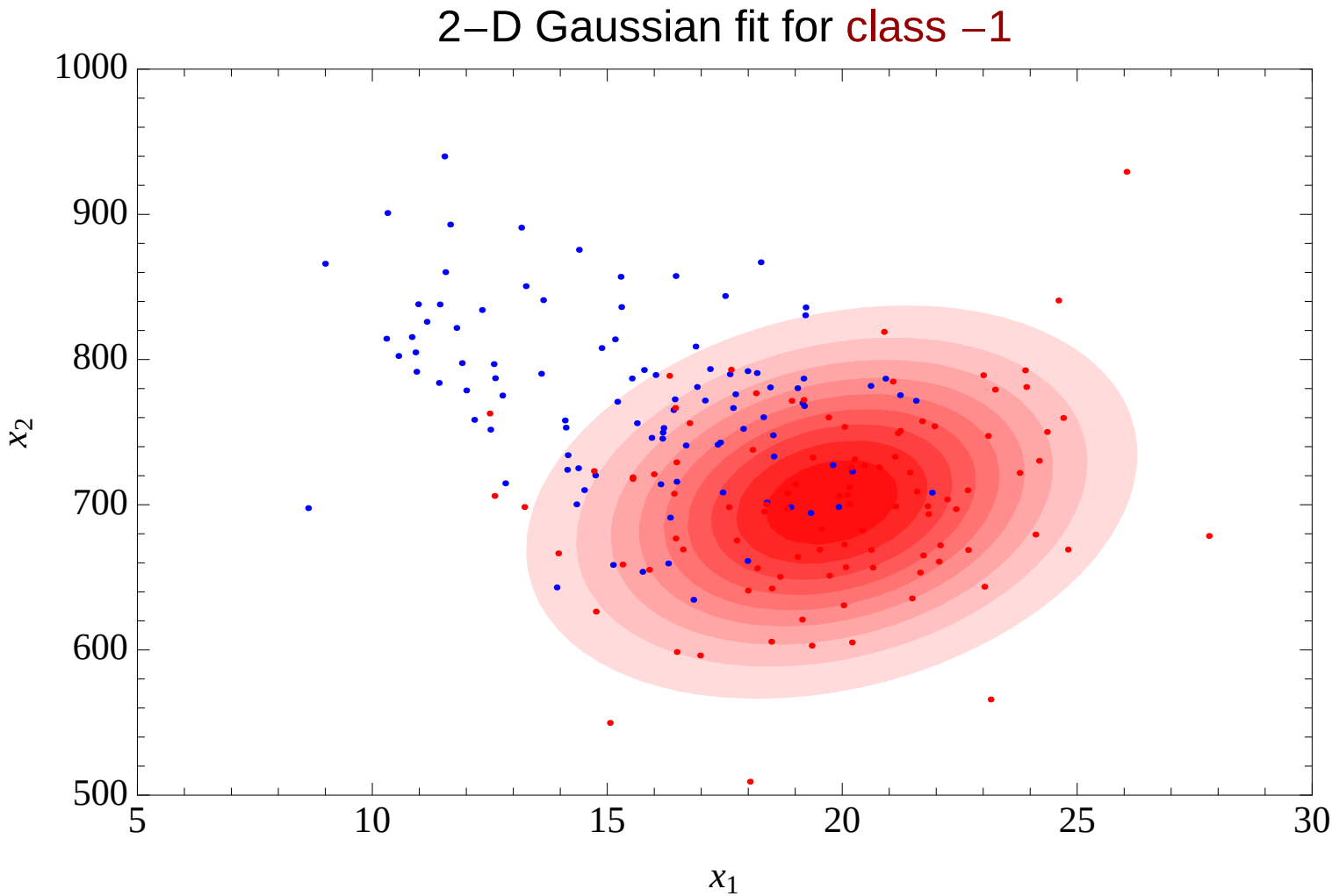

Training and test RMSE's for polinomial fits of different degrees
RMSE
2.0
1.5
1.0
0.5
0.0
0
5
10
15
20
d

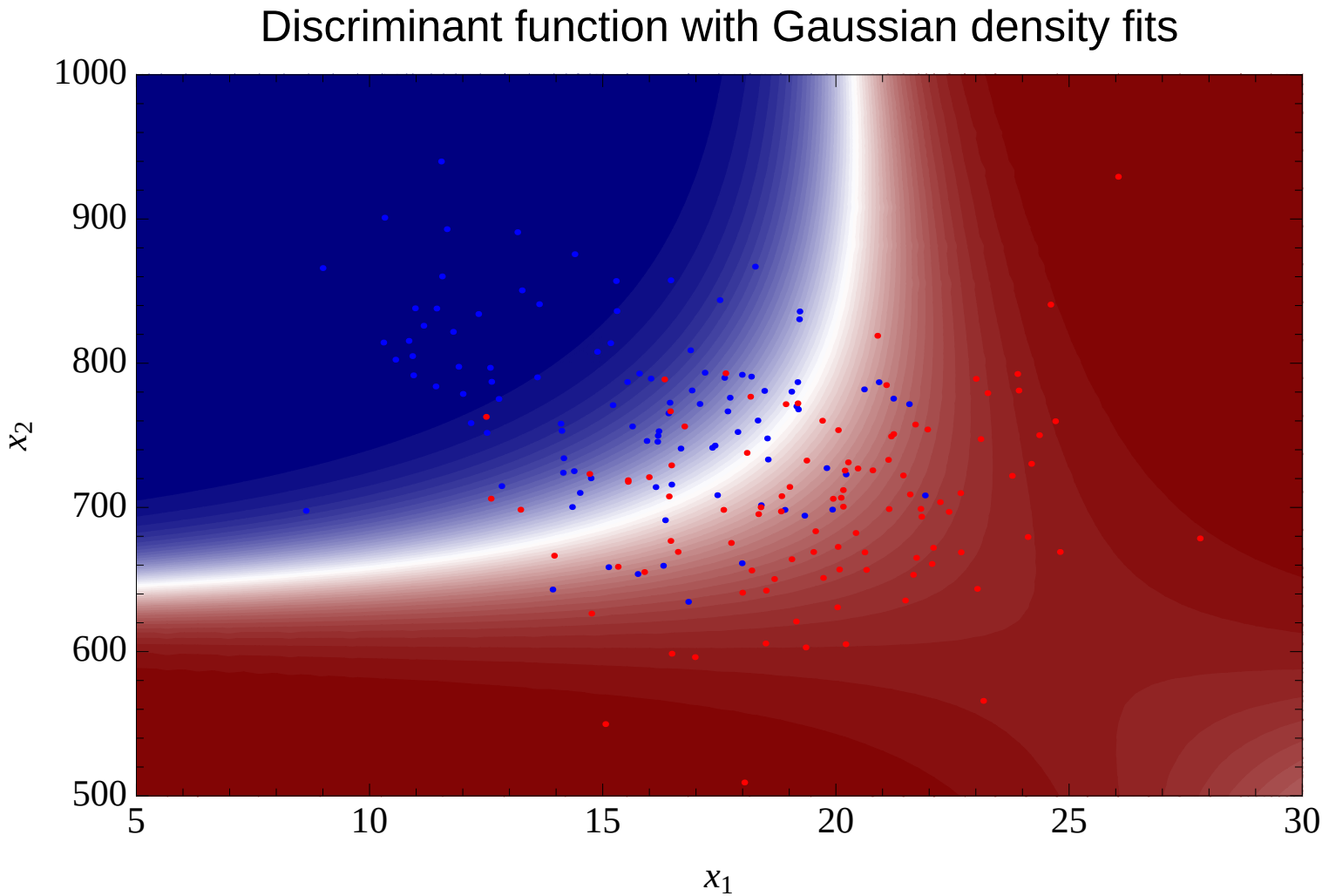
Non-parametric fitting

- Capacity control, regularization
  - trade-off between approximation error and estimation error
  - complexity grows with data size
  - no need to correctly guess the function class


'Two Gaussians' data for 2−class classification
1000
900
800
700
600
500
5
10
15
20
25
30
x_2
x_1


2−D Gaussian fit for class 1
1000
900
800
700
600
500
5
10
15
20
25
30
x_2
x_1


2−D Gaussian fit for class −1
1000
900
800
700
600
500
5
10
15
20
25
30
x_2
x_1


Discriminant function with Gaussian density fits
1000
900
800
700
600
500
x_2
5
10
15
20
25
30
x_1

Outline

- Non-parametric fitting: two simple examples
- The formal model for classification, learning principles
- Classification algorithms (from a user's point of view)
  - perceptron, neural networks (NN)
  - AdaBoost
  - the Support Vector Machine (SVM)
- Machine learning research motivated by HEP applications

Classification

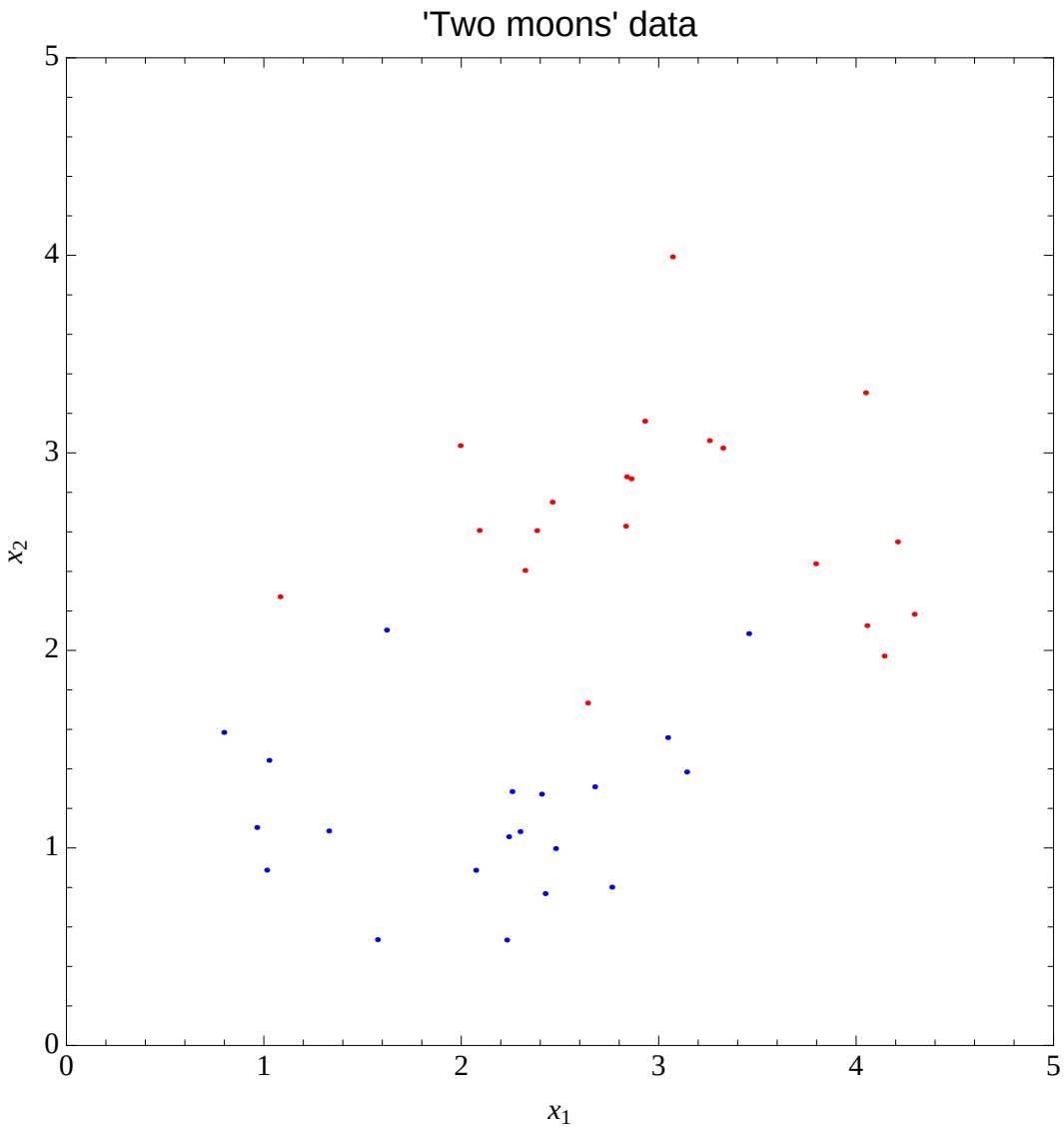
- Terminology
  - Conditional densities: $p(\mathbf{x} \mid Y = 1)$, $p(\mathbf{x} \mid Y = -1)$
  - Prior probabilities: $P(Y = 1)$, $P(Y = -1)$
  - Posterior probabilities: $P(Y = 1 \mid \mathbf{x})$, $P(Y = -1 \mid \mathbf{x})$

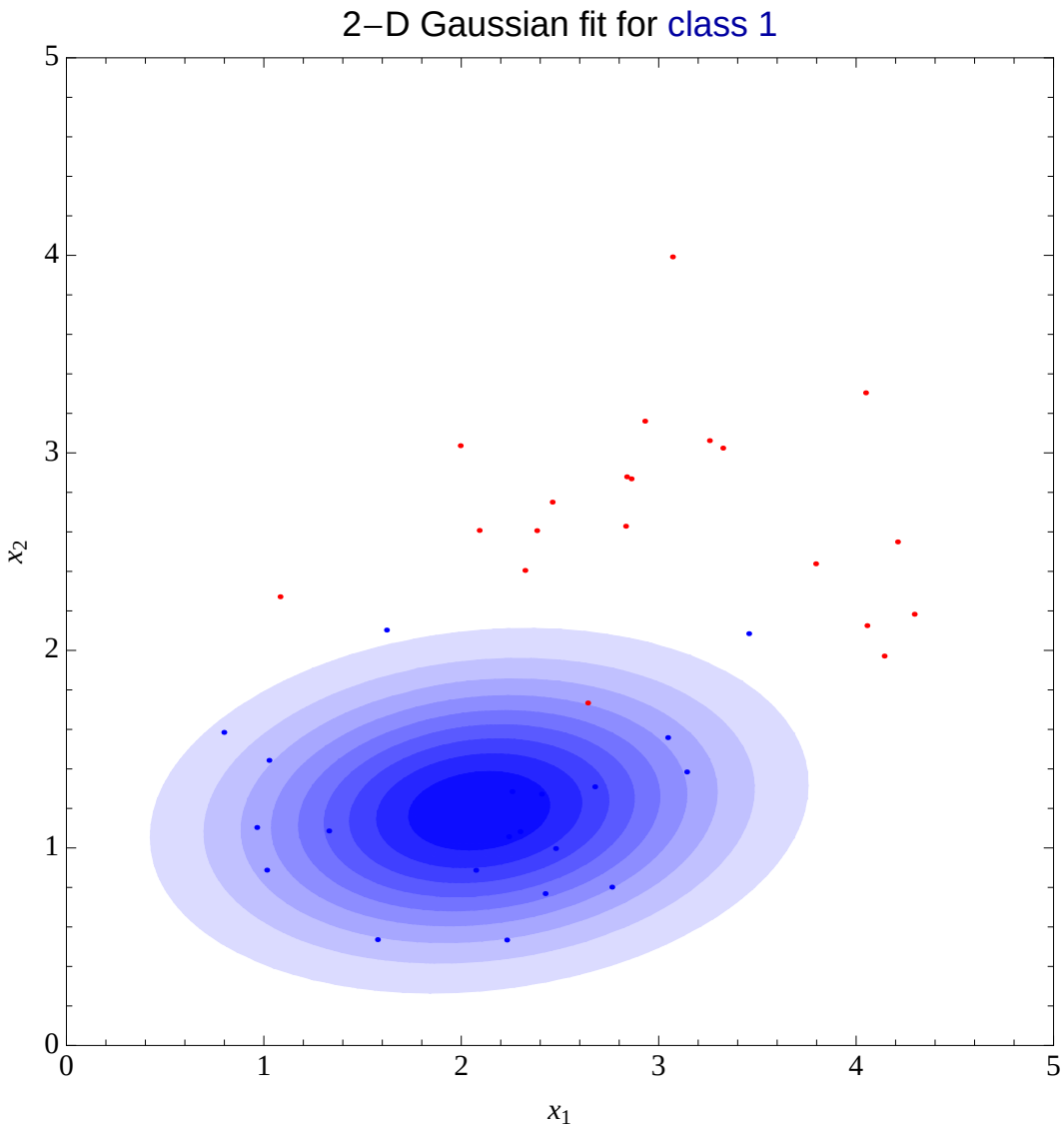
- Bayes theorem:

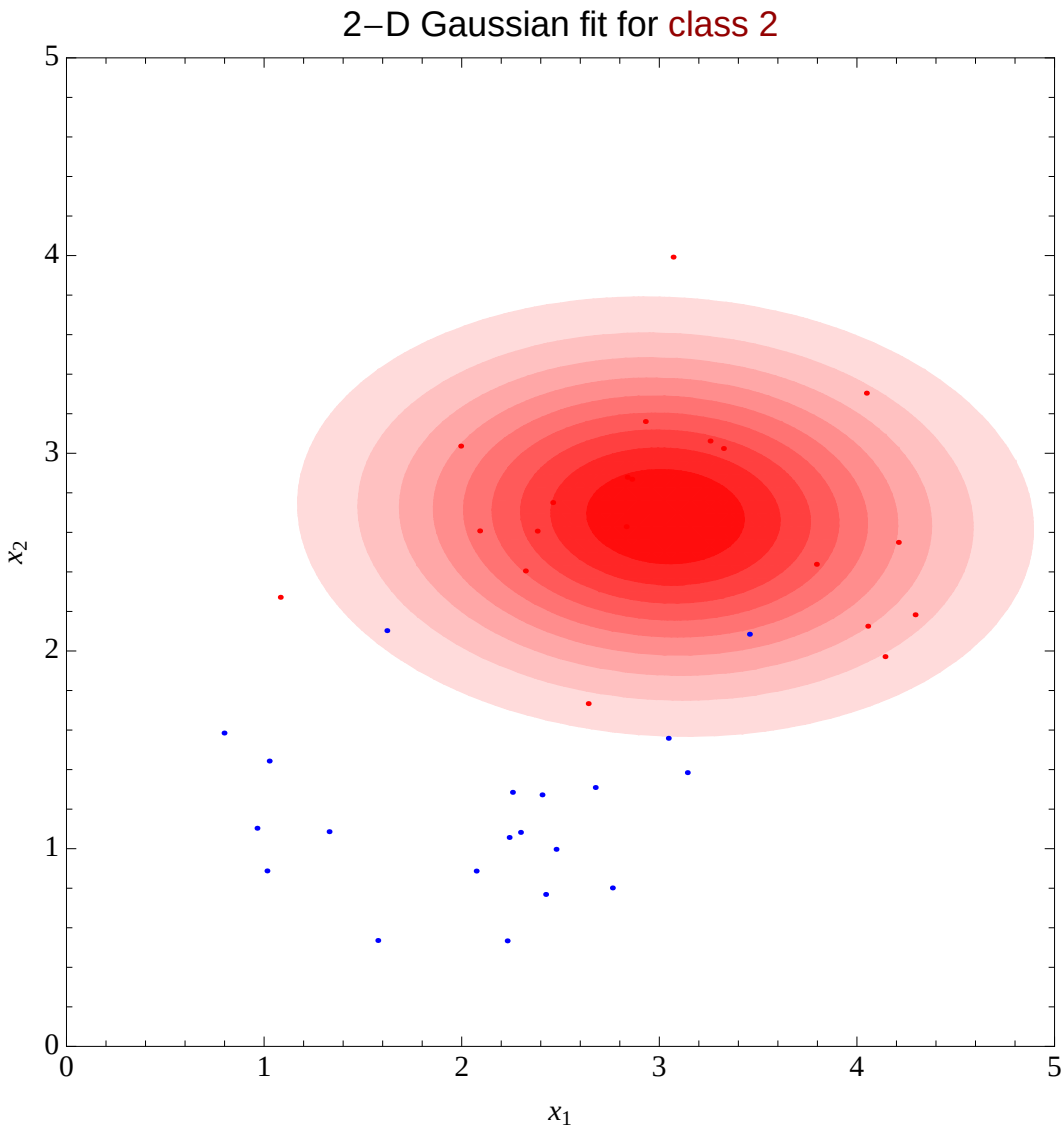
$$P(Y = 1 \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid Y = 1)P(Y = 1)}{p(\mathbf{x})} \propto p(\mathbf{x} \mid Y = 1)P(Y = 1)$$

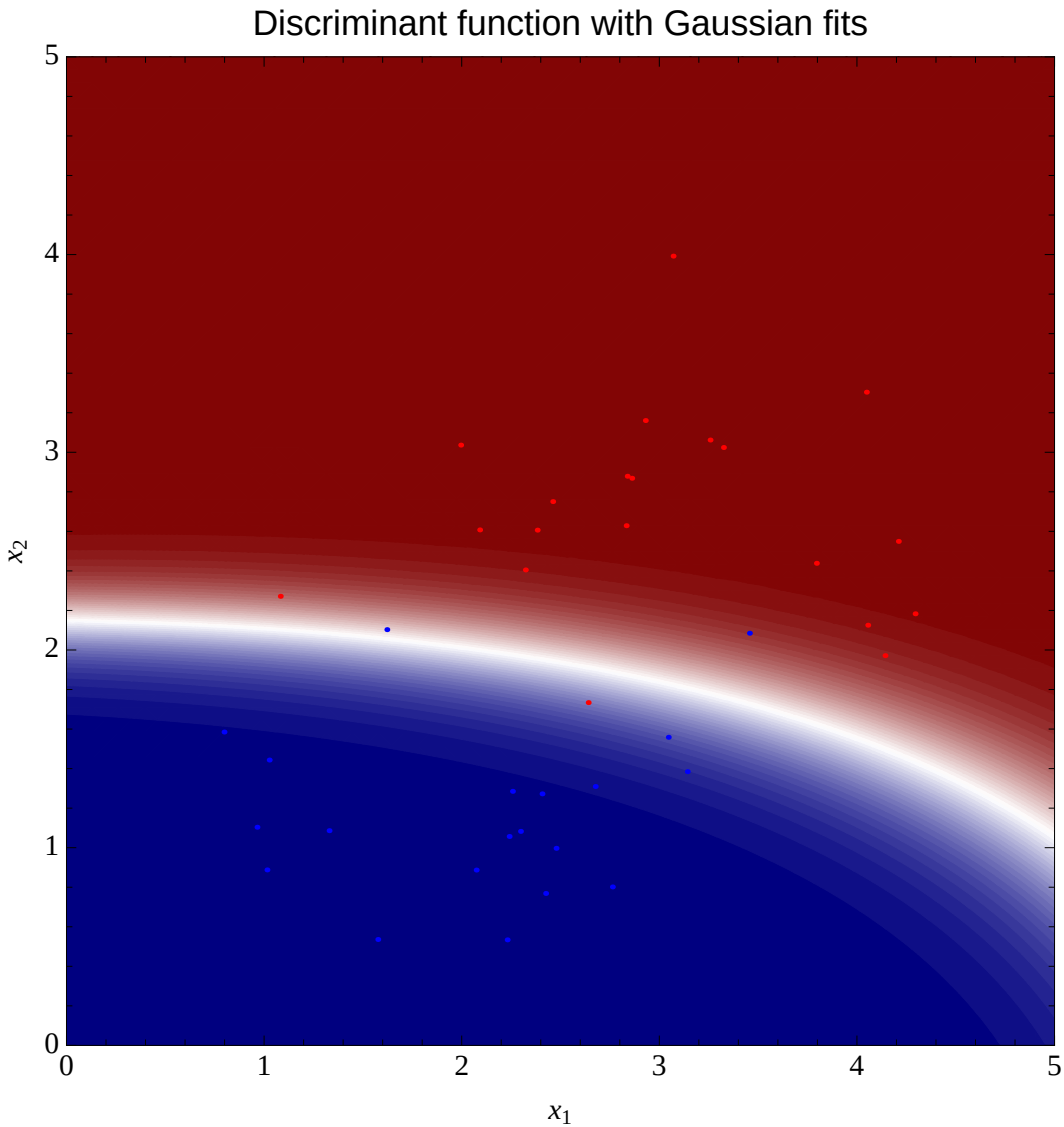
  - Decision:

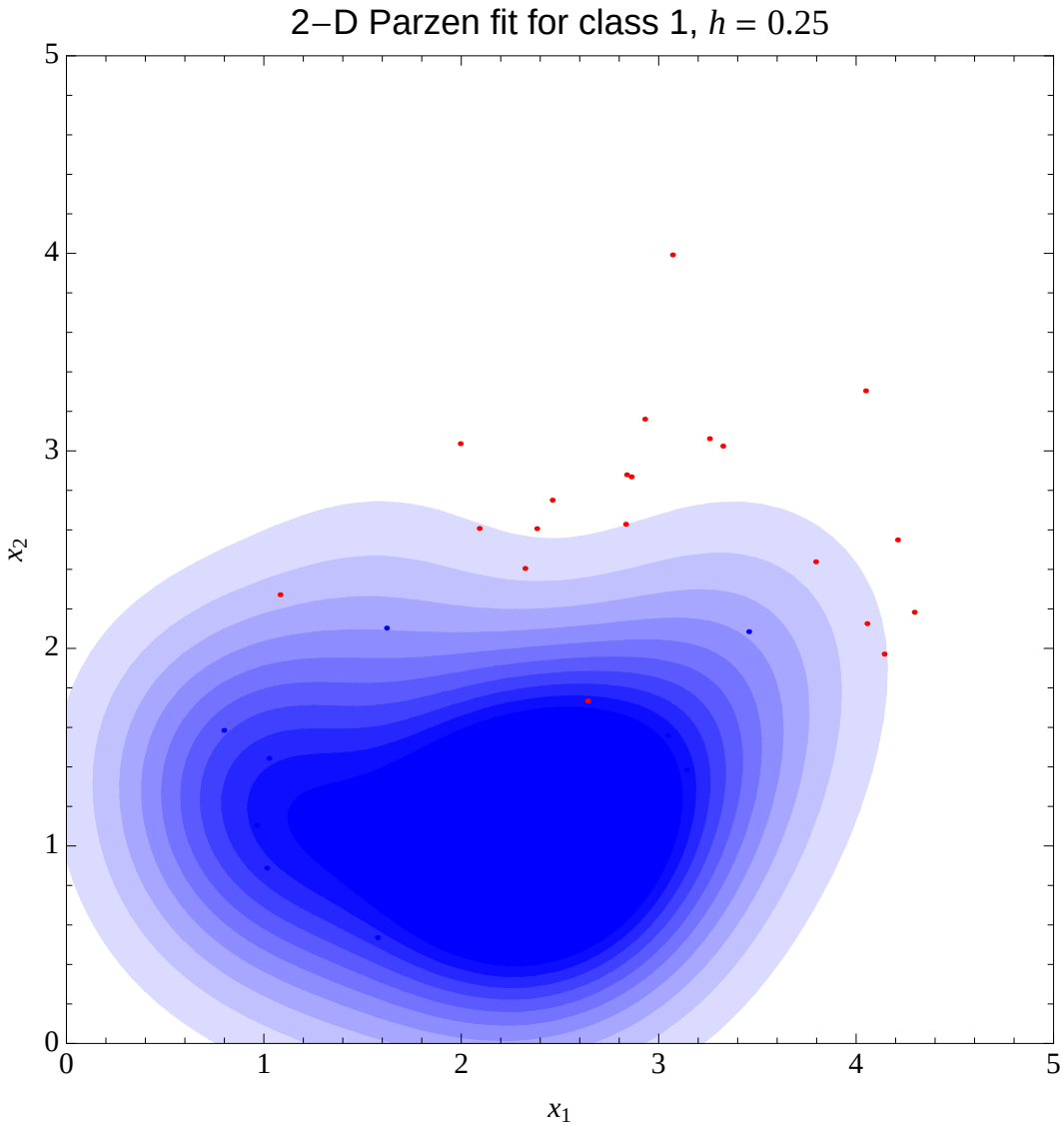
$$g(\mathbf{x}) = \begin{cases} 1 & \text{if } \frac{p(\mathbf{x}|Y=1)P(Y=1)}{p(\mathbf{x}|Y=-1)P(Y=-1)} > 1, \\ -1 & \text{otherwise.} \end{cases}$$

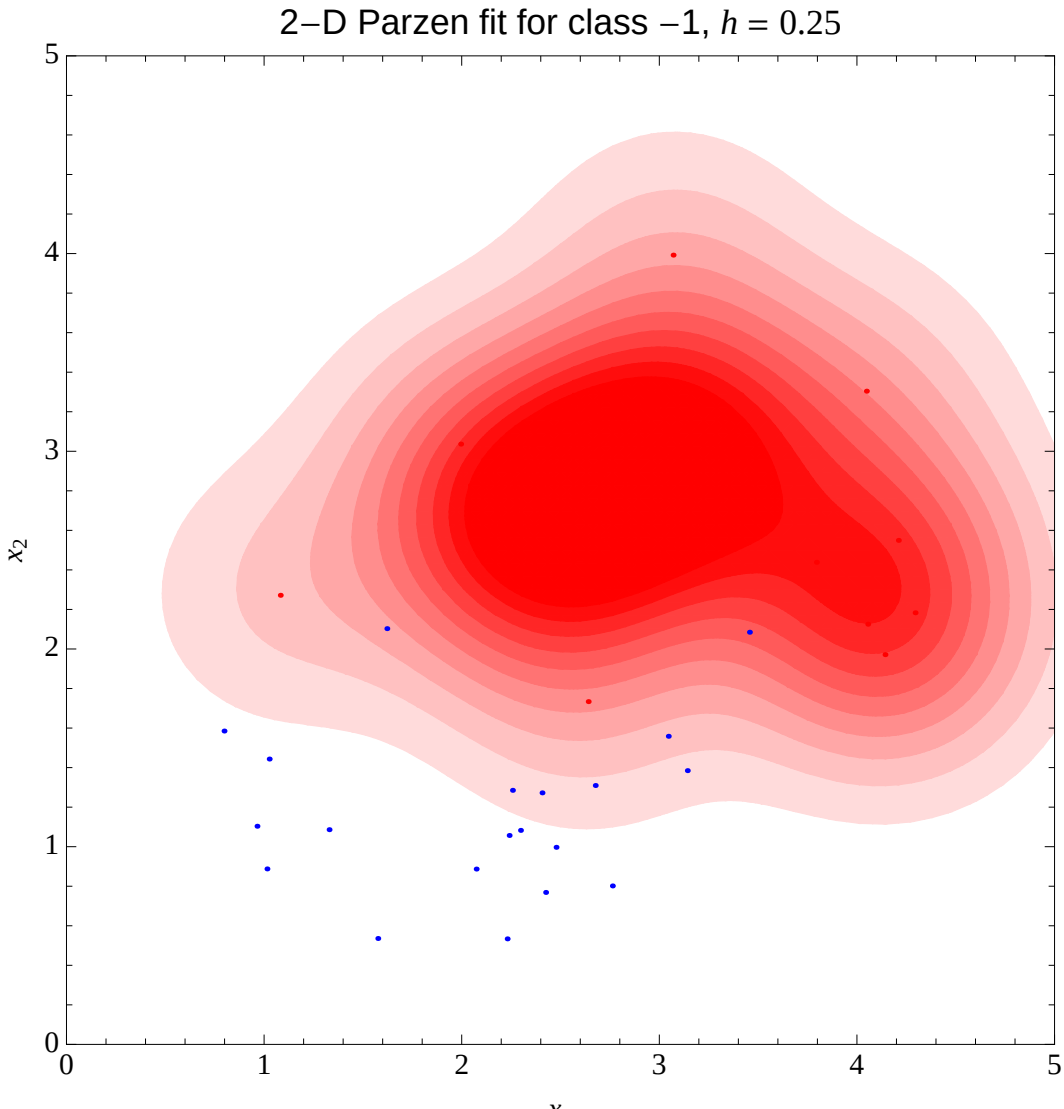

'Two moons' data
x_1
x_2
0
1
2
3
4
5

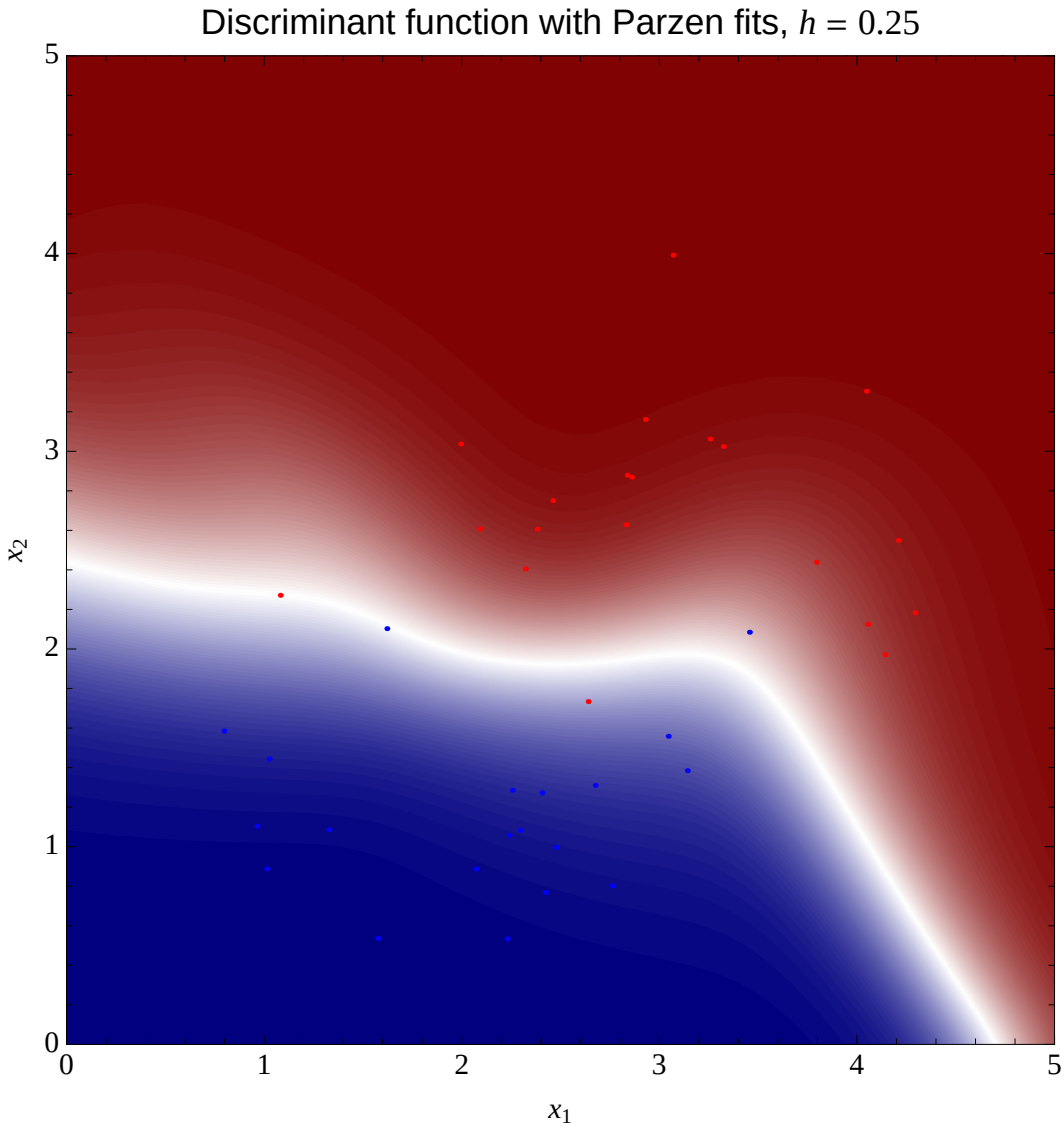

2−D Gaussian fit for class 1
x_1
x_2
0
1
2
3
4
5

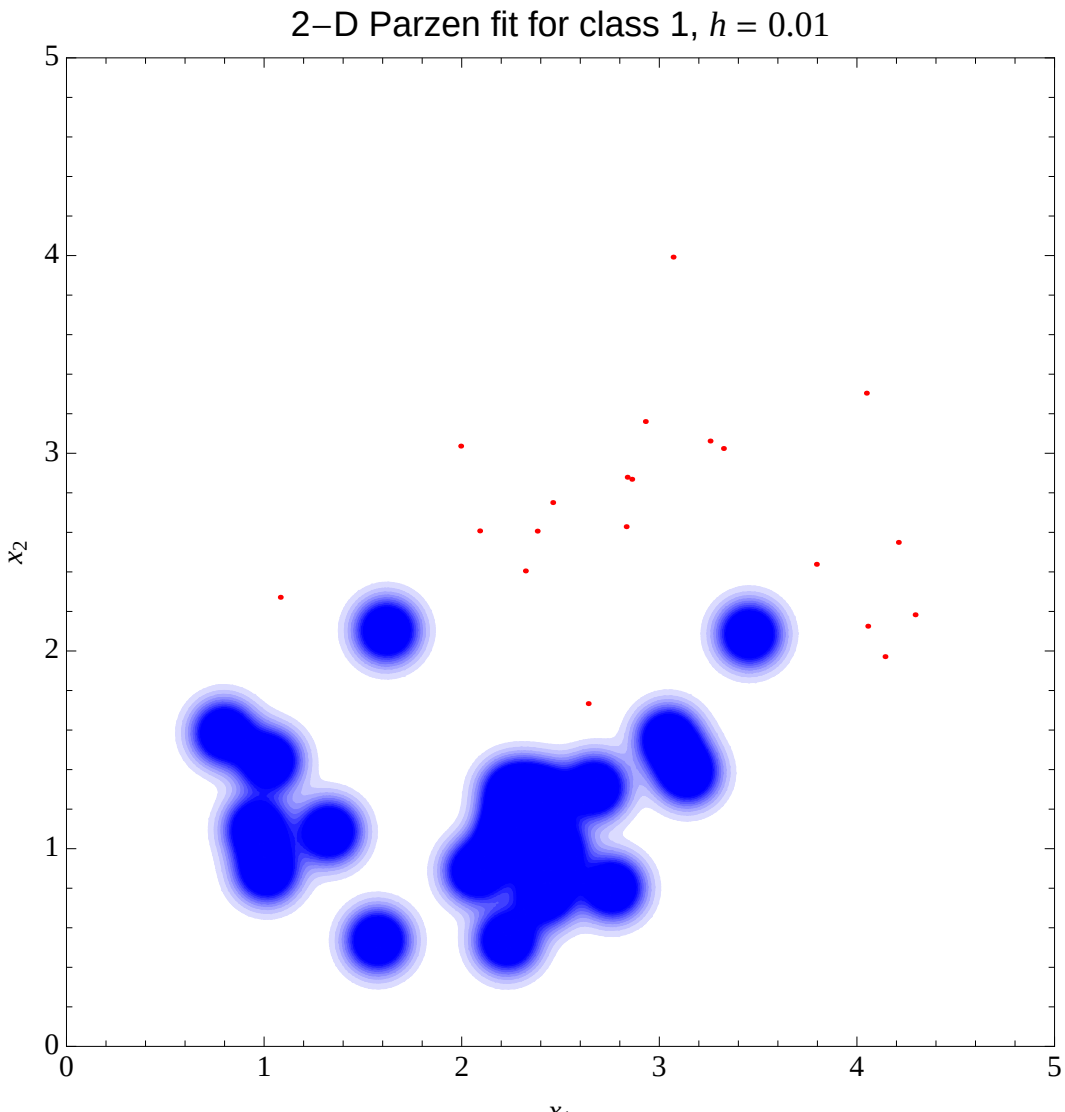

2−D Gaussian fit for class 2
0
1
2
3
4
5
x_1
x_2

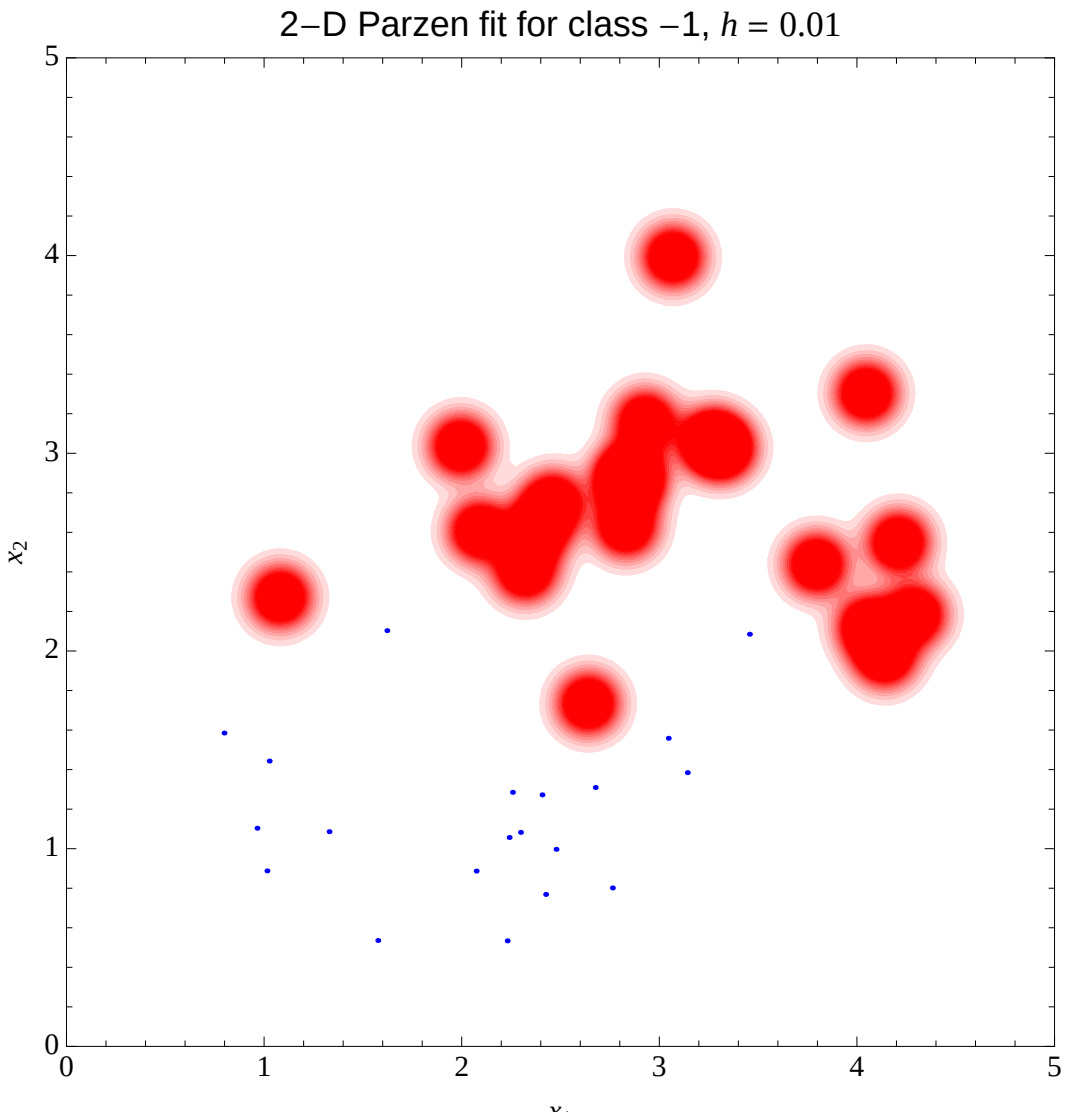

Discriminant function with Gaussian fits
5
4
3
2
1
0
0
1
2
3
4
5
x_2
x_1

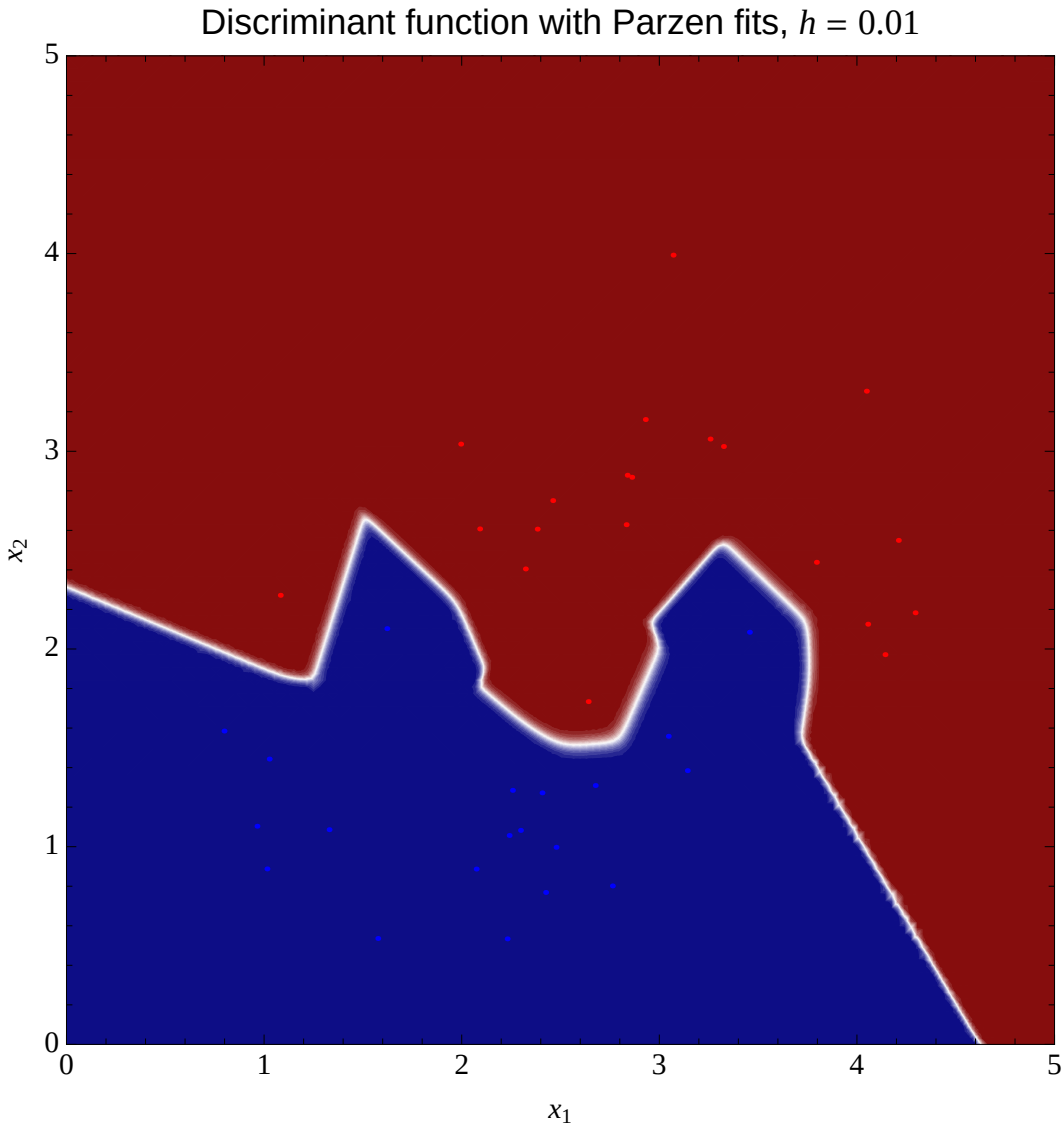

2−D Parzen fit for class 1, $h = 0.25$
x_1
x_2
0
1
2
3
4
5

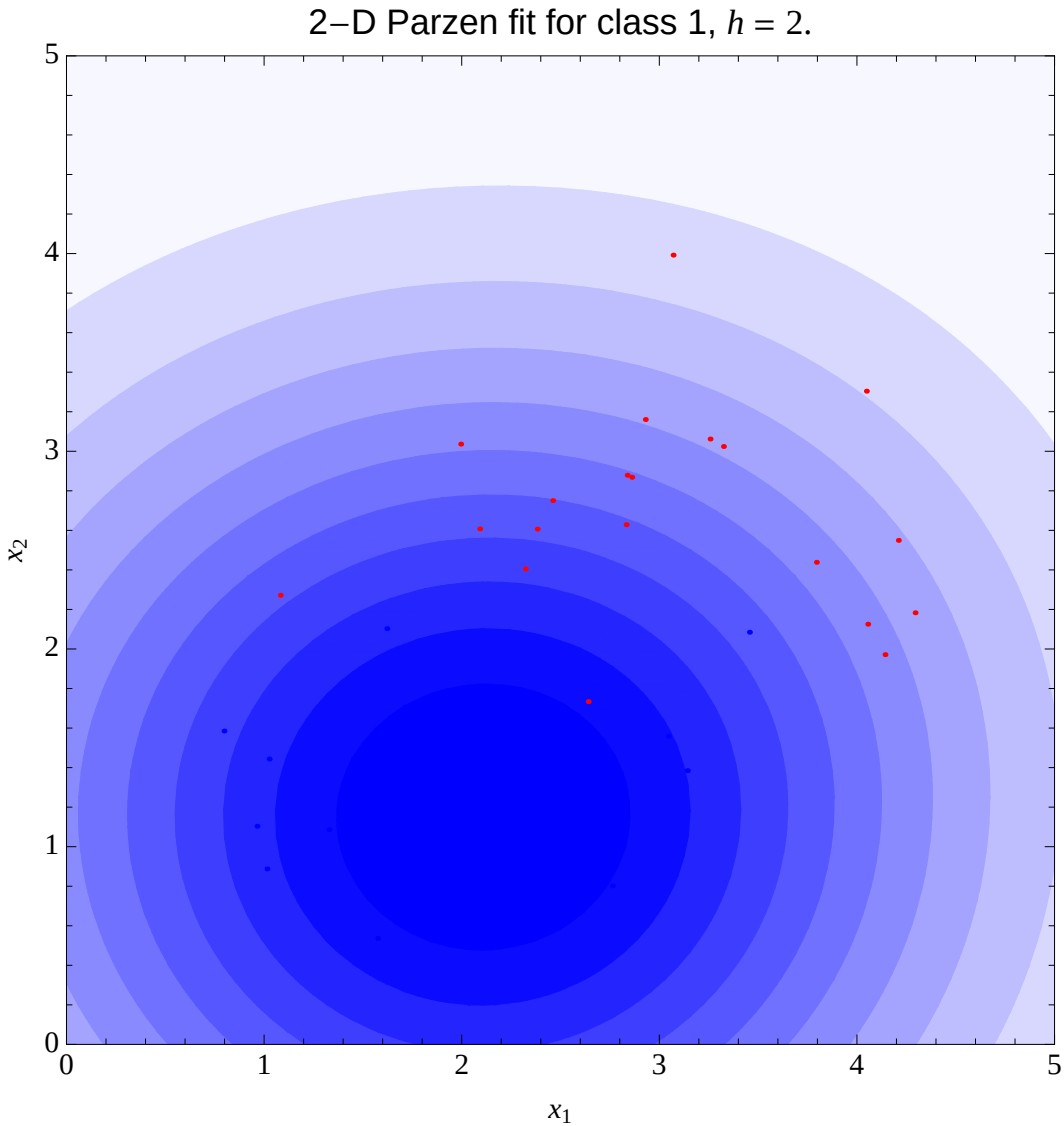

2−D Parzen fit for class −1, $h = 0.25$
x_1
x_2
0
1
2
3
4
5

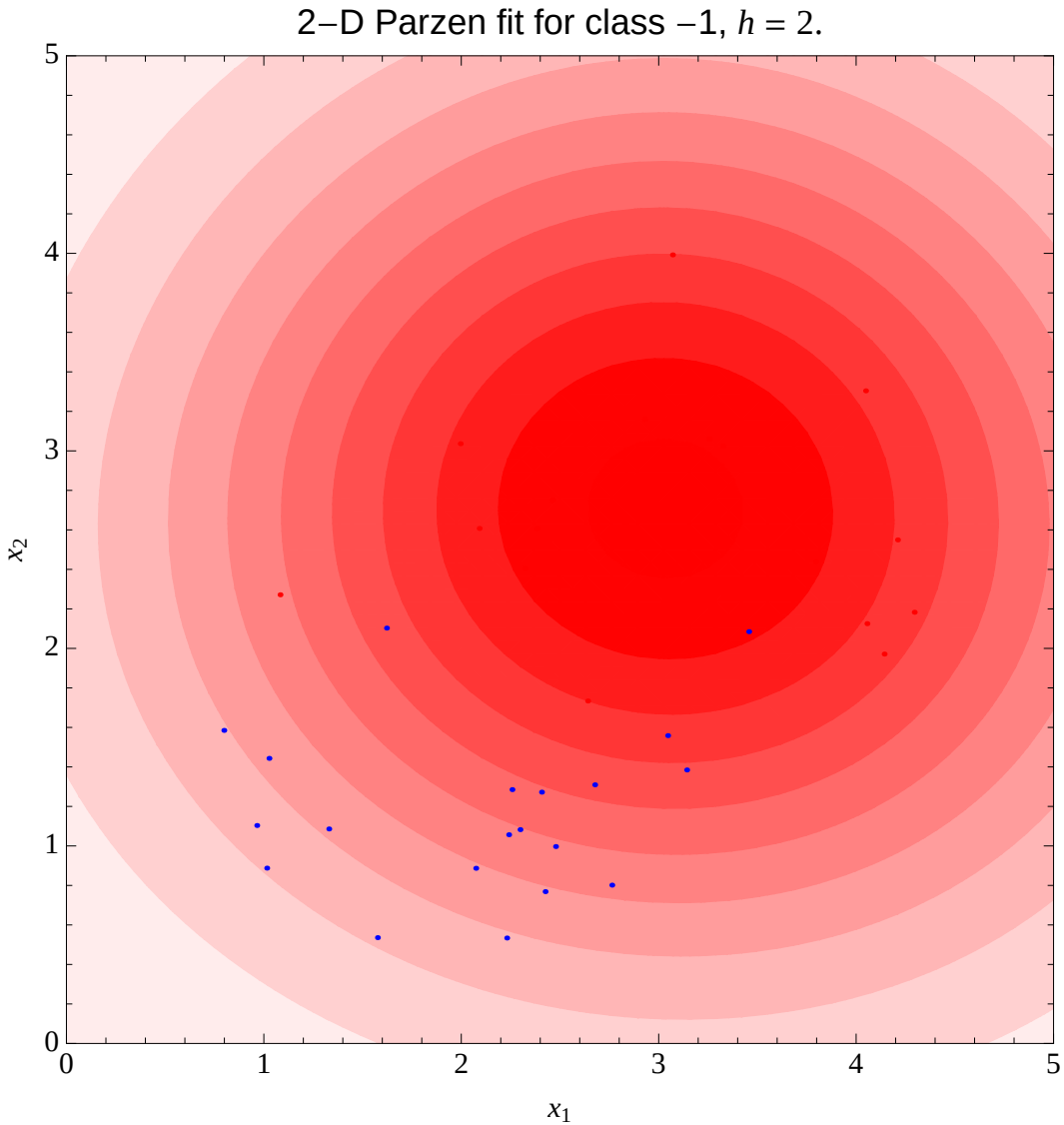

Discriminant function with Parzen fits, $h = 0.25$
x_2
x_1
0
1
2
3
4
5

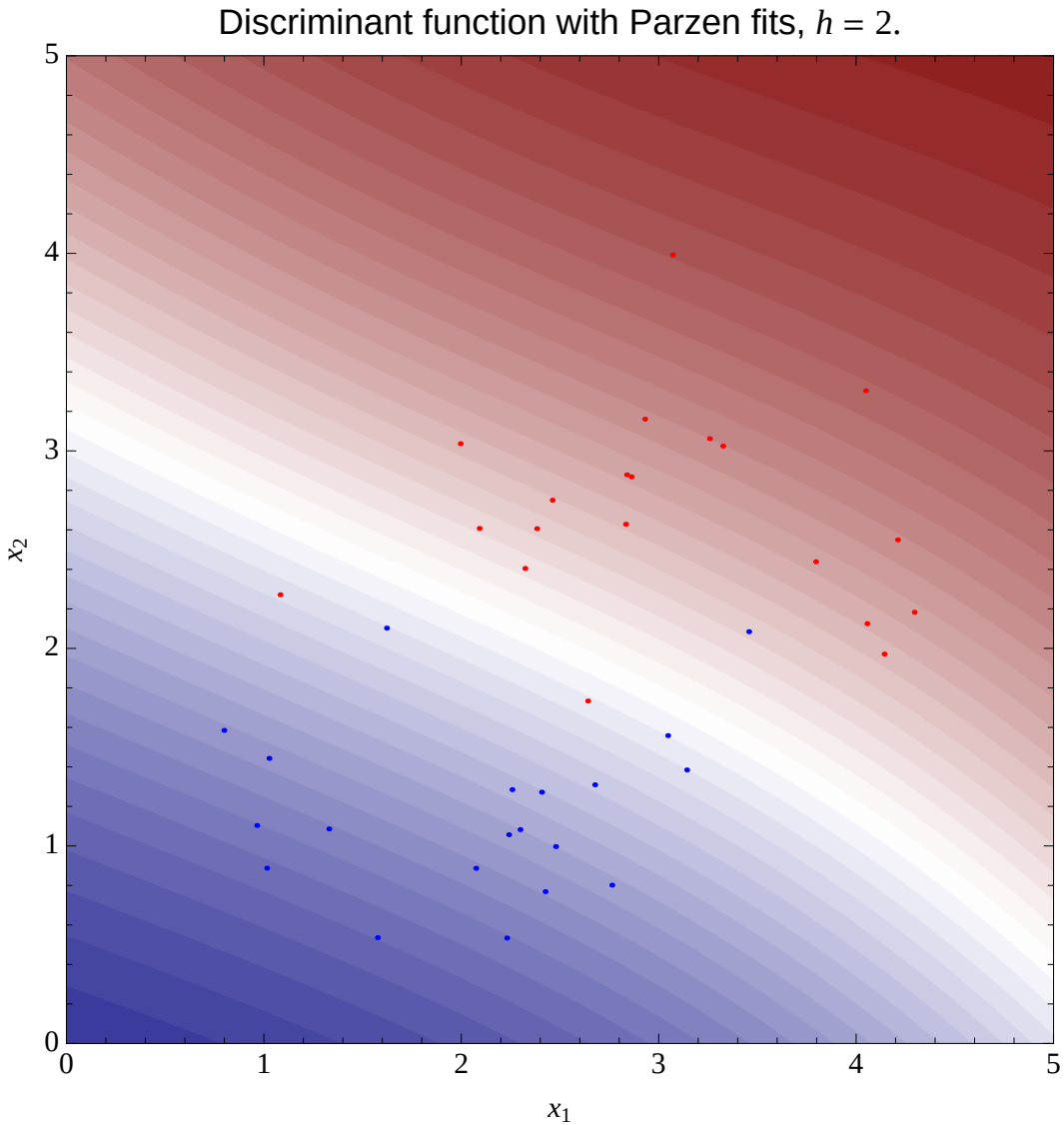

2−D Parzen fit for class 1, $h = 0.01$
x_1
x_2
0
1
2
3
4
5


2−D Parzen fit for class −1, $h = 0.01$
x_1
x_2
0
1
2
3
4
5

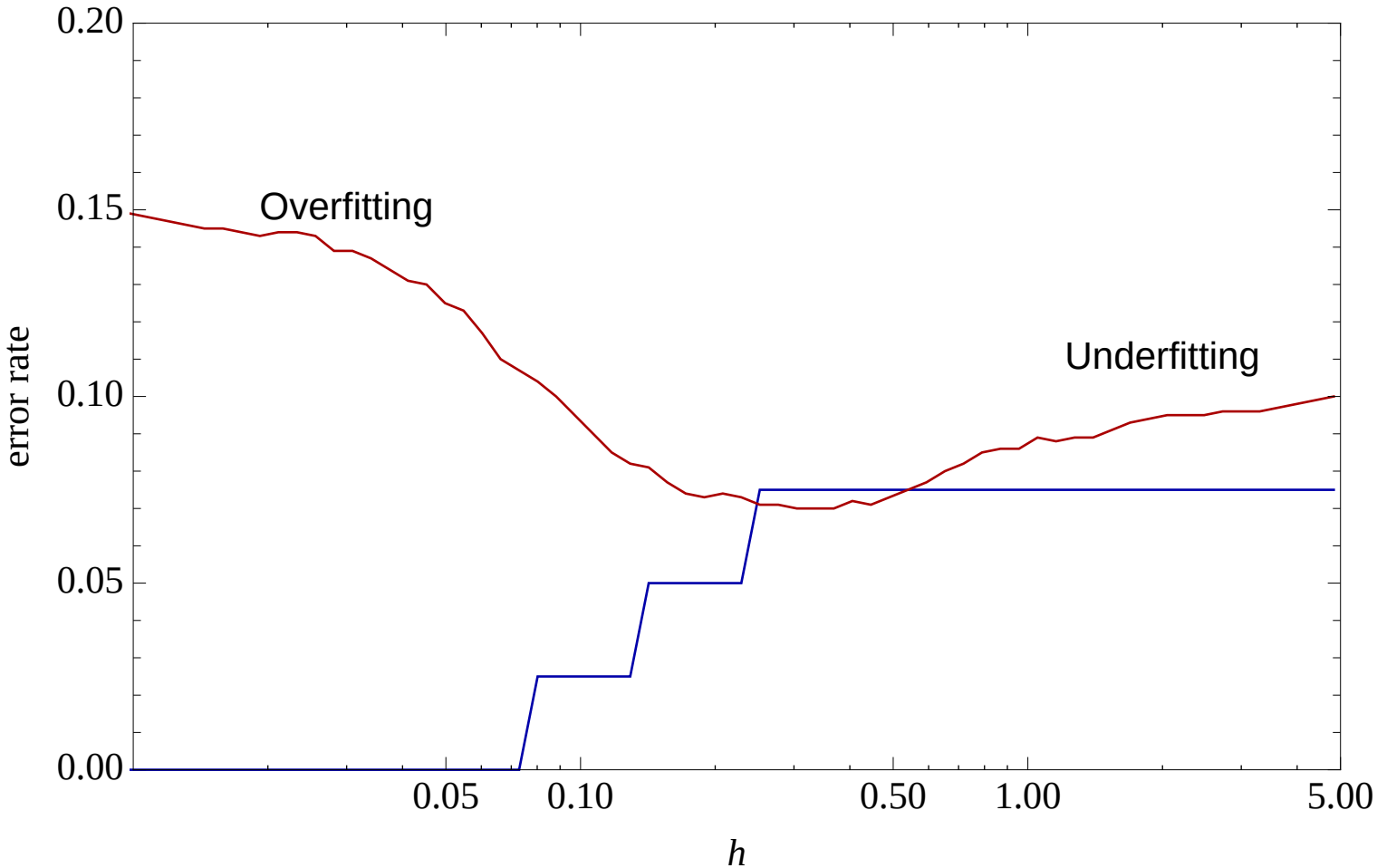

Discriminant function with Parzen fits, $h = 0.01$
x_2
x_1
0
1
2
3
4
5


2−D Parzen fit for class 1, $h = 2$.
x_1
x_2
0
1
2
3
4
5


2−D Parzen fit for class −1, $h = 2$.
x_1
x_2
0
1
2
3
4
5


Discriminant function with Parzen fits, $h = 2$.
x_2
x_1
0
1
2
3
4
5

Training and test error rates



Curse of dimensionality

- Capacity/complexity control becomes a real issue in high-dimensional spaces
  - in a 10000-dimensional space a linear function has 10000 parameters!
  - we need a lot of training points to "fill" the space
- Examples
  - images, music, language, text, bioinfo (genetics, proteomics)
- We prefer to learn the discriminant function directly, without going through the density estimation step

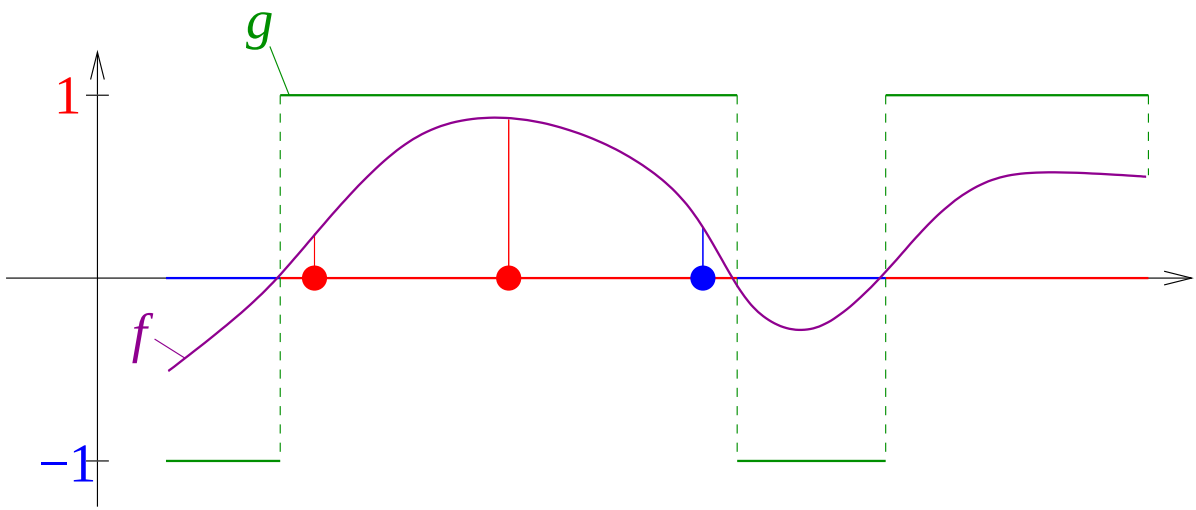
The classification model

- Observation vector: $\mathbf{x} \in \mathbb{R}^d$
- Class label: $y \in \{-1, 1\}$ (or $y \in \{1, \ldots, K\}$)
- Classifier: $g : \mathbb{R}^d \to \{-1, 1\}$
- Discriminant function: $f : \mathbb{R}^d \to [-1, 1]$
  - $\longrightarrow$ classifier

$$g(\mathbf{x}) = \begin{cases} 1, & \text{if } f(\mathbf{x}) \geq 0, \\ -1, & \text{if } f(\mathbf{x}) < 0 \end{cases}$$

  - decision boundary: $\{\mathbf{x} : f(\mathbf{x}) = 0\}$

The classification model



- Discriminant function: $f : \mathbb{R}^d \to [-1, 1]$
- $\longrightarrow$ classifier

$$g(\mathbf{x}) = \begin{cases} 1, & \text{if } f(\mathbf{x}) \geq 0, \\ -1, & \text{if } f(\mathbf{x}) < 0 \end{cases}$$

- decision boundary: $\{\mathbf{x} : f(\mathbf{x}) = 0\}$

The classification model

- Learning from data
  - training set : $D_n = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$
  - function class : $\mathcal{F}$
  - learning algorithm : $\text{ALGO} : \left(\mathbb{R}^d \times \{-1, 1\}\right)^n \to \mathcal{F}$

    $$\text{ALGO}(D_n) \mapsto f$$

  - goal: small generalization error $R(g) = P\left[g(\mathbf{X}) \neq Y\right] = P\left[f(\mathbf{X})Y \leq 0\right]$
  - learning principle: minimize the training error

    $$\widehat{R}(g) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\{g(\mathbf{x}_i) \neq y_i\}$$

The classification model

- goal: small generalization error

$$R(g) = P\left[g(\mathbf{X}) \neq Y\right]$$

- Learning principle: minimize the training error

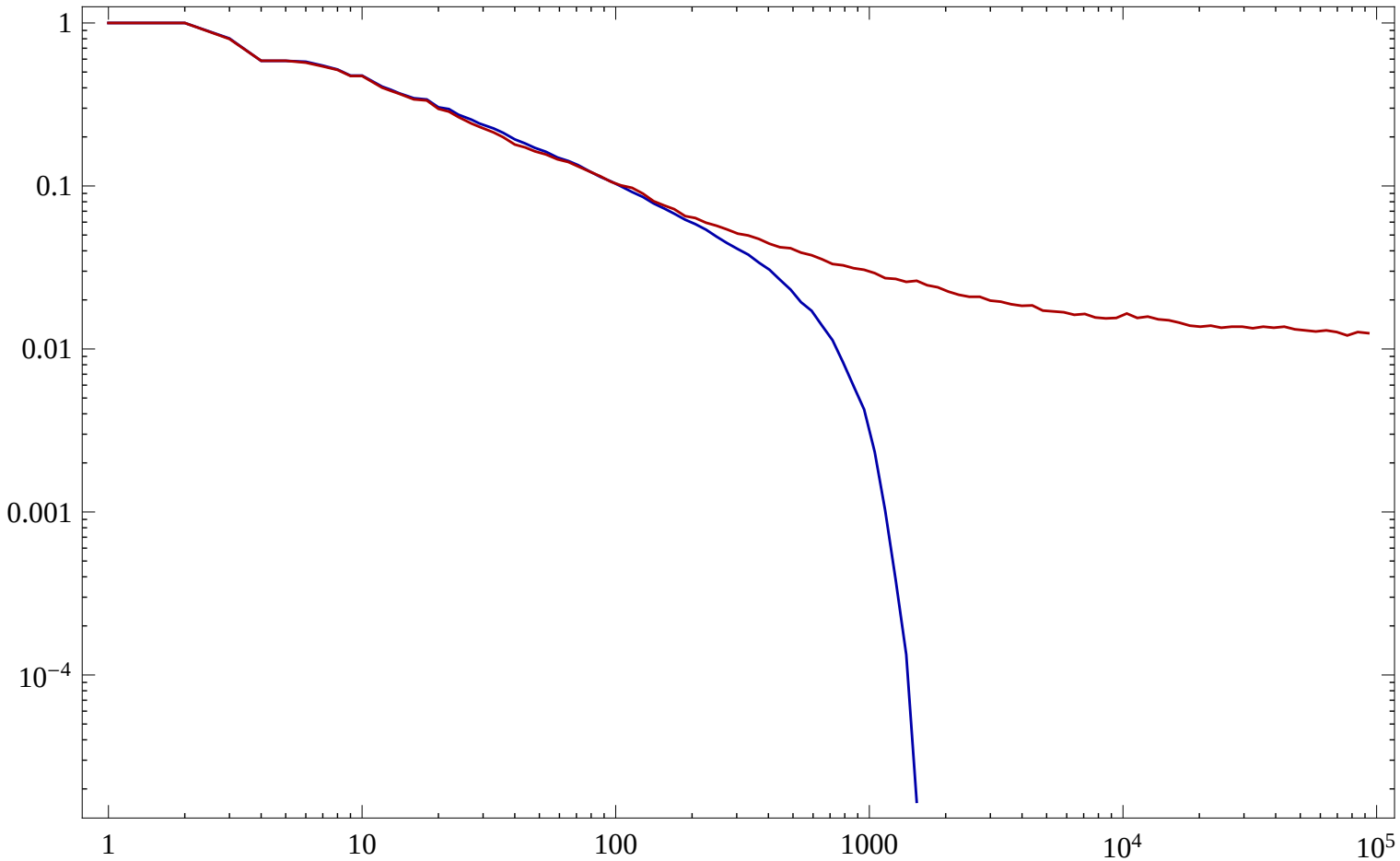
$$\widehat{R}(g) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}\{g(\mathbf{x}_i) \neq y_i\}$$

- Generalization error bounds

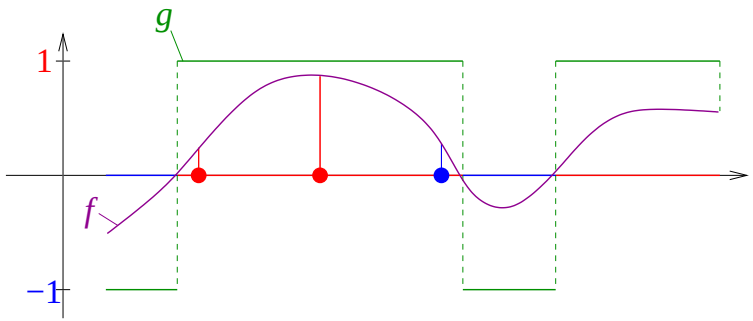
$$\text{“ } R(g) \leq \widehat{R}(g) + O\left(\frac{\dim_{\mathrm{VC}}(\mathcal{F})\log n}{n}\right) \text{ ”}$$

The classification model

AdaBoost on MNIST: training and test error rates



The classification model

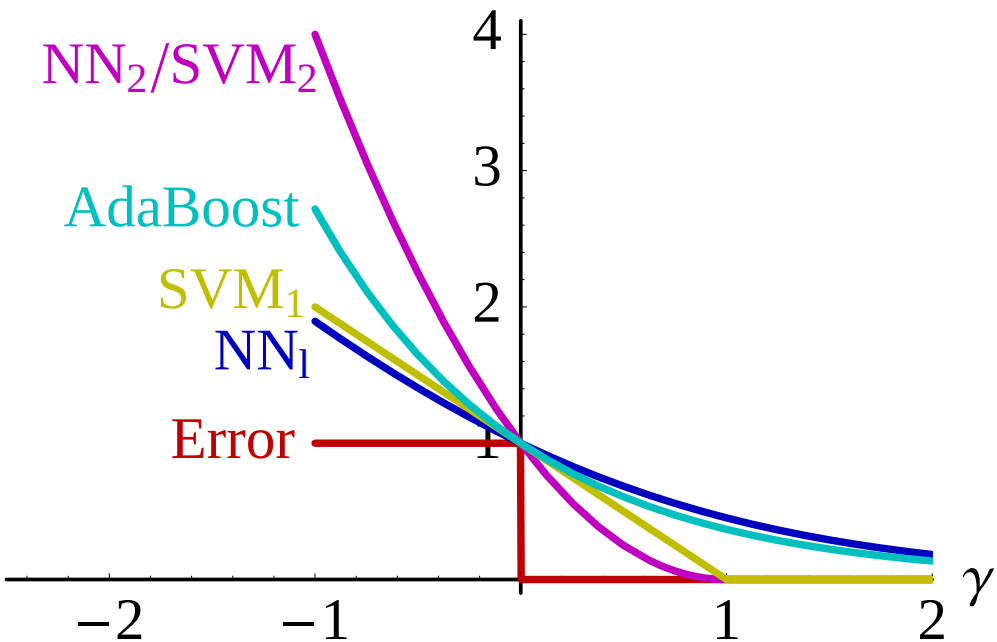


- Margin: $\gamma = y \cdot f(\mathbf{x})$
  - classification error $\equiv$ negative margin
  - the magnitude of a positive margin quantifies the confidence
  - learning principle: minimize a smooth loss function over the margin

$$\widehat{R}_\gamma(f) = \frac{1}{n}\sum_{i=1}^{n} L\big(f(\mathbf{x}_i)y_i\big)$$

The classification model

- Margin loss functions



Outline

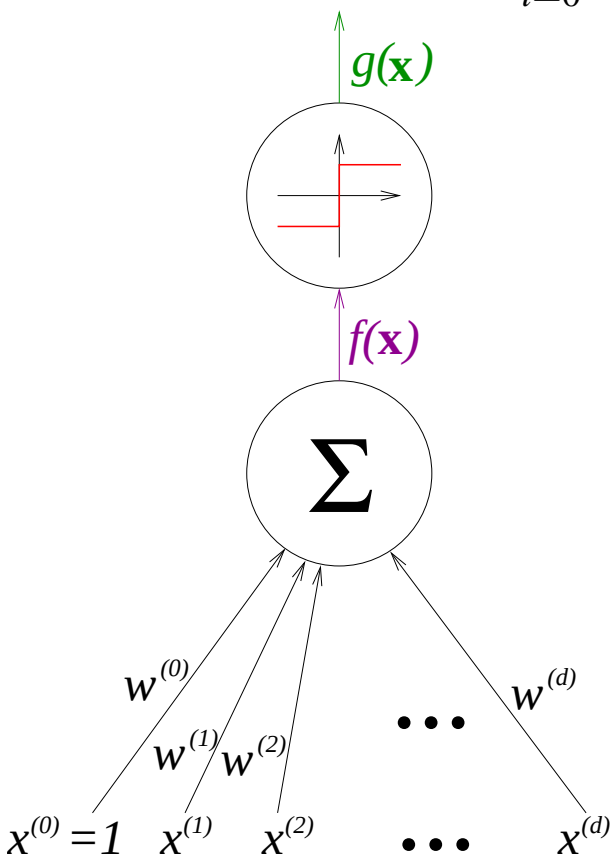
- Non-parametric fitting: two simple examples
- The formal model for classification, learning principles
- Classification algorithms (from a user's point of view)
  - perceptron, neural networks (NN)
  - AdaBoost
  - the Support Vector Machine (SVM)
- Machine learning research motivated by HEP applications

History

- Algorithms
  - 1958: Perceptron [Rosenblatt, ’58] – [Minsky–Papert ’69]
  - 1986: Multilayer perceptrons (neural networks) and the back-propagation algorithm [Rumelhart–Hinton–Williams, ’86]
  - 1995: Support vector machines [Boser–Guyon–Vapnik, ’92], [Cortes–Vapnik, ’95]
  - 1997: boosting, AdaBoost [Freund, ’95], [Freund–Schapire, ’97]

The perceptron

- Linear discriminant functions: $f(\mathbf{x}) = \sum_{i=0}^{d} w^{(i)} \cdot x^{(i)} = \langle \mathbf{w}, \mathbf{x} \rangle$



The perceptron

- Linear discriminant functions: $f(\mathbf{x}) = \sum_{i=0}^{d} w^{(i)} \cdot x^{(i)} = \langle \mathbf{w}, \mathbf{x} \rangle$

- Algorithm
  - simple iterative error correction
  - convergence if the data is linearly separable
  - oscillation for linearly non-separable data

Generalized linear discriminant functions

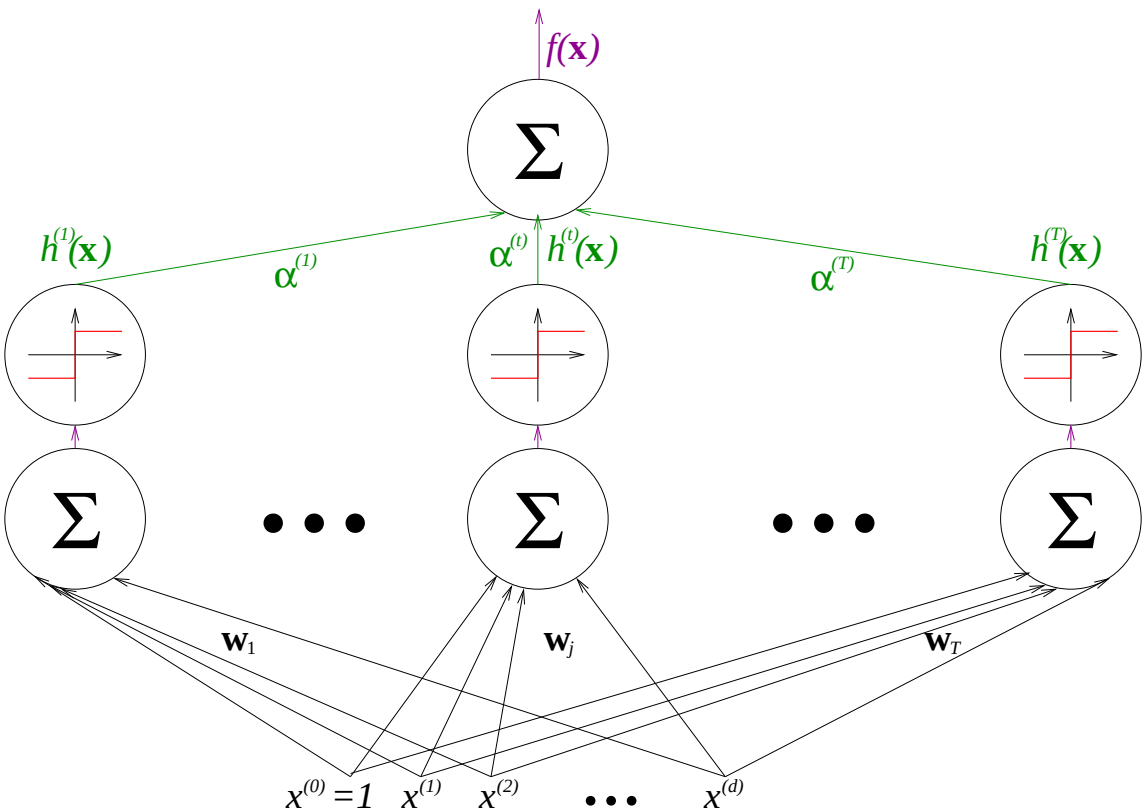
- Model:

$$f(\mathbf{x}) = \sum_{j=1}^{N} \alpha^{(j)} h^{(j)}(\mathbf{x})$$

- $h^{(j)} : \mathbb{R}^d \to [-1, 1]$
  - simple classifiers/discriminant functions, features, experts
- $\alpha^{(j)} \in \mathbb{R}^+$
  - weight of the expert $h^{(j)}$ in the final vote

Multilayer perceptron (neural net)

- Model: $f(\mathbf{x}) = \sum_{j=1}^{N} \alpha^{(j)} \sigma(\langle \mathbf{w}_j, \mathbf{x} \rangle)$



Multilayer perceptron (neural net)

- Model: $f(\mathbf{x}) = \sum_{j=1}^{N} \alpha^{(j)} \sigma(\langle \mathbf{w}_j, \mathbf{x} \rangle)$

- Algorithm:
  - gradient descent optimization
  - differentiable error functions $\rightarrow$ margin loss
  - differentiable activation function σ: the sigmoid
  - local minima, “engineering”, parameters to tune
  - fast, works well if well-tuned
  - versatile: multi-class classification, regression, density estimation

AdaBoost

- Model:

$$f(\mathbf{x}) = \sum_{j=1}^{N} \alpha^{(j)} h^{(j)}(\mathbf{x})$$

  - no restriction on the form of $h^{(j)}(\mathbf{x})$
  - often "decision stumps" :

$$h_{\ell,\theta}(\mathbf{x}) = \begin{cases} +1 & \text{if } x^{(\ell)} \geq \theta, \\ -1 & \text{otherwise} \end{cases}$$

    where $\mathbf{x} = \left(x^{(1)}, \ldots, x^{(d)}\right)$

AdaBoost

- Algorithm
  - extremely simple learning, limited parameter tuning
  - fast
  - the choice of the pool of experts captures the a-priori knowledge
  - no restriction on the form of the simple classifiers
  - multi-class classification is natural, regression is not

Support vector machine

- Model:

$$f(\mathbf{x}) = \sum_{j \in I_{\text{sv}}} \alpha^{(j)} y_j K(\mathbf{x}_j, \mathbf{x})$$

  - $I_{\text{sv}} \subset \{1, \ldots, n\}$ is the set of support vectors
  - $K(\cdot, \cdot)$ is a similarity function (kernel)

- Kernel:

  - $K(\mathbf{x}, \mathbf{x}') = \langle \mathbf{x}, \mathbf{x}' \rangle \longrightarrow f(\mathbf{x})$ is linear
  - $K(\mathbf{x}, \mathbf{x}') = \left(1 + \langle \mathbf{x}, \mathbf{x}' \rangle\right)^d \longrightarrow f(\mathbf{x})$ is a polynom of degree d
  - $K(\mathbf{x}, \mathbf{x}') = \exp\left(-1/h \|mid\mathbf{x} - \mathbf{x}'\|^2\right) \longrightarrow f(\mathbf{x})$ is a Gaussian mixture ($\rightarrow$ Parzen)

Support vector machine

- Model:

$$f(\mathbf{x}) = \sum_{j \in I_{\text{sv}}} \alpha^{(j)} y_j K(\mathbf{x}_j, \mathbf{x})$$

- Algorithm:
  - goal: classification boundary equidistant from classes
  - "sophisticated nearest neighbor"
  - slow and complex quadratic programming optimization
  - turn-key algorithm, very limited parameter tuning
  - no multi-class, no regression

Outline

- Non-parametric fitting: two simple examples
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Discovery, cross section

- First

$$f(x) \sim \frac{P(\text{signal} \mid \mathbf{x})}{P(\text{bg} \mid \mathbf{x})}$$

is estimated, then it is used to find an optimal region A such that

$$\arg\max_{A \in \mathbb{R}^d} \frac{P(\text{signal} \mid \mathbf{x} \in A)}{\sqrt{P(\text{bg} \mid \mathbf{x} \in A)}} \text{ or } \arg\max_{A \in \mathbb{R}^d} \frac{P(\text{signal} \mid \mathbf{x} \in A)}{\sqrt{P(\text{signal or bg} \mid \mathbf{x} \in A)}}$$

- Although $\frac{P(\text{signal}|\mathbf{x})}{P(\text{bg}|\mathbf{x})}$ is related to these goals, it is not the same
- Research goal: modify classification algorithms to directly optimize the modified criteria

Trigger

- Real-time classification: the evaluation of $f(x)$ should be computationally efficient
- Competing goals of accuracy/speed
- Common although not mainstream in ML (object detection, web-page ranking)
- Classical design: cascade classification
- Research goal: explicitly include the accuracy/speed trade-off into training

Final thoughts

- If you can build a generative model for the class densities, do it
- All algorithms are optimized for classification, not hypothesis testing, discovery, trigger, etc.
  - doesn't mean they don't work, but they are probably not optimal
- Non-parametric methods also exist for other objectives (e.g., regression, density estimation)

Software

- mloss.org
- www.cs.waikato.ac.nz/ml/weka
- multiboost.org
- svmlight.joachims.org
- www.csie.ntu.edu.tw/∼cjlin/libsvm
- www.torch.ch

Thank you!

Machines à vecteurs de support

- Idée 1: séparation linéaire avec une marge maximale
  - marge fonctionnelle:

$$\gamma_i = f(\mathbf{x}_i) y_i = (\mathbf{w}^t \mathbf{x}_i + w_0) y_i$$

  - marge géométrique:

$$\gamma_i^{(g)} = \frac{1}{\|\mathbf{w}\|} (\mathbf{w}^t \mathbf{x}_i + w_0) y_i = \frac{1}{\|\mathbf{w}\|} \gamma_i$$

- Optimisations équivalentes
  - maximiser la marge géométrique
  - maximiser la marge fonctionnelle sous la contrainte $\|\mathbf{w}\| = 1$
  - minimiser $\|\mathbf{w}\|$ sous la contrainte $\gamma_i \geq 1$

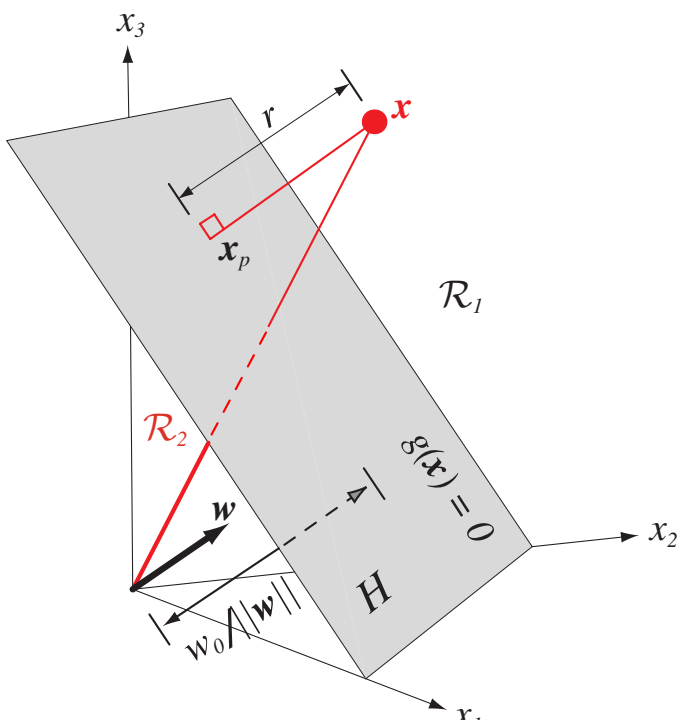
Machines à vecteurs de support

- Géométrie – deux classes
  - $r =$ distance algébrique de $\mathbf{x}$ et H:

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|} \\ g(\mathbf{x}) &= \mathbf{w}^t\mathbf{x} + w_0 = r\|\mathbf{w}\| \\ r &= \frac{g(\mathbf{x})}{\|\mathbf{w}\|} \end{aligned}$$

Machines à vecteurs de support

- Géométrie – deux classes



Machines à vecteurs de support

- Problème d'optimisation:
  - soit $D_n = \big((\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\big)$ linéairement séparable
  - minimiser $\|\mathbf{w}\|^2 = \mathbf{w}^t\mathbf{w}$
  - sous les contraintes $\gamma_i = (\mathbf{w}^t\mathbf{x}_i + w_0)y_i \geq 1, \;\; i = 1, \ldots, n$
- Résultat:
  - l'hyperplan $(\mathbf{w}^t\mathbf{x} + w_0 = 0)$ avec une marge géométrique $\dfrac{1}{\|\mathbf{w}\|}$ maximale

Machines à vecteurs de support

- Problème primal – théorème de Kuhn-Tucker
  - minimiser par rapport à $\mathbf{w}$ et w_0 et maximiser par rapport à $\boldsymbol{\alpha}$:

$$\begin{aligned} L(\mathbf{w}, w_0, \boldsymbol{\alpha}) &= \frac{1}{2}\mathbf{w}^t\mathbf{w} - \sum_{i=1}^{n} \alpha_i(\gamma_i - 1) \\ &= \frac{1}{2}\mathbf{w}^t\mathbf{w} - \sum_{i=1}^{n} \alpha_i\big((\mathbf{w}^t\mathbf{x}_i + w_0)y_i - 1\big) \end{aligned}$$

  - sous les contraintes $\alpha_i \geq 0, \;\; i = 1, \ldots, n$

Machines à vecteurs de support

- Optimisation:
  - les gradients:

$$\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{n} \alpha_i \mathbf{x}_i y_i = \mathbf{0}$$

$$\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial w_0} = \sum_{i=1}^{n} \alpha_i y_i = 0$$

  - resubstitution: maximiser par rapport à $\boldsymbol{\alpha}$ (problème dual):

$$W(\boldsymbol{\alpha}) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^t \mathbf{x}_j - \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^t \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i$$

$$= \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^t \mathbf{x}_j$$

  - sous les contraintes $\alpha_i \geq 0, \;\; i = 1, \ldots, n$ et $\sum_{i=1}^{n} \alpha_i y_i = 0$

Machines à vecteurs de support

- La solution
  - $\mathbf{w}^* = \sum_{i=1}^{n} \alpha_i^* y_i \mathbf{x}_i$
  - $w_0^* = -\frac{1}{2}\left(\max_{y_i=-1} \mathbf{w}^* \mathbf{x}_i + \min_{y_i=1} \mathbf{w}^* \mathbf{x}_i\right)$

Machines à vecteurs de support

- La structure de la solution
  - $\mathbf{w}^*$ est une combinaison linéaire des points d'entraînement
  - théorème de Kuhn-Tucker:

$$\alpha_i^* \left((\mathbf{w}^{*t} \mathbf{x}_i + w_0^*) y_i - 1 \right) = 0, \quad i = 1, \ldots, n$$

  - si $\gamma_i > 1$ alors $\alpha_i^* = 0$
  - si $\alpha_i^* > 0$ alors $\gamma_i = 1$: vecteurs de support
  - $\mathbf{w}^* = \sum_{i \in sv} \alpha_i^* y_i \mathbf{x}_i$
  - $f^*(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i^* y_i \mathbf{x}_i^t \mathbf{x} + w_0^* = \sum_{i \in sv} \alpha_i^* y_i \mathbf{x}_i^t \mathbf{x} + w_0^*$

Machines à vecteurs de support

- La structure de la solution
  - pour $j \in sv$

$$\gamma_j = y_j f^*(\mathbf{x}_j) = y_j \left(\sum_{i \in sv} \alpha_i^* y_i \mathbf{x}_i^t \mathbf{x}_j + w_0^* \right) = 1$$

  - alors

$$\begin{aligned} \mathbf{w}^{*t}\mathbf{w}^* &= \sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i^* \alpha_j^* y_i y_j \mathbf{x}_i^t \mathbf{x}_j = \sum_{j \in sv} \alpha_j^* y_j \sum_{i \in sv} \alpha_i^* y_i \mathbf{x}_i^t \mathbf{x}_j = \sum_{j \in sv} \alpha_j^* (1 - y_j w_0^*) \\ &= \sum_{j \in sv} \alpha_j^* \end{aligned}$$

  - la marge maximale:

$$\gamma^* = \frac{1}{\|\mathbf{w}\|} = \left(\sum_{i \in sv} \alpha_i^* \right)^{-1/2}$$

Machines à vecteurs de support

- Idée 2: le noyau
  - l'optimisation: $W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^t \mathbf{x}_j$
  - la fonction optimale: $f^*(\mathbf{x}) = \sum_{i \in sv} \alpha_i^* y_i \mathbf{x}_i^t \mathbf{x} + w_0^*$
- Remplacer $\mathbf{x}^t \mathbf{x}'$ par une fonction de noyaux $K(\mathbf{x}, \mathbf{x}')$
  - l'optimisation: $W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$
  - la fonction optimale: $f^*(\mathbf{x}) = \sum_{i \in sv} \alpha_i^* y_i K(\mathbf{x}_i, \mathbf{x}) + w_0^*$
  - matrice de Gram: $\mathbf{G}_{i,j} = K(\mathbf{x}_i, \mathbf{x}_j)$
  - équivalent à une transformation non-linéaire dans une espace de traits de dimension très élévée

Machines à vecteurs de support

- Exemples de noyaux
  - linéaire: $K^{\ell}(\mathbf{x},\mathbf{x}') = \mathbf{x}^t\mathbf{x}'$
  - polynômial: $K^{p}_{d}(\mathbf{x},\mathbf{x}') = (\mathbf{x}^t\mathbf{x}' + 1)^d$
  - base radiale: $K^{r}(\mathbf{x},\mathbf{x}') = K(\|\mathbf{x} - \mathbf{x}'\|)$
    - gaussien: $K^{g}_{\gamma}(\mathbf{x},\mathbf{x}') = e^{-\gamma\|\mathbf{x}-\mathbf{x}'\|^2}$
  - réseaux de neurones: $K^{\sigma}(\mathbf{x},\mathbf{x}') = \sigma(s\mathbf{x}^t\mathbf{x}' + c)$
    - sigmoïde: $K^{t}_{s,c}(\mathbf{x},\mathbf{x}') = \tanh(s\mathbf{x}^t\mathbf{x}' + c)$

Machines à vecteurs de support

- Discrimination linéaire généralisée
  - linéaire:

$$f^*(\mathbf{x}) = \mathbf{w}^{*t}\mathbf{x} + w_0^* = \sum_{j=1}^{d} w_j^* x^{(j)} + w_0^* = \sum_{i \in sv} \alpha_i^* y_i \mathbf{x}_i^t \mathbf{x} + w_0^*$$

  - généralisée:

$$f^*(\mathbf{x}) = \sum_{j=1}^{D} w_j^* \phi^{(j)}(\mathbf{x}) + w_0^* = \sum_{i \in sv} \alpha_i^* y_i \sum_{j=1}^{D} \phi^{(j)}(\mathbf{x}_i)\phi^{(j)}(\mathbf{x}) + w_0^*$$

  - produit scalaire dans l'espace de traits:

$$\boldsymbol{\phi}^t(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}') = \sum_{j=1}^{D} \phi^{(j)}(\mathbf{x})\phi^{(j)}(\mathbf{x}')$$

Machines à vecteurs de support

- Discrimination linéaire généralisée
  - exemple:

$$\begin{aligned}
\phi^{(j)}(\mathbf{x}) &= \sqrt{2}x^{(j)}, \quad j = 1, \ldots, d, \\
\phi^{(id+j)}(\mathbf{x}) &= x^{(i)}x^{(j)}, \quad i, j = 1, \ldots, d \\
\phi^{(d^2)}(\mathbf{x}) &= 1
\end{aligned}$$

  - produit scalaire dans l'espace des traits:

$$\begin{aligned}
\boldsymbol{\phi}^t(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}') &= \sum_{j=1}^{d^2} \phi^{(j)}(\mathbf{x})\phi^{(j)}(\mathbf{x}') \\
&= \sum_{j=1}^{d} \sqrt{2}x^{(j)}\sqrt{2}x'^{(j)} + \sum_{i=1}^{d}\sum_{j=1}^{d} x^{(i)}x^{(j)}x'^{(i)}x'^{(j)} + 1 \\
&= 2\mathbf{x}^t\mathbf{x}' + (\mathbf{x}^t\mathbf{x}')^2 + 1 \\
&= (\mathbf{x}^t\mathbf{x}' + 1)^2 = K_2^p(\mathbf{x}, \mathbf{x}')
\end{aligned}$$

Machines à vecteurs de support

- Caractérisation des noyaux
  - $K(\mathbf{x},\mathbf{x}') = \boldsymbol{\phi}^t(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}') = \sum_{j=1}^{D} \phi^{(j)}(\mathbf{x})\phi^{(j)}(\mathbf{x}')$
  - commutativité: $K(\mathbf{x},\mathbf{x}') = K(\mathbf{x}',\mathbf{x})$
  - inégalité de Cauchy-Schwartz:

$$\begin{aligned} K(\mathbf{x},\mathbf{x}')^2 &= \left(\boldsymbol{\phi}^t(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}')\right)^2 \\ &\leq \|\boldsymbol{\phi}(\mathbf{x})\|^2 \|\boldsymbol{\phi}(\mathbf{x}')\|^2 \\ &= \boldsymbol{\phi}^t(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}) \cdot \boldsymbol{\phi}^t(\mathbf{x}')\boldsymbol{\phi}(\mathbf{x}') \\ &= K(\mathbf{x},\mathbf{x})K(\mathbf{x}',\mathbf{x}') \end{aligned}$$

Machines à vecteurs de support

- Théorème de Mercer:
  - $\boldsymbol{\phi}^t(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}') = K(\mathbf{x},\mathbf{x}')$
- Conditions
  - diagonaliser la matrice de Gram: $\mathbf{G}_{i,j} = K(\mathbf{x}_i,\mathbf{x}_j) = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}$
  - valeurs propres: λ_t, vecteurs propres: $\mathbf{v}_t$
  - condition suffisante: $\mathbf{G}$ est positif semi-definit ($\forall t : \lambda_t > 0$) pour tout $\mathcal{X}_n = (\mathbf{x}_1,\ldots,\mathbf{x}_n)$
  - D peut être ∞!!!

Machines à vecteurs de support

- Idée 3: les variables d'écart (slack variables)
  - cas non-séparable
- Permettre des erreurs:
  - minimiser $\|\mathbf{w}\|^2 = \mathbf{w}^t\mathbf{w}$
  - sous les contraintes $\gamma_i = (\mathbf{w}^t\mathbf{x}_i + w_0)y_i \geq 1 - \xi_i, \;\; i = 1, \ldots, n$
  - où $\xi_i \geq 0, \;\; i = 1, \ldots, n$
  - minimiser l'erreur $\equiv$ minimiser le nombre de points avec $\xi_i > 0$: NP-difficile

Machines à vecteurs de support

- Problème soluble 1: minimiser $\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i^2$
  - on peut supprimer la contrainte de positivité des ξ_i
  - C est un hyper-paramètre réglé par la validation croisée (par exemple)

Machines à vecteurs de support

- Problème primal
  - minimiser par rapport à $\mathbf{w}$, $\boldsymbol{\xi}$ et w_0 et maximiser par rapport à $\boldsymbol{\alpha}$:

$$L(\mathbf{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}) = \frac{1}{2}\mathbf{w}^t\mathbf{w} + \frac{C}{2}\sum_{i=1}^{n}\xi_i^2 - \sum_{i=1}^{n}\alpha_i\left[(\mathbf{w}^t\mathbf{x}_i + w_0)y_i - 1 + \xi_i\right]$$

  - sous les contraintes $\alpha_i \geq 0, \;\; i = 1, \ldots, n$
  - les gradients:

$$\begin{aligned}
\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial \mathbf{w}} &= \mathbf{w} - \sum_{i=1}^{n}\alpha_i\mathbf{x}_i y_i = \mathbf{0} \\
\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial \boldsymbol{\xi}} &= C\boldsymbol{\xi} - \boldsymbol{\alpha} = \mathbf{0} \\
\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial w_0} &= \sum_{i=1}^{n}\alpha_i y_i = 0
\end{aligned}$$

Machines à vecteurs de support

- Problème dual
  - resubstitution: maximiser par rapport à $\boldsymbol{\alpha}$:

$$\begin{aligned} W(\boldsymbol{\alpha}) &= \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j) + \frac{1}{2C} \boldsymbol{\alpha}^t \boldsymbol{\alpha} - \frac{1}{C} \boldsymbol{\alpha}^t \boldsymbol{\alpha} \\ &= \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j) - \frac{1}{2C} \boldsymbol{\alpha}^t \boldsymbol{\alpha} \\ &= \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \left(K(\mathbf{x}_i, \mathbf{x}_j) + \frac{1}{C} \delta_{i,j} \right) \end{aligned}$$

  - sous les contraintes $\alpha_i \geq 0, \;\; i = 1, \ldots, n$ et $\sum_{i=1}^{n} \alpha_i y_i = 0$

Machines à vecteurs de support

- La solution
  - $\mathbf{w}^* = \sum_{i=1}^{n} \alpha_i^* y_i \mathbf{x}_i = \sum_{i \in sv} \alpha_i^* y_i \mathbf{x}_i$
  - $f^*(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i^* y_i K(\mathbf{x}_i, \mathbf{x}) + w_0^* = \sum_{i \in sv} \alpha_i^* y_i K(\mathbf{x}_i, \mathbf{x}) + w_0^*$
  - w_0^* est choisi tel que $\gamma_i = f(\mathbf{x}_i) y_i \geq 1 - \xi_i = 1 - \frac{\alpha_i^*}{C}$
  - la marge obtenue: $\gamma = \left(\sum_{i \in sv} \alpha_i^* - \frac{1}{C} \alpha^{*t} \alpha^* \right)^{-1/2}$

Machines à vecteurs de support

- Problème soluble 2: minimiser $\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i$

- Problème primal

  - minimiser par rapport à $\mathbf{w}$, $\boldsymbol{\xi}$ et w_0 et maximiser par rapport à $\boldsymbol{\alpha}$:

$$L(\mathbf{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \mathbf{r}) = \frac{1}{2}\mathbf{w}^t\mathbf{w} + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i\left[(\mathbf{w}^t\mathbf{x}_i + w_0)y_i - 1 + \xi_i\right] - \sum_{i=1}^{n} r_i\xi_i$$

  - sous les contraintes $\alpha_i \geq 0, r_i \geq 0 \;\; i = 1, \ldots, n$

Machines à vecteurs de support

- Problème dual
  - les gradients:

$$\begin{aligned}
\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial \mathbf{w}} &= \mathbf{w} - \sum_{i=1}^{n} \alpha_i \mathbf{x}_i y_i = \mathbf{0} \\
\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial \boldsymbol{\xi}} &= C - \boldsymbol{\alpha}_i - r_i = 0 \\
\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial w_0} &= \sum_{i=1}^{n} \alpha_i y_i = 0
\end{aligned}$$

Machines à vecteurs de support

- Problème dual
  - resubstitution: maximiser par rapport à $\boldsymbol{\alpha}$:

$$W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

  - sous les contraintes $\alpha_i \geq 0, r_i \geq 0, C - \boldsymbol{\alpha}_i - r_i = 0 \;\; i = 1, \ldots, n$ et $\sum_{i=1}^{n} \alpha_i y_i = 0$
  - $\equiv$ sous les contraintes $0 \leq \alpha_i \leq C$ (contraintes de boîte)

Machines à vecteurs de support

- La solution
  - $\mathbf{w}^* = \sum_{i=1}^{n} \alpha_i^* y_i \mathbf{x}_i = \sum_{i \in sv} \alpha_i^* y_i \mathbf{x}_i$
  - $f^*(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i^* y_i K(\mathbf{x}_i, \mathbf{x}) + w_0^* = \sum_{i \in sv} \alpha_i^* y_i K(\mathbf{x}_i, \mathbf{x}) + w_0^*$
  - w_0^* est choisi tel que $\gamma_i = f(\mathbf{x}_i) y_i = 1$ pour tous $i : 0 < \alpha^* < C$
  - la marge obtenue: $\gamma = \left(\sum_{i,j \in sv} \alpha_i^* \alpha_j^* y_i y_j K(\mathbf{x}_i, \mathbf{x}_j) \right)^{-1/2}$