Algorithms of Scientific Computing

Hierarchical Methods and Sparse Grids
– Classification and Data Mining –

Michael Bader

Technische Universität München

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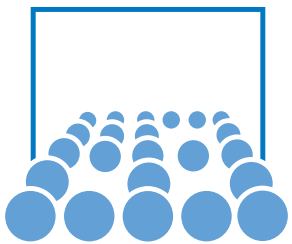


Classification in Data Mining

Now for something completely different?

- We consider another application: classification in data mining (our contribution to “Big Data”)
- Aim is extraction of new and (hopefully) useful information (out of data bases, etc.)

- We consider *predictive modelling* in data mining:
  - Forecast values on new, previously unseen data
  - Prediction based on given set of data points (training data)

Problem Setting: Binary Classification

Classification aims to

- assign a "correct" class label $k \in K$
- to all data points $\vec{x}$ in some d-dimensional feature space Ω
- based on set S of pre-classified data points for training

$$S := \{(\vec{x}_i, y_i) \in \Omega \times K\}_{i=1}^{m}$$

- Here: binary classification, for us $K := \{+1, -1\}$

Tasks (examples):

- Is person male or female?
  (dimensions: shoe size, body height, ...)?
- Is customer of bank credit-worthy?
  (dimensions: income, type of house, ...)?
- Will personalized advertising pay off for a certain person?
  (dimensions: interests, previous purchases, ...)

Classification

Classical approaches

- Decision trees
- Rule-based classifiers (decision rules)
- Instance-based classifiers (k-Nearest Neighbour, ...)
- Probabilistic (Bayes) classifiers
- Based on function representation (artificial neural networks, support vector machines, ...)

Problem

- All depend at least quadratically on size of training set (think of classification based on comparisons of data points)
- Approach based on discretization of Ω (i.e., approximate S by a function) would allow linear training time
- roadblock: curse of dimensionality
  $\Rightarrow$ possible solution: sparse grids! (to be discussed ...)

Sparse Grid Classification

- Training set (normalized)

$$S := \left\{ (\vec{x}_i, y_i) \in [0,1]^d \times \{+1, -1\} \right\}_{i=1}^{m}$$

- Assume: training data obtained by randomly sampling of unknown function f disturbed by noise
- Reconstruct piecewise d-linear sparse grid approximation u of f:

$$f_N(\vec{x}) = \sum_{i=1}^{N} v_i \phi_i(\vec{x})$$

  $\rightsquigarrow$ our well known "coefficients and basis functions" approach
- To determine class at new data location $\vec{x}$:
  - Compute $f_N(\vec{x})$
  - Predict class $+1$, if $f_N(\vec{x}) \geq 0$; otherwise -1

Sparse Grid Classification

- Solve regularized least squares problem

$$f_N \stackrel{!}{=} \arg\min_{f_N \in V_N} \left(\frac{1}{m} \sum_{i=1}^{m} \left(y_i - f_N(\vec{x}_i) \right)^2 + \lambda \| \nabla f_N \|_{L_2}^2 \right)$$

  with $\|g\|_{L_2}^2 := \int g^2 \, \mathrm{d}\vec{x}$

- Aims:
  - Be close to training data: minimize quadratical error
  - Prevent overfitting: minimize gradient (or similar property) to avoid oscillations due to noise in training data
  - Parameter λ to control trade-off

- Derive system of linear equations:
  - We plug in our sparse-grid approximation of f_N
  - And minimize by setting each first derivative $\partial / \partial v_i$ to zero

From Minimization to System of Linear Equations

$\Rightarrow$ N linear equations for N unknowns

$$\left(\frac{1}{m}BB^T + \lambda C\right)\vec{v} = \frac{1}{m}B\vec{y}\,,$$

- With matrices C and B

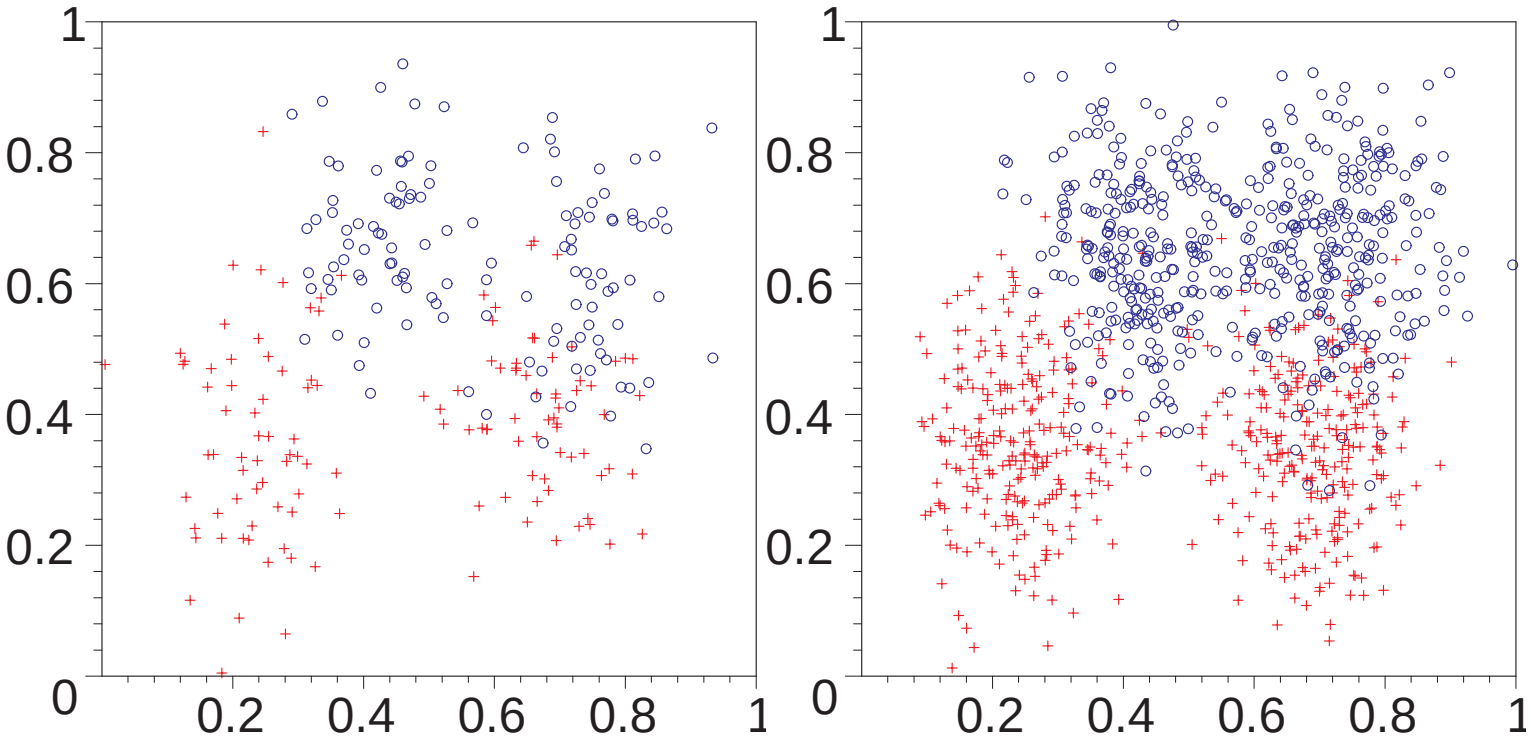
$$(C)_{ij} = \langle \nabla\phi_i(\vec{x}), \nabla\phi_j(\vec{x})\rangle_{L_2}, \qquad (B)_{ij} = \phi_i(\vec{x}_j)$$

- B and C need to simple to set up
- applying B to vector $\vec{y}$ should be cheap, e.g. $\mathcal{O}(Nm)$ operations (and even better)
- we will need efficient algorithms to solve the system of equations!

$\Rightarrow$ **how to choose basis functions $\phi_i(\vec{x})$ and thus classifier f_N?**

Example 1 – Ripley Data Set

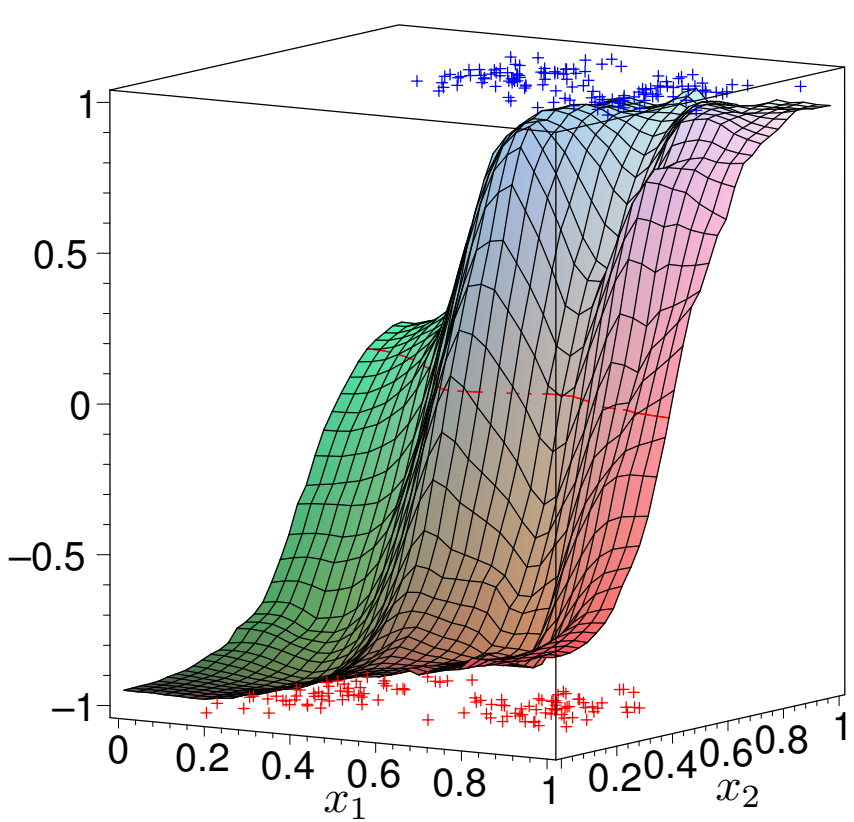
- Artificial, *2d* data set, frequently used as a benchmark (mixture of Gaussian distributions plus noise)
- 250 points for training, 1000 to test on

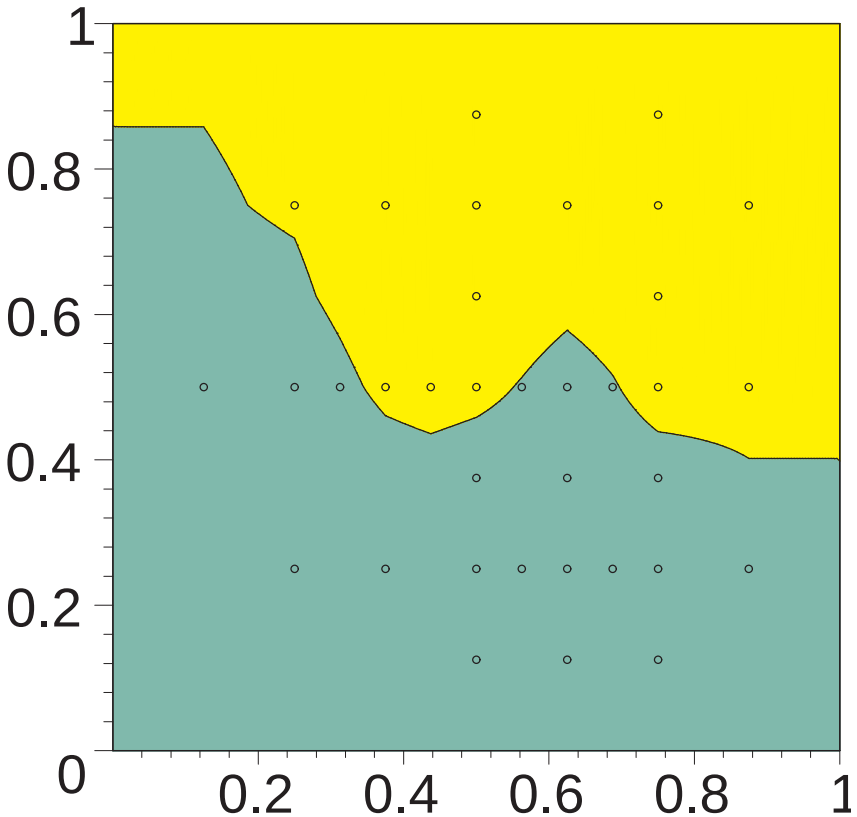


- Constructed to contain 8% of noise

Outlook – Ripley Data Set (Using Sparse Grids)

- Compute adaptive sparse grid classifier, e.g.:



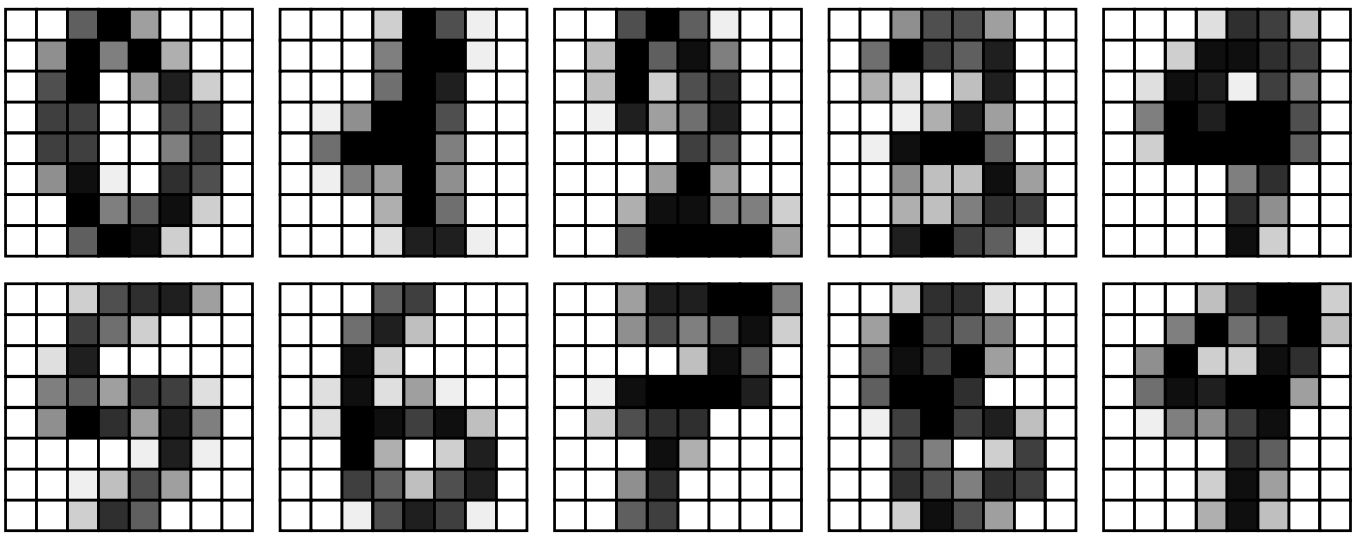


- Best accuracy: 91.5% on test data (max. 92%)
- Suitable treatment of boundary needed

Example 2 – Optidigits

Now for something really high-dimensional...

- Optical recognition of handwritten digits:
  Classify images of handwritten digits
- 64-dimensional data set of gray-values (0,1,...,16)



Outlook – Optidigits (Using Sparse Grids)

- Construct ten different binary classifiers
  (one digit ($+1$) against all others (-1))
- Take the one with highest prediction (function value)

$\Rightarrow$ Best accuracy: 97.7% correctly classified

Summary

- Even high-dimensional problems ("real problems" are often not that high-dimensional) can be successfully solved
- Typically requires to adapt sparse grids to given problem
  - What to do with the boundary (3 points per dim. equiv. to 3^d $\rightsquigarrow$ already really large for $d = 64$)?
  - Adaptive refinement!
  - Consider dependency of algorithms in d, N, and m
    (not only exponential parts can hurt!)
  - ...