Klasifikace pomocí hloubky dat – nové nápady

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Z. Fabián: Vzpomínka na Compstat 2010 aneb večeře na Pařížské radnici, Informační Bulletin ČStS, 4/2017

Nápad pořádat konferenci v Paříži se dustojně řadí k nápadu pořádat mistrovství světa v Kataru nebo letní olympiádu v Letňanech. ...



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Outliers in \mathbb{R}^1





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Outliers in \mathbb{R}^2 – any idea?



1st idea – Mahalanobist distance



1st idea – Mahalanobist distance – non-elliptical case



1st idea – Mahalanobist distance – non-elliptical case



Halfspace depth in \mathbb{R}^1

$$D(x) = \min \{P(X \le x), P(X \ge x)\}$$

Example: univariate normal distribution N(μ, σ^2)



Halfspace depth in \mathbb{R}^d

projection pursuit approach

$$D(\mathbf{x}) = \inf_{\mathbf{u}:\|\mathbf{u}\|=1} D(\mathbf{u}^T \mathbf{x}).$$



The **halfspace depth** of a point $x \in \mathbb{R}^d$ with respect to a probability measure P on \mathbb{R}^d is defined as the minimum probability mass carried by any closed halfspace containing x, that is

 $D(\mathbf{x}; P) = \inf \{ P(H) : H \text{ a closed halfspace}, \mathbf{x} \in H \}$

- The depth provides so called central-outward ordering of data
- The deepest point extends the notion of median into a higher dimensions.

Problem of classification

The Bayes classifier

$$class(\mathbf{x}) = \arg \max_{i} f_i(\mathbf{x}) \pi_i.$$

produces smallest possible number of misclassified points (total over all groups)

When Bayes misclassifies the centre of the distribution...

$$egin{aligned} P_1 &= \mathcal{N}(0,1), P_2 &= \mathcal{N}(1,1) \ \pi_1 &= 0.7, \pi_2 &= 0.3 \end{aligned}$$



Hey, Bayes, be fair to x_2 ! lognormal distribution from N(0, 1)



 $\begin{aligned} \text{quantile}_{0.05} &= x_1, \qquad f(x_1) = 0.53 \\ \text{quantile}_{0.95} &= x_2, \qquad f(x_2) = 0.02 \end{aligned}$

Basics in decision theory

- ► Distributions P_i defined on ℝ^d, with densities f_i and prior probabilities π_i, i = 1,..., K.
- A classifier divides the space \mathbb{R}^d into K disjoint parts $A_i, i = 1, ..., K, \bigcup_{i=1}^K A_i = \mathbb{R}^d$ such that any $\mathbf{x} \in \mathbb{R}^d$ is assigned to P_i iff $\mathbf{x} \in A_i$.
- Cost function

$$c_{ij}(\boldsymbol{x}) = \begin{cases} c_i(\boldsymbol{x}) & \text{if } j \neq i, \\ 0 & \text{if } j = i. \end{cases}$$

Total cost

$$\min\sum_{i=1}^{K}\sum_{j\neq i}\int_{A_j}c_i(\boldsymbol{x})f_i(\boldsymbol{x})\pi_i d\boldsymbol{x}.$$

Optimal classifier

$$class(\mathbf{x}) = \arg\max_{i} c_i(\mathbf{x}) f_i(\mathbf{x}) \pi_i.$$

Bayes classifier and its 2 new competitors

$$class(\mathbf{x}) = \arg\max_{i} c_i(\mathbf{x}) f_i(\mathbf{x}) \pi_i.$$

1. Bayes classifier: $c_i(x) = 1$

$$class_B(\mathbf{x}) = \arg\max_i f_i(\mathbf{x})\pi_i$$

2. Depth-weighted classifier: $c_i(\mathbf{x}) = D(\mathbf{x}; P_i)$

 $class_D(\mathbf{x}) = \arg\max_i D(\mathbf{x}; P_i) f_i(\mathbf{x}) \pi_i$

3. Rank-weighted classifier: $c_i(\mathbf{x}) = F_i(D(\mathbf{x}; P_i))$, where F_i is CDF of $D(\mathbf{X}; P_i), \mathbf{X} \sim P_i$

 $class_R(\mathbf{x}) = \arg\max_i F_i(D(\mathbf{x}; P_i))f_i(\mathbf{x})\pi_i$

Toy example

- ► $P_1 = Unif[0, 100], \pi_1 = 0.5,$ $P_2 = Unif[50, 250], \pi_2 = 0.5.$
- Classification on the overlapping part of supports: Bayes classifier:

$$class_B(x) = 1$$
 for $x \in [50, 100]$

Depth-weighted classifier:

$$class_D(x) = egin{cases} 1 & ext{for } x \in [50, 90), \\ 2 & ext{for } x \in (90, 100]. \end{cases}$$



Example 1: Uniform distributions, red: $P_1 = Unif[0, 100]$; blue: $P_2 = Unif[50, 250]$, $\pi_1 = \pi_2 = 0.5$. The Bayes classifier: x = 100, $P(class(x) \neq i|x \in P_i) = 0.125$,

 $\begin{aligned} P(class(x) \neq 1 | x \in P_1) &= 0, \ P(class(x) \neq 2 | x \in P_2) = 0.25. \\ \text{The depth-weighted classifier: } x &= 90, \ P(class(x) \neq i | x \in P_i) = 0.15, \\ P(class(x) \neq 1 | x \in P_1) = 0.1, \ P(class(x) \neq 2 | x \in P_2) = 0.2. \end{aligned}$

The first question (or two)

- To what extent do the new (depth-weighted) classifiers differ from the Bayes classifier?
- How large might the corresponding difference in the average misclassification rate be?

Difference in the case of elliptical symmetry

Let us assume:

- (P1): f_i(x) = k_ig(M_i(x)), where g is a strictly decreasing function, k_i > 0 are constants, and M_i(x) = ((x − α_i)'B_i⁻¹(x − α_i))^{1/2} with B_i positive definite, α_i ∈ ℝ^d, denotes the generalized distance of the point x from the center of the distribution P_i.
- (P2) $D(\mathbf{x})$ is an affine invariant depth. Then, given (P1), $D_i(\mathbf{x}) = D(\mathbf{x}; P_i)$ is a fixed decreasing function of generalized distance, that can be expressed as $D_i(\mathbf{x}) = h(M_i(\mathbf{x}))$, where h is a strictly decreasing function.

Denote

Then

- The Bayes classifier assigns \mathbf{x} to P_1 if $G(\mathbf{x}) > \pi$,
- The depth-weighted classifier assigns \mathbf{x} to P_1 if $H(\mathbf{x})G(\mathbf{x}) > \pi$.

Difference in the case of elliptical symmetry



The classifiers differ when π is between $G(\mathbf{x})$ and $H(\mathbf{x})G(\mathbf{x})$. For the fixed π , the region where the classifiers differ is

$$RD(\pi) = \big\{ \mathbf{x} \in \mathbb{R}^d : H(\mathbf{x})G(\mathbf{x}) < \pi < G(\mathbf{x}) \text{ or } G(\mathbf{x}) < \pi < H(\mathbf{x})G(\mathbf{x}) \big\}.$$

Let (P1) and (P2) hold for P_1 and P_2 . Then $P(class_B(\boldsymbol{X}) \neq class_D(\boldsymbol{X})) = 0 \Leftrightarrow \pi_1 k_1 = \pi_2 k_2.$ Difference in the case of elliptical symmetry – example

$$P_1 = N(-1, 1), P_2 = N(1, 1)$$



Next question

- To what extent does the performance of the new classifiers depend on the choice of depth function?
- Which depth function results in the smallest (biggest) differences from the Bayes classifier?

Difference between the depth-based classifiers using halfspace and projection depths

$$P_1 = Unif[0, 100], \pi_1 = 0.5,$$

 $P_2 = Unif[50, 250], \pi_2 = 0.5.$



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Rank-weighted classifier

• Depth-weighted classifier: $c_i(\mathbf{x}) = D(\mathbf{x}; P_i)$

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class_D(\mathbf{x}) = \arg\max_i D(\mathbf{x}; P_i) f_i(\mathbf{x}) \pi_i
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► Rank-weighted classifier: $c_i(\mathbf{x}) = F_i(D(\mathbf{x}; P_i))$, where F_i is CDF of $D(\mathbf{X}; P_i)$, $\mathbf{X} \sim P_i$

$$class_R(\mathbf{x}) = \arg\max_i F_i(D(\mathbf{x}; P_i))f_i(\mathbf{x})\pi_i$$

Let (P1) and (P2) hold for P_1 and P_2 and any two depth functions $D(\cdot)$ and $D^*(\cdot)$. Then $class_R(\mathbf{x})$ is the same for both $D(\cdot)$ and $D^*(\cdot)$ with probability one.

Robustness of the newly proposed classifiers



• $(1-\alpha)\pi_1$ for P_1 ,

- $\alpha \pi_1$ for the contamination of P_1
- π_2 for the non-contaminated P_2 .

Assume $z_0 = z$, $\pi_2 < \alpha \pi_1$.

Robustness of the newly proposed classifiers



• $(1 - \alpha)\pi_1$ for P_1 ,

- $\alpha \pi_1$ for the contamination of P_1
- π_2 for the non-contaminated P_2 .

Assume $z_0 = z$, $\pi_2 < \alpha \pi_1$.

- ► $f_2(x)\pi_2 < f_1(x)\pi_1$ for all $x \in (2z, 4z)$. Misclass. rate for group 2 is 1.
- ► $D_2(x)f_2(x)\pi_2 > D_1(x)f_1(x)\pi_1$ for $x > 2z + \sqrt{2\pi_2}z$ Misclass. rate for group 2 is π_2

Simulation study – settings

	Group 1		Group 2	
Ex.	Distribution	Parameters	Distribution	Parameters
1	Normal	0, Σ ₀	Normal	1, Σ ₀
2	Normal	0, Σ ₀	Normal	1, 4Σ ₀
3	Cauchy	0 , Σ ₀	Cauchy	1, Σ ₀
4	Cauchy	0, Σ ₀	Cauchy	1, 4Σ ₀
5	Bivar. exponen.	1, 1	Shifted bivar. expon. (+1)	1, 1
6	Bivar. exponen.	1, 1/2	Shifted bivar. expon. (+1)	1/2, 1
7	Normal	0, /	Bivar. exponential	1, 1
8	Skewed normal	$\left(\begin{smallmatrix}1\\2\end{smallmatrix}\right), \left(\begin{smallmatrix}1&0\\0&7\end{smallmatrix}\right), \left(\begin{smallmatrix}-2\\-5\end{smallmatrix}\right)$	Skewed normal	$\left(\begin{smallmatrix} 0\\ -1 \end{smallmatrix}\right), \left(\begin{smallmatrix} 1 & 0\\ 0 & 5 \end{smallmatrix}\right), \left(\begin{smallmatrix} 1\\ 5 \end{smallmatrix}\right)$

Where
$$\mathbf{\Sigma}_0 = \left(egin{array}{cc} 1 & 1 \\ 1 & 4 \end{array}
ight).$$

Percentage of points classified differently than by the Bayes classifier



Increase of AMR versus percentage of points classified differently than by the Bayes classifier



Conclusion

- We suggest to weight misclassification cost according to the centrality of a misclassified point measured either by its depth w.r.t. the distribution from which it comes (depth-weighted classifier) or by its rank w.r.t. the distribution from which it comes (rank-weighted classifier).
- In particular cases, the new classifiers does not differ from the Bayes classifier. Simulation study showed that increase in AMR is much smaller than percentage of points classified differently.
- Both classifiers depend on the depth function which they are using. In particular cases rank-weighted classifier does not depend on the used depth function.
- Presence of the depth term in the depth-based classifiers may substantially increase robustness of the procedure.

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Happy end

