Imbalanced Classification. Multiclass Classification

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Outline

1. Imbalanced Classification
2. Multi-Class Classification: General Strategies and Particular Models
3. Multi-Class Classification with Naive Bayes Classifier
4. Appendix. Materials for Additional Study: Nonparametric Estimation

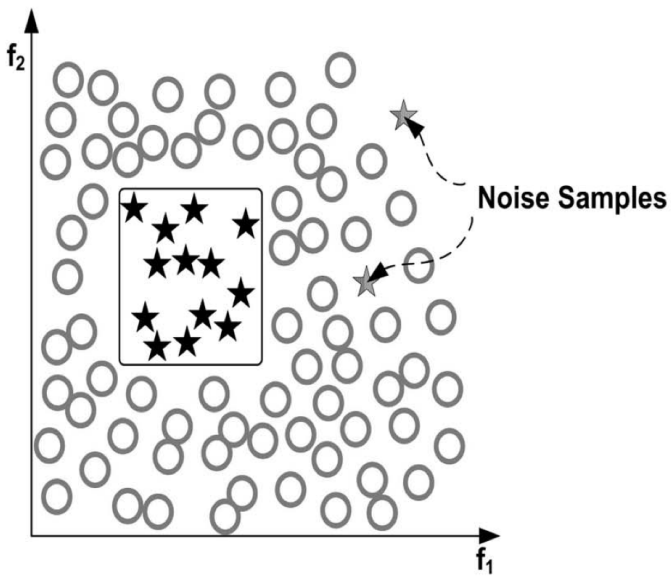
1 Imbalanced Classification

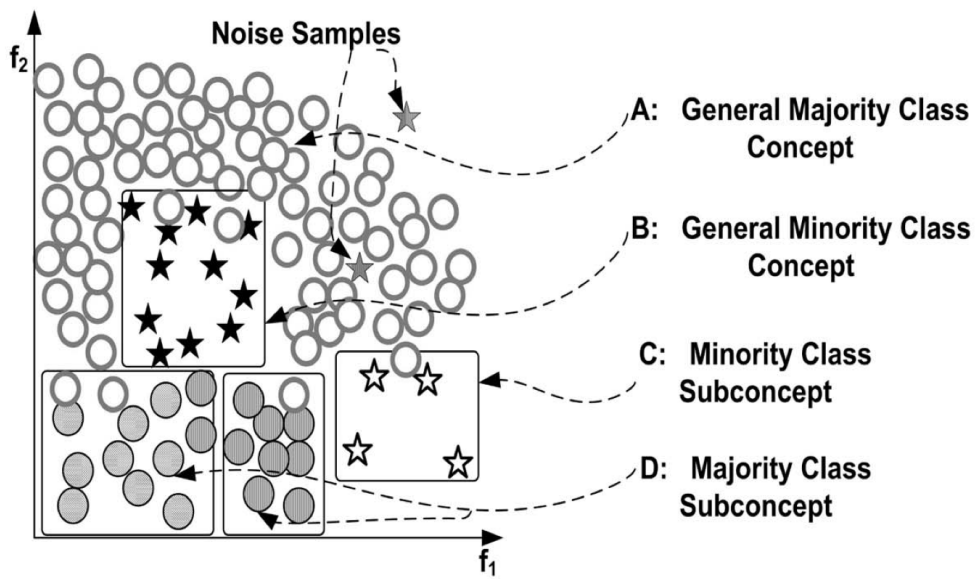
2 Multi-Class Classification: General Strategies and Particular Models

3 Multi-Class Classification with Naive Bayes Classifier

4 Appendix. Materials for Additional Study: Nonparametric Estimation

- Between-class imbalance (relative imbalance)
- Relative imbalance vs. imbalance due to rare instances or "absolute rarity"
- Data complexity vs. imbalanced data vs. small sample size





- Binary classification: often dataset has "natural" imbalance
- Minor class (of **prime** interest) vs. major class: e.g. classification of "cancerous" vs. "healthy" mammography image
- Standard classifiers (SVM, kNN, log. reg., etc.): classes are equally important $\Rightarrow$ results are biased towards the major class
- Poor prediction of minor class while the average quality can be good:
  - target events occurs in 1% of all cases
  - classifier always gives a 'no-event' answer
  - it is wrong just 1% of all cases

- Approaches to increase importance of the minor class:
  - Adapt a probability threshold for classifiers,
  - Modify a loss function, e.g., by assigning more weight to the minor class error,
  - Resample a dataset in order to soften or remove class imbalance
- We focus on resampling: convenient, allows to use standard classifiers
- The main aim:
  - review and compare main resampling methods,
  - compare strategies of resampling amount (i.e., how many observations to add or drop) selection,
  - explore their influence on quality of classification

- Dataset $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, where $\mathbf{x}_i \in \mathbb{R}^d$, $y_i \in \{-1, +1\}$
- $C_{+1}(S) = \{(\mathbf{x}_i, y_i) \in S \mid y_i = +1\}$ is a major class,
- $C_{-1}(S) = \{(\mathbf{x}_i, y_i) \in S \mid y_i = -1\}$ is a minor class, i.e. $|C_{+1}(S)| > |C_{-1}(S)|$
- Imbalance ratio $IR(S) = \frac{|C_{-1}(S)|}{|C_{+1}(S)|}$, $IR(S) \leq 1$

Learning a classifier

- Learn a classifier using imbalanced training sample S
- The dataset S is resampled using a method r:
  - some observations in S are dropped, or
  - some new synthetic observations are added to S
- The result of resampling is a dataset $r(S)$ with $IR(r(S)) > IR(S)$
- Standard classification model f is learned on $r(S)$ to construct a classifier $f_{r(S)} : \mathbb{R}^d \to \{-1, +1\}$

- Performance is determined by a predefined classifier quality metrics $Q(f_{S_{train}}, S_{test})$ (e.g. AUC under Precision-Recall curve):
  - input classifier $f_{S_{train}}$,
  - testing dataset S_{test},
  - the higher value is the better
- M-fold cross-validation is used to estimate Q^{CV} on S

Resampling method r:

1. Takes input:
   - dataset S;
   - resampling multiplier $m > 1$ for resulting imbalance ratio $IR(r(S)) = m \cdot IR(S)$;
   - additional parameters, specific for the method
2. Add synthesized objects to the minor class (oversampling), or drop objects from the major class (undersampling), or both
3. Outputs resampled dataset $r(S)$ with imbalance ratio $IR(r(S)) = m \cdot IR(S)$

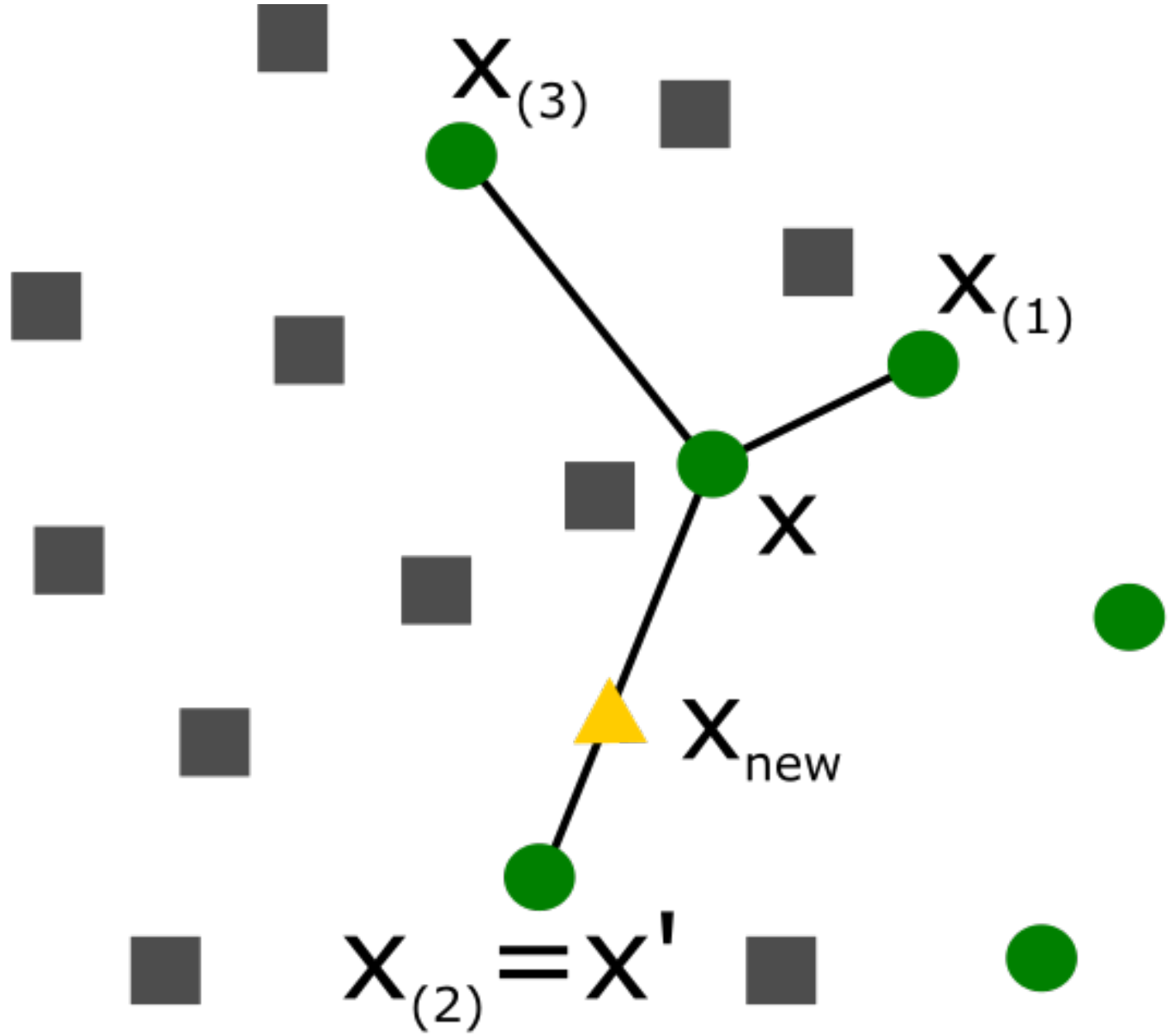
Random Oversampling (ROS)

- ROS, also known as bootstrap oversampling
- No additional input parameters
- It adds to the minor class new $(m-1)|C_{-1}(S)|$ objects
- Each of objects is drawn from uniform distribution on $C_{-1}(S)$

Random Undersampling (RUS)

- No additional input parameters
- It chooses random subset of $C_{+1}(S)$ with $|C_{+1}(S)|\frac{m-1}{m}$ elements and drops it from the dataset
- All subsets of $C_{+1}(S)$ have equal probabilities to be chosen

Synthetic Minority Oversampling Technique (SMOTE)



Synthetic Minority Oversampling Technique (SMOTE)

- Input parameter: k (number of neighbors)
- Oversampling, it adds to the minor class new synthesized objects
- Initialize: $S_{new} := \emptyset$. Repeat $(m-1)|C_{-1}(S)|$ times:
  1. Select randomly $\mathbf{x}_i \in C_{-1}(S)$
  2. Find k minor class NN of $\mathbf{x}_i$, randomly select $\mathbf{x}'_i$ from them
  3. Select randomly $\mathbf{x}_{new}$ on the segment connecting $\mathbf{x}_i$ and $\mathbf{x}'_i$
  4. $S_{new} := S_{new} \cup \{(\mathbf{x}_{new}, -1)\}$
- Add objects to the dataset: $r(S) = S \cup S_{new}$

Artificial Data

- Artificial pool of data with ~ 1000 datasets
- Artificial datasets were drawn from a Gaussian mixture distribution
- Each of two classes is represented as a Gaussian mixture with not more than 3 components
- Number of features varies from 6 to 40, size of dataset from 200 to 1000, IR from 0.05 to 0.35

Real Data

- Real pool of data with ~ 100 datasets
- Different areas: biology, medicine, engineering, sociology
- All features are numeric or binary, their number varies from 3 to 1000
- Size of dataset varies from 200 to 1000, IR from 0.02 to 0.75

- For each dataset we varied classifier model, resampling method and resampling multiplier
- We used Bootstrap, RUS and SMOTE with $k = 5$
- We varied resampling multiplier m from 1.25 to 10.0
- We used Decision Trees, k-Nearest Neighbors, and Logistic Regression with ℓ_1 regularization
- Optimal parameters of a classifier were selected by cross-validation

- Accuracy measure = Area under precision-recall curve Q_{PRC}
- We performed 10-fold cross-validation and calculated Q_{PRC}^{CV} — average of Q_{PRC}

Resampling Multiplier Selection

- Two strategies of resampling multiplier selection:
  - equalizing strategy, EqS: select multiplier providing balanced classes ($IR = 1$) in resulting dataset
  - CV-search, CVS: select optimal multiplier (i.e., providing maximum of $\overline{Q^{CV}}$) by cross-validation
- The equalizing strategy seems to be reasonable as it removes class imbalance which we initially tried to tackle. It is quick and widely used
- CV-search may provide better quality but it is more time-consuming

- $\{r_1, \ldots, r_n\}$ — the set of considered methods (e.g. resampling methods)
- $\{S_1, \ldots S_T\}$ — the set of tasks (datasets),
- q_{ti} — the quality of the method i on the dataset t,
- $p_i(\beta)$ is a fraction of tasks, on which the method i is worse than the best one not more than β times:

$$p_i(\beta) = \frac{1}{T}\left|\left\{t : q_{ti} \geq \frac{1}{\beta}\max_i q_{ti}\right\}\right|, \ \beta \geq 1$$

Dolan-More Curves

- $p_i(1)$ is a fraction of datasets where the method i is the best
- A graph of $p_i(\beta)$ on β is called Dolan-More curve for the method i
- The higher the curve, the better the method!

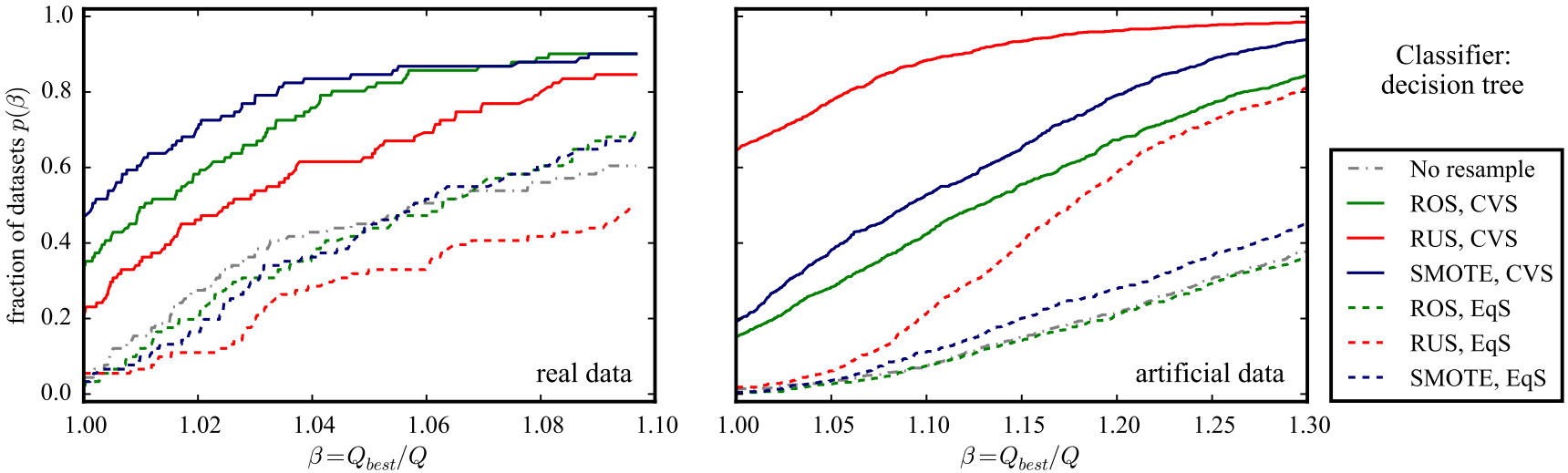
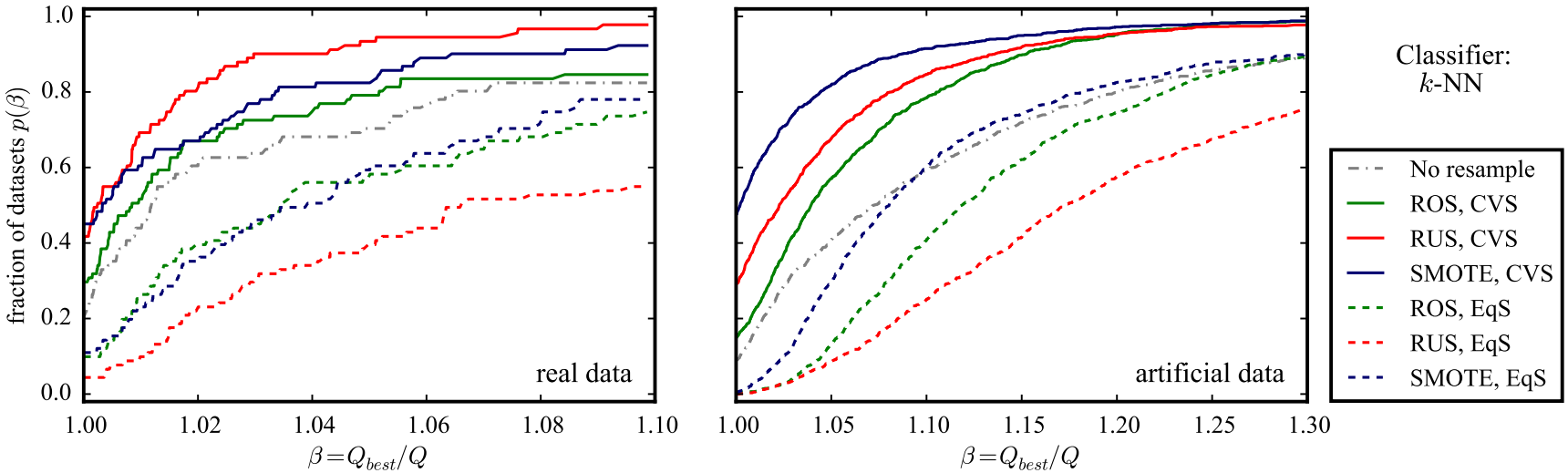


Figure – Dolan-More curves for metric Q^{CV}_{PRC}



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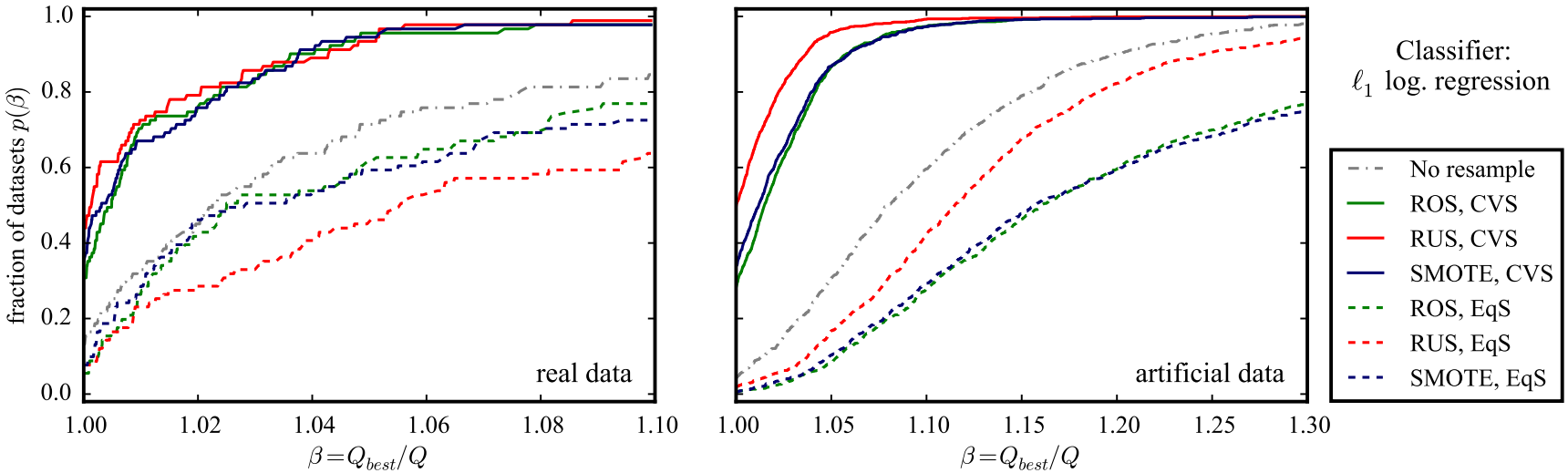

Figure – Dolan-More curves for metric Q^{CV}_{PRC}

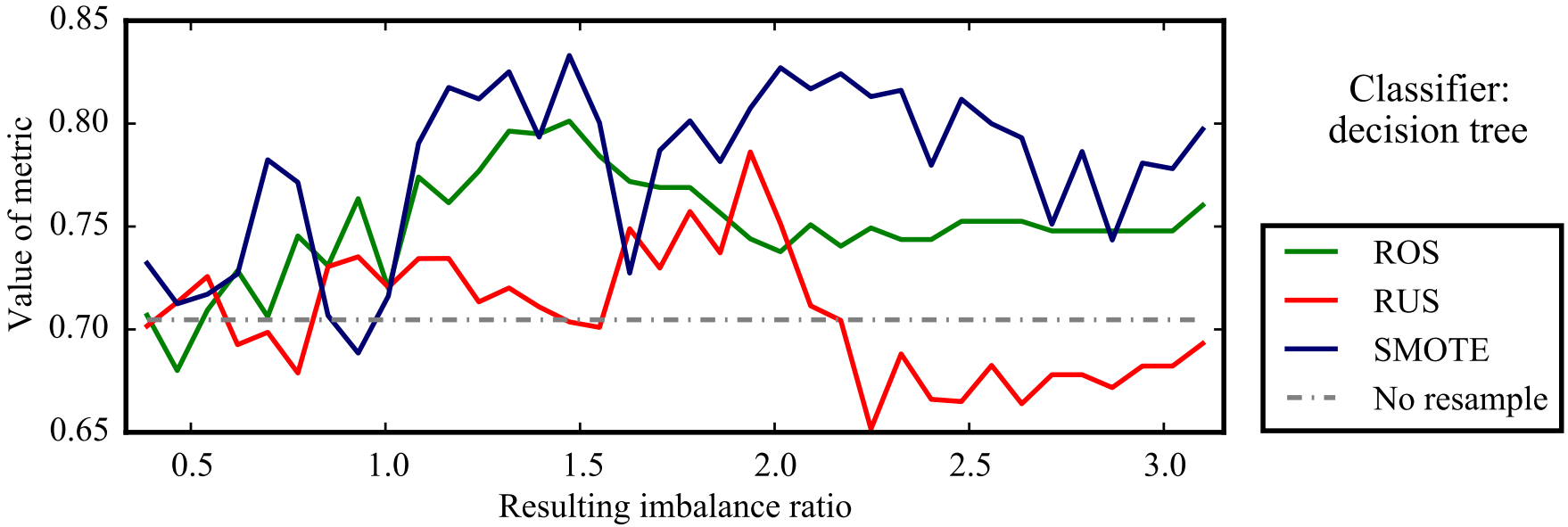

Figure – Value of Q_{PRC}^{CV} vs. resulting value of IR for dataset "Delft pump 1x3"

Comments

- Resampling with CV-search of multiplier provides better results, especially for Decision trees and Logistic regression
- The equalizing strategy (EqS) shows much lower quality, especially in case of k-Nearest neighbors and Logistic regression
- There is no method that would always outperform the others
- Classification without resampling is the best choice in some cases. E.g., for Logistic regression it is about 15% of real datasets and 5% of artificial
- Resampling improves classification of imbalanced datasets in most cases if a method and a multiplier are selected properly

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Multi-Class Classification Problem

- **Training sample**: i.i.d. generated by D

$$S = \{(\mathbf{x}_i, y_i)\}_{i=1}^{m} \in X^m \times Y^m, \; y = f(\mathbf{x})$$

  - mono-label case: $\mathrm{Card}(Y) = K$
  - multi-label case: $Y = \{-1, +1\}^K$
- **Problem**: find classifier $h : X \to Y$ swith small generalization error
  - mono-label case: $R_D(h) = \mathbb{E}_{\mathbf{x} \sim D}\left[1_{h(\mathbf{x}) \neq f(\mathbf{x})}\right]$
  - multi-label case: $R_D(h) = \mathbb{E}_{\mathbf{x} \sim D}\left[\frac{1}{K}\sum_{j=1}^{K} 1_{[h(\mathbf{x})]_j \neq [f(\mathbf{x})]_j}\right]$
  - **Remark**: Precision/Recall with Micro/Macro averaging!

Comments

- Usually $K \leq 100$
- If $K \gg 1$ then some other methods are used, e.g. ranking
- Big values of K increases computational burden
- In general, classes are not balanced

- **Technique**
  - for each class $k \in Y$ learn a binary classifier

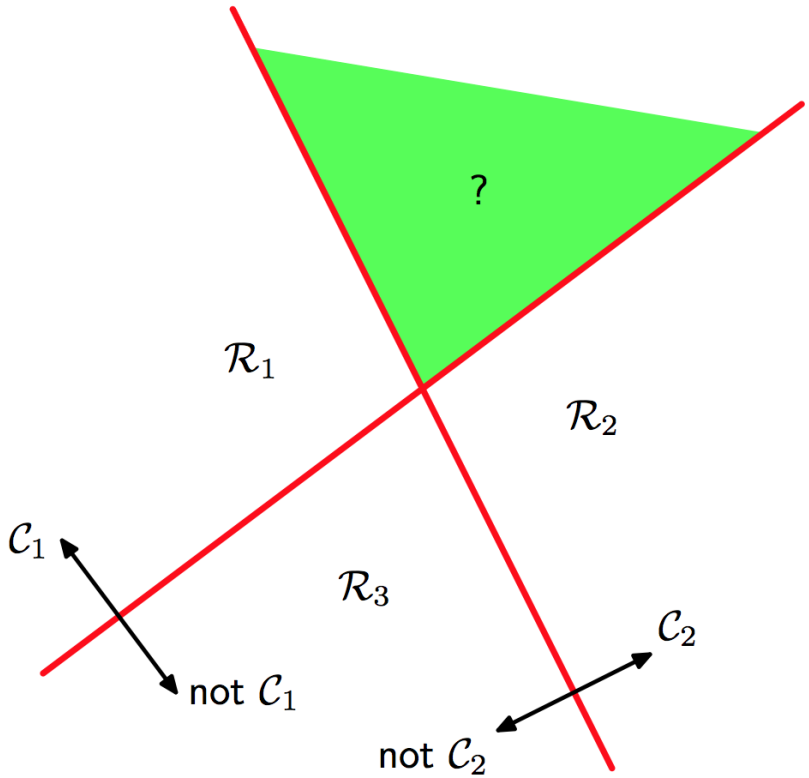
$$h_k(\mathbf{x}) = \text{sign}(f_k(\mathbf{x}))$$

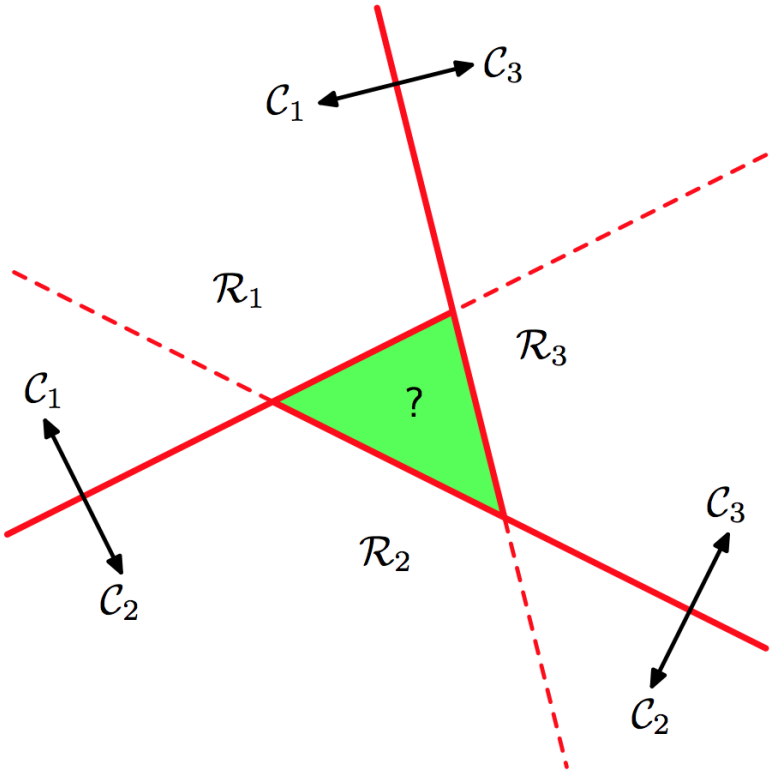
  - combine binary classifiers via voting, e.g. majority voting

$$h : \mathbf{x} \to \arg\max_{k \in Y} f_k(\mathbf{x})$$

- **Comments**
  - calibration: classifiers scores are not comparable
  - simple and frequently used in practice, computational advantages in some cases

One-vs-All





Consider the use of $K - 1$ classifiers each of which solves a two-class problem of separating points in a particular class from points not in that class. This approach leads to regions of input space that are ambiguously classified

- **Technique**
  - for each pair $(k, k') \in Y$, $k \neq k'$ learn a binary classifier $h_{k,k'} : X \to \{0, 1\}$
  - combine binary classifiers via majority vote

$$h(\mathbf{x}) = \arg\max_{k' \in Y} |\{k : h_{k,k'}(\mathbf{x}) = 1\}|$$

- **Comments**
  - computational complexity: train $K(K-1)/2$ binary classifiers
  - overfitting: size of a training sample can be small for a given pair of classifiers

Approach based on Error-Correcting Codes

- 8 classes, codes of length 6

codes

classes	1	2	3	4	5	6
1	0	0	0	1	0	0
2	1	0	0	0	0	0
3	0	1	1	0	1	0
4	1	1	0	0	0	0
5	1	1	0	0	1	0
6	0	0	1	1	0	1
7	0	0	1	0	0	0
8	0	1	0	1	0	0

$f_1(x)$	$f_2(x)$	$f_3(x)$	$f_4(x)$	$f_5(x)$	$f_6(x)$
0	1	1	0	1	1

new example x

- Assign L-long binary code word to each class, i.e. represent each class as

$$\mathbb{C} = [\mathbb{C}_{k,j}] \in \{0,1\}^{[1,K]\times[1,L]}$$

- Learn a binary classifier $f_j : X \to \{0,1\}$ for each column. Example $\mathbf{x}$ in class k is labeled with $\mathbb{C}_{k,j}$
- Classifier output:

$$\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_L(\mathbf{x})),$$

- Final classifier

$$h : \mathbf{x} \to \arg\min_{k \in Y} d_{\text{Hamming}} \left(\mathbb{C}_{k,.}, \mathbf{f}(\mathbf{x})\right)$$

Comments

- One-vs-all approach is the most widely used
- No clear empirical evidence of the superiority of other approaches
- Large structured multi-class problems are often treated as ranking problems
- Above we considered how to reduce multi-class classification to the binary case.
- Also we can incorporate a multi-class structure explicitly into a classification algorithm, see e.g. multi-class logistic regression or multi-class SVM (below)

Particular Model: Multi-class Logistic Regression

- Linear Classifier in a multi-class case, i.e. $|Y| > 1$
- Probability of an object to belong to some class y is equal to

$$p(y|\mathbf{x};\mathbf{w}) = \frac{\exp(\mathbf{w}_y^\top \mathbf{x})}{\sum_{z\in Y}\exp(\mathbf{w}_z^\top \mathbf{x})} = \mathrm{SoftMax}_{y\in Y}(\mathbf{w}_y^\top \mathbf{x})$$

- Regularized logistic regression

$$\overline{L}(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m}\log p(y_i|\mathbf{x}_i,\mathbf{w}) - \frac{\lambda}{2}\sum_{y\in Y}\|\mathbf{w}_y\|^2 \to \max_{\mathbf{w}}$$

- **Optimization problem**

$$\min_{\mathbf{w},\xi} \frac{1}{2}\sum_{k=1}^{K}\|\mathbf{w}_k\|^2 + C\sum_{i=1}^{m}\xi_i$$

$$s.t.\ \mathbf{w}_{y_i}\mathbf{x}_i^\top - \mathbf{w}_k\mathbf{x}_i^\top + \delta_{y_i,k} \geq 1 - \xi_i,\ \xi_i \geq 0$$

$$(i,k) \in [1,m] \times Y$$

- **Decision function**:

$$h:\ \mathbf{x} \to \arg\max_{k\in Y}(\mathbf{w}_k \cdot \mathbf{x}^\top) = \arg\max_{k\in Y}\left(\sum_{i=1}^{m}\alpha_{i,k}(\mathbf{x}_i \cdot \mathbf{x}^\top)\right),$$

  where $\{\alpha_{i,k}\}_{i=1}^{m},\ k \in Y$ are dual variables
- Complex constraints, $m \cdot K$ size

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Probabilistic model

- Naive Bayes (NB) is a conditional probability model
- Given an object to be classified, represented by features $\mathbf{x} = (x_1, \ldots, x_d)$, Bayes classifier assigns probabilities

$$p(y|x_1, \ldots, x_d)$$

  for each of K possible classes $y \in Y = \{1, \ldots, K\}$
- The conditional probability can be decomposed as

$$p(y|\mathbf{x}) = \frac{p(y)p(\mathbf{x}|y)}{p(\mathbf{x})} \sim p(y)p(\mathbf{x}|y),\ y \in Y$$

- The maximum a posteriori (MAP) decision rule

$$\widehat{y} = \arg \max_{y \in \{1,\ldots,K\}} p(y)p(\mathbf{x}|y)$$

- How to model $p(\mathbf{x}|y)$?

- Let us decompose $p(y, \mathbf{x})$. Using the chain rule we get that

$$
\begin{aligned}
& p(y, x_1, \ldots, x_d) = p(x_1, \ldots, x_d, y) \\
& = p(x_1 | x_2, \ldots, x_d, y) \cdot (x_2, \ldots, x_d, y) \\
& = p(x_1 | x_2, \ldots, x_d, y) \cdot p(x_2 | x_3, \ldots, x_d, y) \cdot p(x_3, \ldots, x_d, y) = \; = \\
& \ldots = \\
& = p(x_1 | x_2, \ldots, x_d, y) \cdot \ldots \cdot p(x_{d-1} | x_d, y) \cdot p(x_d | y) \cdot p(y)
\end{aligned}
$$

- Usually $d \gg 1$ or a feature can take on a large number of values $\Leftrightarrow$ we assume independence of features
- The "naive" conditional independence: assume that each feature x_j is conditionally independent of every other feature x_s given the category y, i.e.

$$p(x_j | x_{j+1}, \ldots, x_d, y) = p(x_j | y)$$

- The joint model

$$p(y|\mathbf{x}) \sim p(y) \prod_{j=1}^{d} p(x_j|y),\ y \in Y$$

- Normalized model

$$p(y|\mathbf{x}) = \frac{1}{Z} p(y) \prod_{j=1}^{d} p(x_j|y),\ y \in Y$$

where $Z = p(\mathbf{x}) = \sum_{y \in Y} p(y)p(\mathbf{x}|y)$

- The maximum a posteriori (MAP) decision rule

$$\widehat{y} = \arg \max_{y \in \{1,\ldots,K\}} p(y) \prod_{j=1}^{d} p(x_j|y)$$

Event model of the Naive Bayes classifier

- How to define individual models for $p(x_j|y)$?
- We can use any parametric distribution model for $p(x_j|y)$!
- E.g. if x_j is continuous, we can use a Gaussian distribution, i.e.

$$p(x_j = v|y = k) = (2\pi\sigma_{jk}^2)^{-1/2} e^{-(v-\mu_{jk})^2/2\sigma_{jk}^2}$$

- Parameters $(\mu_{jk}, \sigma_{jk}^2)$ are estimated using a subsample S_{jk} of the initial sample $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$

$$S_{jk} = \{x_{ij} : (\mathbf{x}_i, y_i) \in S,\, y_i = k, i = 1, \ldots, m\}$$

Event model of the Naive Bayes classifier

- We can use various discrete distributions in case some features are categorical
- Multinomial NB: feature x_j counts the number of times event j was observed in a particular instance
- If J is a set of indexes of categorical features, then we can model their joint multimomial distribution as

$$p(x_j, j \in J | y = k) = \frac{(\sum_{j \in J} x_j)!}{\prod_{j \in J} x_j!} \prod_{j \in J} p_{kj}^{x_j}$$

- In log-scale we get a linear classifier

$$\log p(y = k | x_j, j \in J) \sim \log p(y = k) + \sum_{j \in J} x_j \cdot \log p_{kj} = b + \mathbf{w}_k \mathbf{x}_J^\top,$$

with $\mathbf{w}_k = (\log p_{kj}, j \in J)$ and $\mathbf{x}_J = (x_j, j \in J)$

Event model of the Naive Bayes classifier

- Analogously we can define Bernoulli NB: x_j is a boolean expressing the occurrence or absence of the jth term from the vocabulary

$$p(x_j, j \in J | y = k) = \prod_{j \in J} p_{kj}^{x_j} (1 - p_{kj})^{(1 - x_j)}$$

- In order to learn NB:
  - Define models for $p(\mathbf{x}|y)$
  - Estimate parameters of these models using corresponding subsampls, extracted w.r.t. values of y
  - Use MAP to predict $\widehat{y}$

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Nonparametric Estimation: Problem Statement

- $S = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \sim F$ is a given sample, $\mathbf{x} \in \mathbb{R}^1$
- $F(\mathbf{x})$ is an absolutely continuous CDF with an unknown density $p(\mathbf{x})$
- We estimate $p(\mathbf{x})$ in the point $\mathbf{x}$, i.e. construct $\widehat{p}_m(\mathbf{x}) = \widehat{p}_m(\mathbf{x}|S)$
- Typical parametric assumption

$$p \in \{p(\mathbf{x}; \boldsymbol{\theta}), \boldsymbol{\theta} \in \Theta\}, \Theta \subset \mathbb{R}^p$$

- Now we do not use such assumption $\Rightarrow$ Nonparametric Estimation

- We estimate $\widehat{p}_m(\mathbf{x})\,\forall \mathbf{x} \in \mathbb{R}^1$

Definition

Mean Integrated Squared Error:

$$MISE(\widehat{p}_m, p) = \mathbb{E}_p \left[\int_{\mathbb{R}} (\widehat{p}_m(\mathbf{x}) - p(\mathbf{x}))^2 d\mathbf{x} \right]$$

Histogram

- We consider interval $\{\mathbf{x}_1, \dots \mathbf{x}_m\} \in [a, b)$ and divide it into N equal bins Δ_i of size $h = \frac{b-a}{N}$:

$$\Delta_i = [a + ih, a + (i+1)h), i = 0, 1, \dots, N-1$$

- Let ν_i be a number of data points, belonging to Δ_i

Definition

$$\widehat{p}_m(\mathbf{x}) = \begin{cases} \frac{\nu_0}{mh}, & \mathbf{x} \in \Delta_0, \\ \dots & \\ \frac{\nu_{N-1}}{mh}, & \mathbf{x} \in \Delta_{N-1}; \end{cases} = \frac{1}{mh} \sum_{i=0}^{N-1} \nu_i 1\{\mathbf{x} \in \Delta_i\}$$

- For $\mathbf{x} \in \Delta_j$ and small h:

$$\mathbb{E}_p \widehat{p}_m(\mathbf{x}) = \frac{\mathbb{E}_p \nu_j}{mh} = \frac{\int_{\Delta_j} p(\mathbf{z}) d\mathbf{z}}{h} \approx \frac{p(\mathbf{x})h}{h} = p(\mathbf{x})$$

  At the same time

$$\text{Var}\left(\widehat{p}_m(\mathbf{x})\right) = \frac{\int_{\Delta_j} p(\mathbf{z}) d\mathbf{z} \left(1 - \int_{\Delta_j} p(\mathbf{z}) d\mathbf{z}\right)}{mh^2}$$

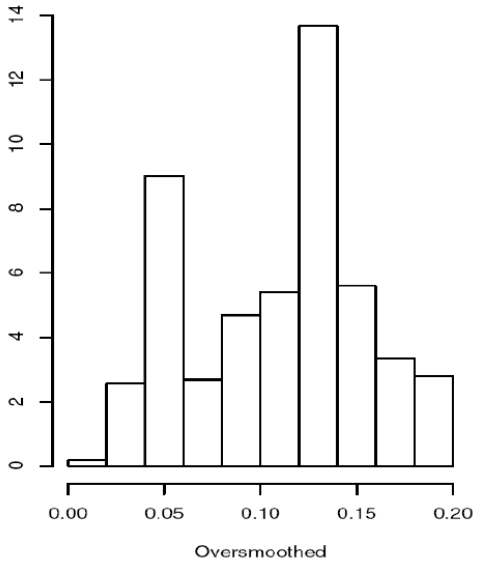
- We can prove that mean integrated squared error

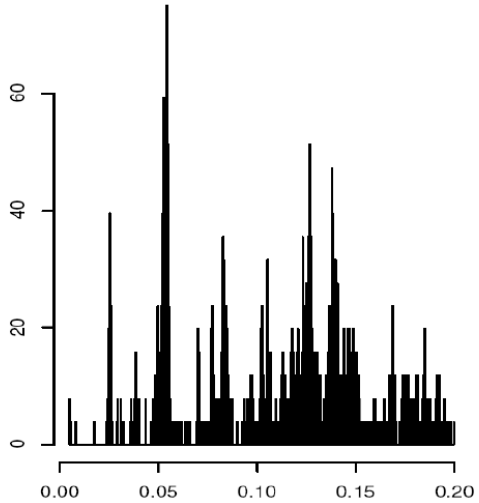
$$MISE(\widehat{p}_m, p) \approx \left(\int_{\mathbb{R}} [p'(\mathbf{x})]^2 d\mathbf{x} \right) \frac{h^2}{12} + \frac{1}{mh}$$

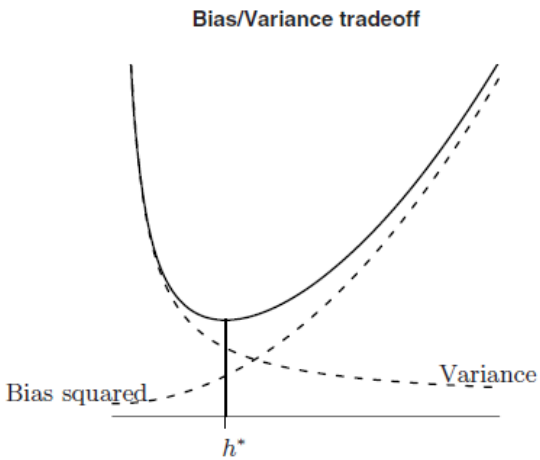
- The bigger h we use the bigger bias and smaller variance we get, and vice versa: Bias-Variance Tradeoff
- Too big h = oversmoothing, too small h = undersmoothing
- Thus for a histogram with optimal h, we get that

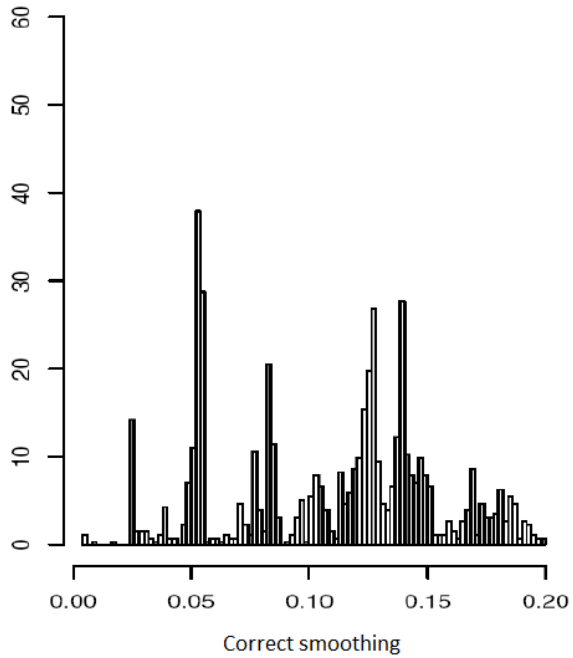
$$MISE = O(m^{-\frac{2}{3}})$$

Smoothing Selection: Example









KDE allows to get smoother estimate (compared to histogram based ones) with faster convergence rates

Definition

Kernel is a function K, such that

$$K(\mathbf{x}) \geq 0, \int_{\mathbb{R}} K(\mathbf{x})d\mathbf{x} = 1, \int_{\mathbb{R}} \mathbf{x}K(\mathbf{x})d\mathbf{x} = 0, \sigma_K^2 \equiv \int_{\mathbb{R}} \mathbf{x}^2 K(\mathbf{x})d\mathbf{x} < \infty$$

Examples

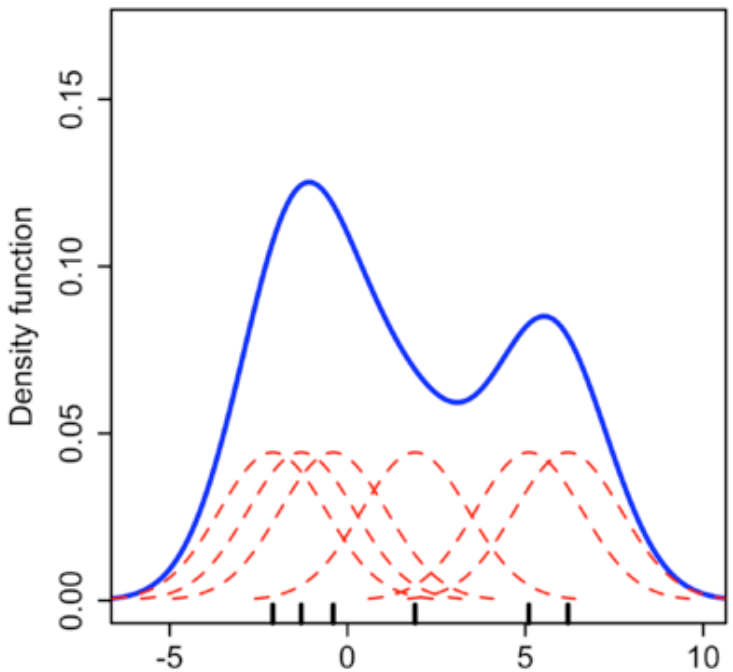
- $K(x) = \frac{1}{2}\mathbb{I}\{|x| < 1\}$ — rectangular kernel
- $K(x) = (1 - |x|)\mathbb{I}\{|x| < 1\}$ — triangle kernel
- $K(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$ — Gaussian kernel
- $K(x) = \frac{3}{4}(1 - x^2)\mathbb{I}\{|x| < 1\}$ — Epanechnikov kernel

Definition

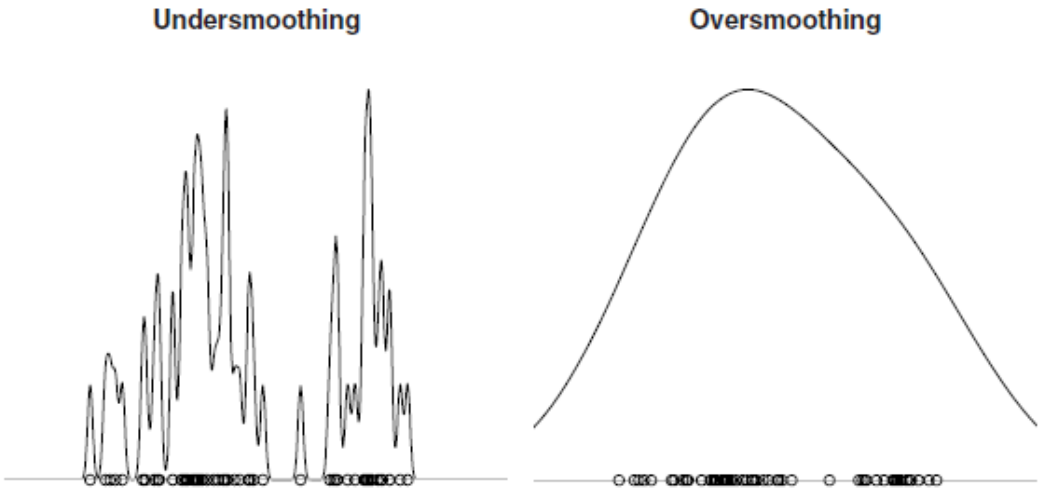
KDE has the form

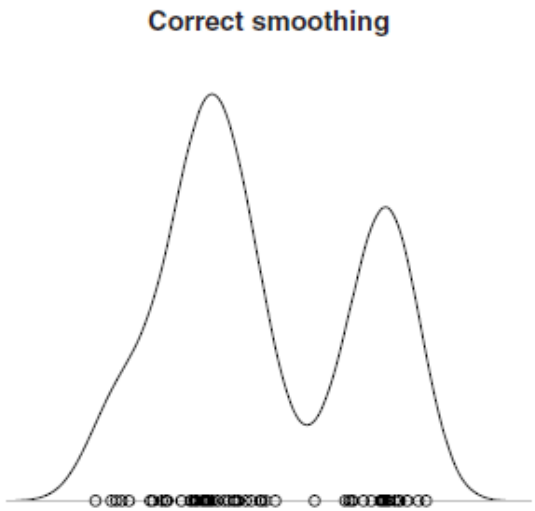
$$\widehat{p}_m(\mathbf{x}) = \frac{1}{mh} \sum_{i=1}^{m} K\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right),$$

h is a kernel width



Kernel width selection: Example





- Multidimensional case, i.e. $\mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d$ is a point in $\mathbb{R}^d$.
- Thus $i-$th observation is an d-dimensional vector:

$$\mathbf{x}_i = (x_{i1}, \ldots x_{id})$$

- Let $h = (h_1, \ldots, h_d)$ be a vector of kernel widths
- Then

$$\widehat{p}_m(\mathbf{x}) = \frac{1}{mh_1 \cdot \ldots \cdot h_d} \sum_{i=1}^{m} \left[\prod_{j=1}^{d} K\left(\frac{x_j - x_{ij}}{h_j} \right) \right]$$

Curse of Dimensionality

- Optimal rate of convergence is $O(m^{-\frac{4}{4+d}})$: if d increases convergence rate decreases

- Let us consider a table with values of m necessary to get the mean squared estimation error in $\mathbf{x}_0 = 0$ less than 0.1 depending on d for a multidimensional normal density and optimal kernel width:

d	1	2	3	4	5	6	7	8	9
m	4	19	67	223	768	2790	10700	43700	187000

- Here d is a dimension, m is a sample size

Nonparametric regression: Definition

- Let us consider m observations: $S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$, generated from a joint density $p(\mathbf{x}, y)$
- These observations are generated by the model

$$y_i = f(\mathbf{x}_i) + \varepsilon_i,$$

  where ε_i is an i.i.d white noise, $\mathbb{E}\varepsilon_i = 0$, $\mathbb{V}(\varepsilon_i) = \sigma^2$
- We should estimate a regression function

$$f(\mathbf{x}) = \mathbb{E}(y|\mathbf{x}) = \int_{\mathbb{R}} yp(y|\mathbf{x})dy = \frac{\int_{\mathbb{R}} yp(\mathbf{x}, y)dy}{\int_{\mathbb{R}} p(\mathbf{x}, y)dy} = \frac{\int_{\mathbb{R}} yp(\mathbf{x}, y)dy}{p(\mathbf{x})}$$

Definition

Let K denote a kernel, and

- $\widehat{p}_m(\mathbf{x})$ be a kernel density estimate, obtained using $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$,
- $\widehat{p}_m(\mathbf{x}, y)$ be a kernel density estimate, obtained using $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$.

If $\widehat{p}_m(\mathbf{x}) \neq 0$, then

$$\widehat{f}_m^{NW}(\mathbf{x}) = \frac{\int_{\mathbb{R}} y \widehat{p}_m(\mathbf{x}, y) dy}{\widehat{p}_m(\mathbf{x})}$$

We can notice that Nadaraya-Watson estimate can be used also in case when $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$ are some fixed and deterministic values, e.g. $\mathbf{x}_i = \frac{i}{m}$

We use Nadaraya-Watson estimate for $f(\mathbf{x})$:

Definition

Nadaraya-Watson estimate has the form

$$\widehat{f}_m^{NW}(\mathbf{x}) = \sum_{i=1}^{m} w_i(\mathbf{x}) y_i,$$

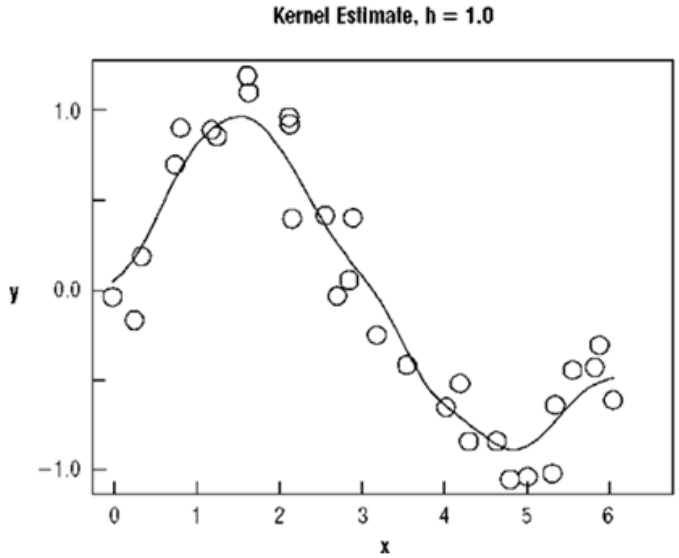
where

$$w_i = \frac{K(\frac{\mathbf{x}-\mathbf{x}_i}{h})}{\sum_{j=1}^{m} K(\frac{\mathbf{x}-\mathbf{x}_j}{h})},$$

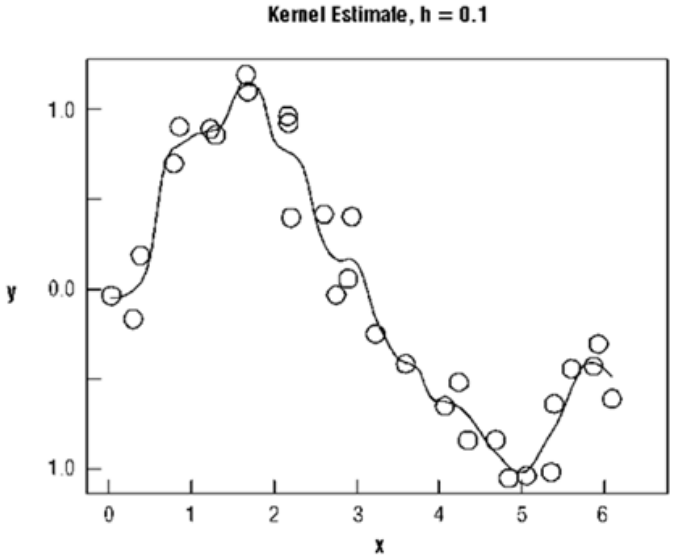
and K is a some kernel function

Thus, the estimate is a weighted sum of y_i, where any point, close to $\mathbf{x}$, has a big weight

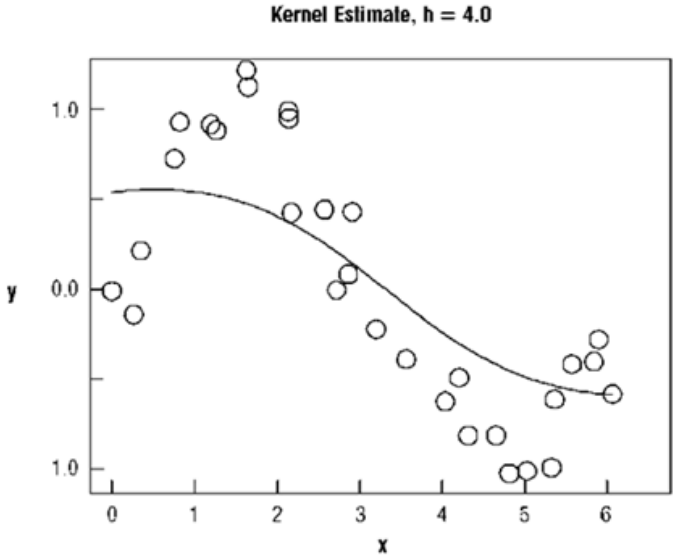
Nonparametric regression: Example



Correct smoothing



Undersmoothing



Oversmoothing

Definition

Bias: $\text{bias}(\mathbf{x}_0) = \mathbb{E}_p \widehat{p}_m(\mathbf{x}_0) - p(\mathbf{x}_0)$

We get the following decomposition

Lemma

$$MSE(\widehat{p}_m, p, \mathbf{x}_0) = \text{bias}^2(\mathbf{x}_0) + \mathbb{V}_p(\widehat{p}_m(\mathbf{x}_0)) =$$
$$= [\mathbb{E}_p \widehat{p}_m(\mathbf{x}_0) - p(\mathbf{x}_0)]^2 + \mathbb{E}_p[\widehat{p}_m(\mathbf{x}_0) - \mathbb{E}_p \widehat{p}_m(\mathbf{x}_0)]^2$$

Lemma

$$MISE(\widehat{p}_m, p) = \int_{\mathbb{R}} \text{bias}^2(\mathbf{x}) d\mathbf{x} + \int_{\mathbb{R}} \mathbb{V}_p(\widehat{p}_m(\mathbf{x})) dx$$

We will use these statements when constructing optimal density estimates

KDE: MISE

A shape of K influence quality of estimate not so significant compared to a value of h

Theorem

$$MISE(\widehat{p}_m, p) \approx \frac{1}{4}\sigma_K^4 h^4 \int_{\mathbb{R}} (p''(\mathbf{x}))^2 d\mathbf{x} + \frac{1}{mh} \int_{\mathbb{R}} (K(\mathbf{x}))^2 d\mathbf{x}$$

For an optimal kernel width we get that $MISE(\widehat{p}_m, p) = O\left(m^{-\frac{4}{5}}\right)$

Optimal Width

- Again we can not calculate h^* in practice, since it depends on unknown values of $r(\mathbf{x})$, $p(\mathbf{x})$
- Then we should minimize the risk estimate w.r.t. h

$$\widehat{\mathcal{J}}(h) = \sum_{i=1}^{m} (y_i - \widehat{r}^{NW}_{(-i)}(\mathbf{x}_i))^2,$$

where $\widehat{r}^{NW}_{(-i)}$ is a Nadaraya-Watson estimate, constructed using the sample, from which the observation $(\mathbf{x}_i, y_i)$ is excluded

Theorem

$$\widehat{\mathcal{J}}(h) = \sum_{i=1}^{m} \left(y_i - \widehat{r}^{NW}(\mathbf{x}_i)\right)^2 \frac{1}{\left(1 - \frac{K(0)}{\sum_{j=1}^{m} K\left(\frac{\mathbf{x}_i - \mathbf{x}_j}{h}\right)}\right)^2}$$