Depth and depth-based classification

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Machine Learning

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Linear discriminant analysis

- **Assumptions:** Two classes are normally distributed with the same covariance matrix, *i.e.* $X|Y = j \sim N(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$, $j = 0, 1$ or

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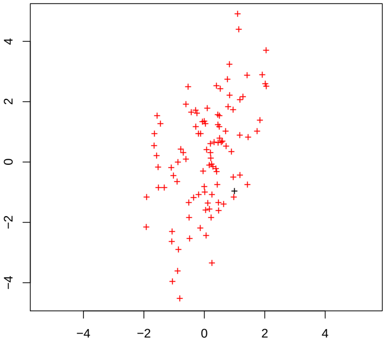
- Equivalently one can write

$$g(\boldsymbol{x}) = \begin{cases} 1 & d^2_{Mah}(\boldsymbol{x}, \boldsymbol{\mu}_0; \boldsymbol{\Sigma}_0) > d^2_{Mah}(\boldsymbol{x}, \boldsymbol{\mu}_1; \boldsymbol{\Sigma}_1)\,, \\ 0 & \text{else}\,. \end{cases}$$

Mahalanobis distance

- Regard a data set $\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n\} \subset \mathbb{R}^d$ and a point $\boldsymbol{x} \in \mathbb{R}^d$.



- How central (or representative) is $\boldsymbol{x}$ with respect to $\boldsymbol{X}$?

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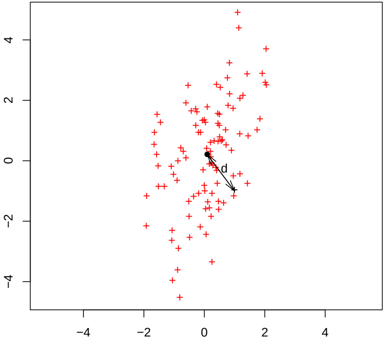

- Euclidean distance from $\boldsymbol{x}$ to $\boldsymbol{\mu}_{\boldsymbol{X}}$:

$$d^2_{Eucl}(\boldsymbol{x}, \boldsymbol{\mu}_{\boldsymbol{X}}) = (\boldsymbol{x} - \boldsymbol{\mu}_{\boldsymbol{X}})^\top (\boldsymbol{x} - \boldsymbol{\mu}_{\boldsymbol{X}}) \,.$$

- Sample mean: $\boldsymbol{\mu}_{\boldsymbol{X}} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_i$.

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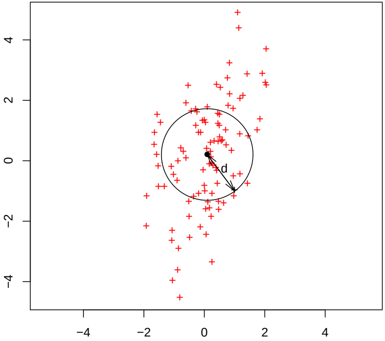

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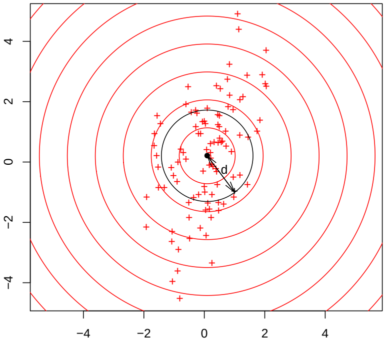

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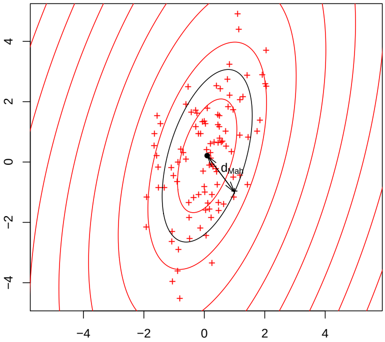

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- Sample mean: $\boldsymbol{\mu}_{\boldsymbol{X}} = \frac{1}{n}\sum_{i=1}^n \boldsymbol{x}_i$.
- Sample covariance matrix: $\boldsymbol{\Sigma}_{\boldsymbol{X}} = \frac{1}{n-1}\sum_{i=1}^n (\boldsymbol{x}_i - \boldsymbol{\mu}_{\boldsymbol{X}})(\boldsymbol{x}_i - \boldsymbol{\mu}_{\boldsymbol{X}})^\top$.

Mahalanobis depth (Mahalanobis, 1936)

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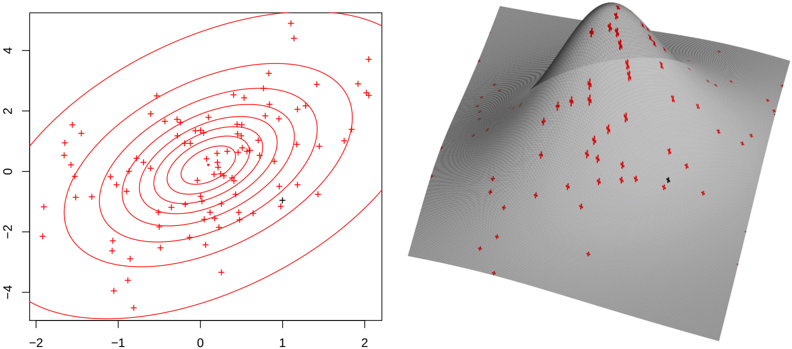

- **Mahalanobis depth** of $\boldsymbol{x}$ = a *centrality measure*:

$$D^{Mah(n)}(\boldsymbol{x}|\boldsymbol{X}) = \frac{1}{1 + d^2_{Mah}(\boldsymbol{x}, \boldsymbol{\mu}_{\boldsymbol{X}}; \boldsymbol{\Sigma}_{\boldsymbol{X}})} = \frac{1}{1 + (\boldsymbol{x} - \boldsymbol{\mu}_{\boldsymbol{X}})^\top \boldsymbol{\Sigma}_{\boldsymbol{X}}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_{\boldsymbol{X}})}$$

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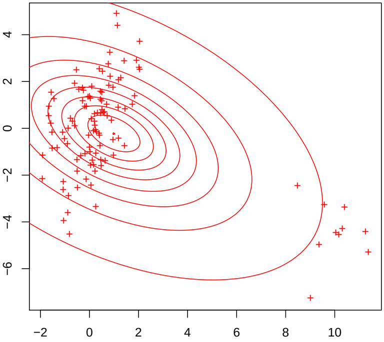

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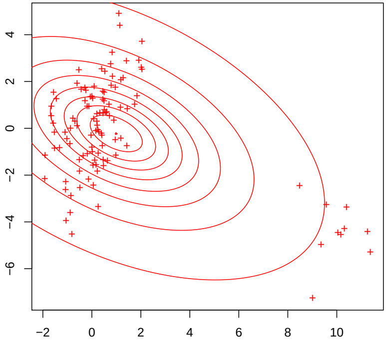

- Robust estimates for $\boldsymbol{\mu_X}$ and $\boldsymbol{\Sigma_X}$ can be used, like *minimum covariance determinant* estimator; this is not the topic of the lecture.

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- Tukey depth of $\boldsymbol{x} \in \mathbb{R}^d$ with respect to a d-variate random vector X distributed as P is defined as the smallest probability mass of a closed halfspace containing $\boldsymbol{x}$:

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- Thus, Tukey depth of $\boldsymbol{x}$ with respect to a data set $\boldsymbol{X} = \{\boldsymbol{x}_1, ..., \boldsymbol{x}_n\} \subset \mathbb{R}^d$ can be formulated as:

$$D^{Tuk(n)}(\boldsymbol{x}|\boldsymbol{X}) = \frac{1}{n} \min_{\boldsymbol{u} \in S^{d-1}} \sharp\{i : \boldsymbol{u}'\boldsymbol{x}_i \geq \boldsymbol{u}'\boldsymbol{x}\}.$$

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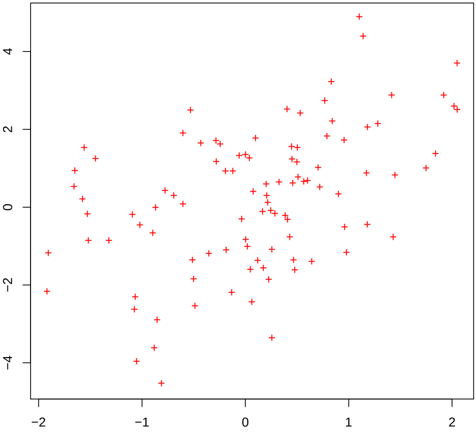

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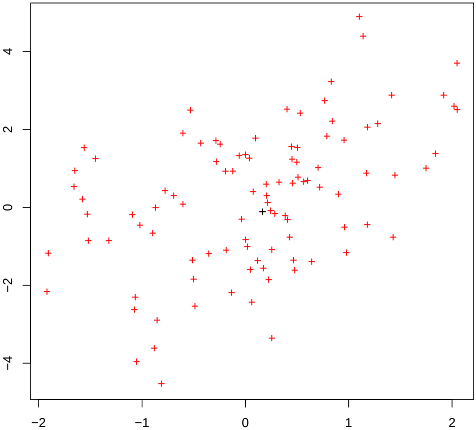

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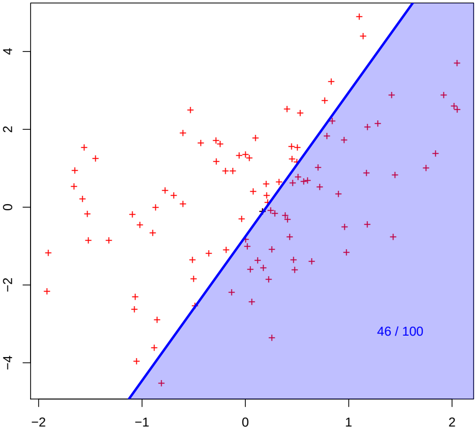

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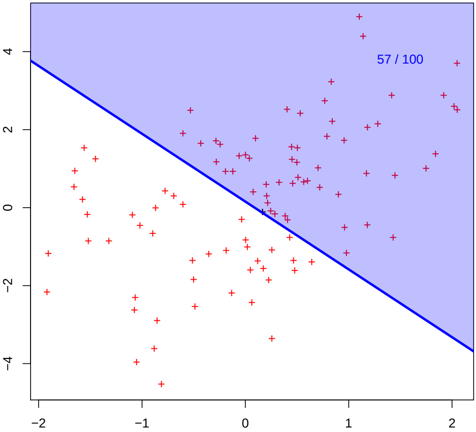

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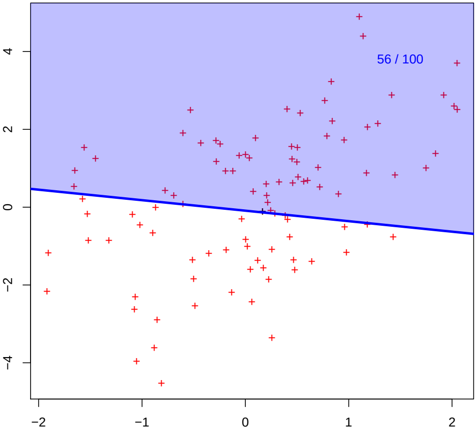

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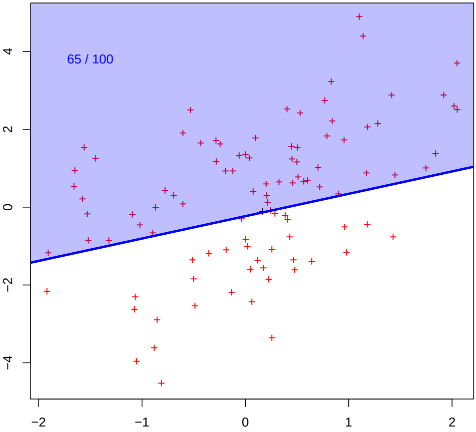

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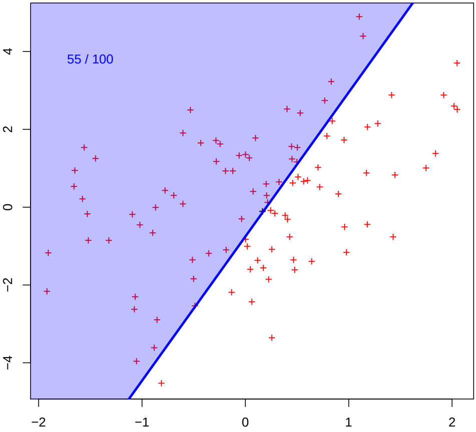

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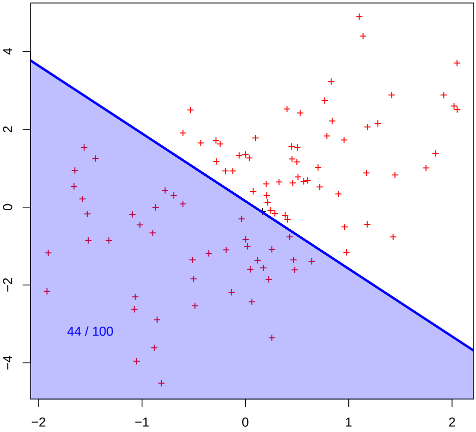

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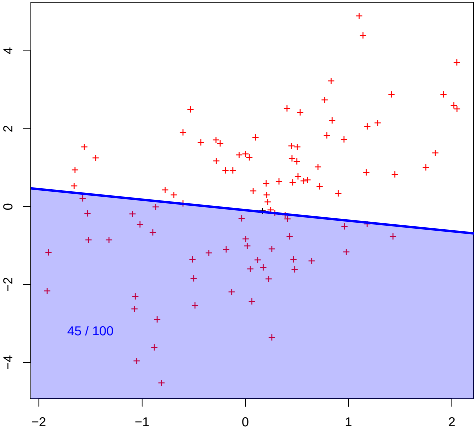

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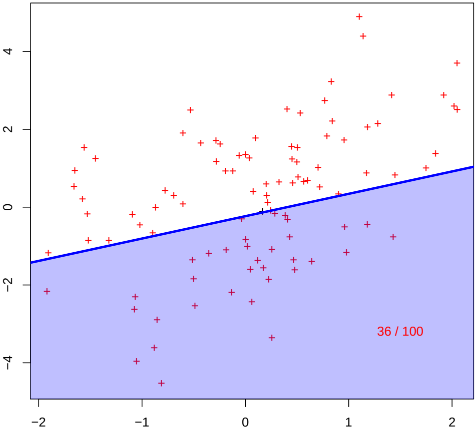

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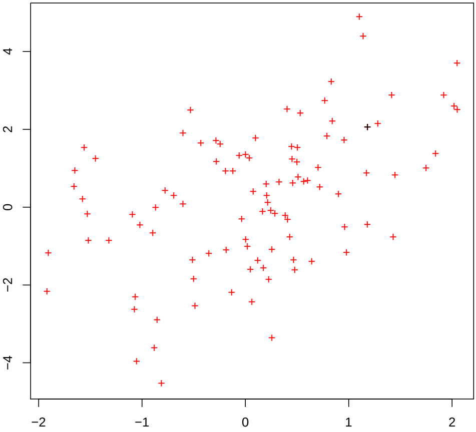

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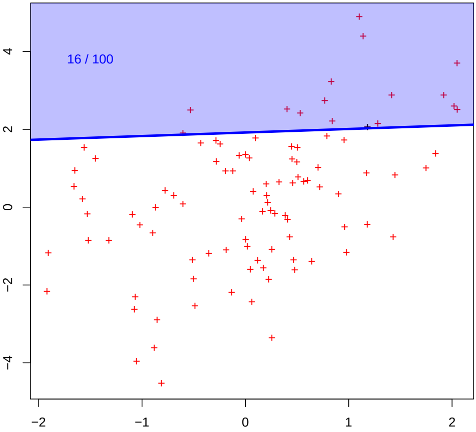

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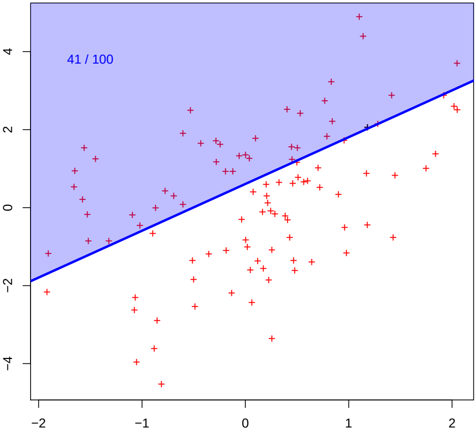

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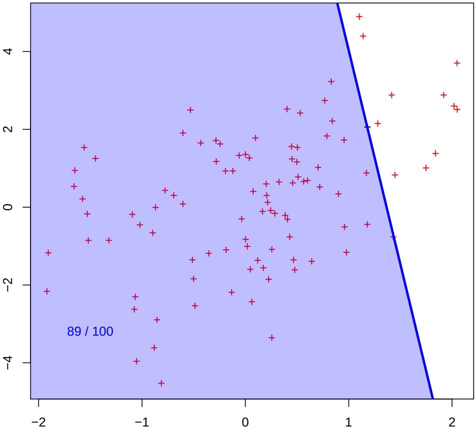

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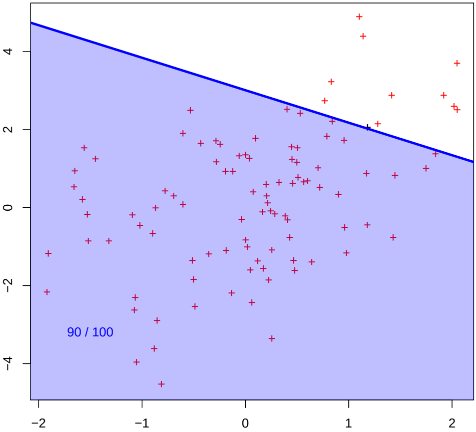

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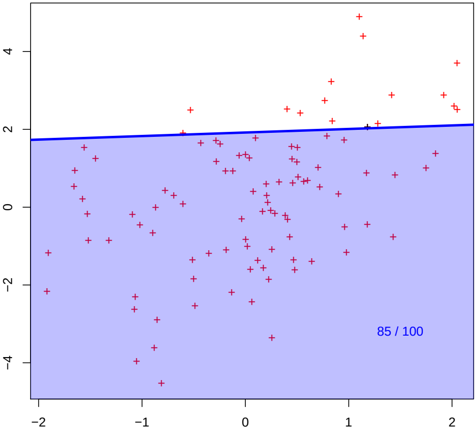

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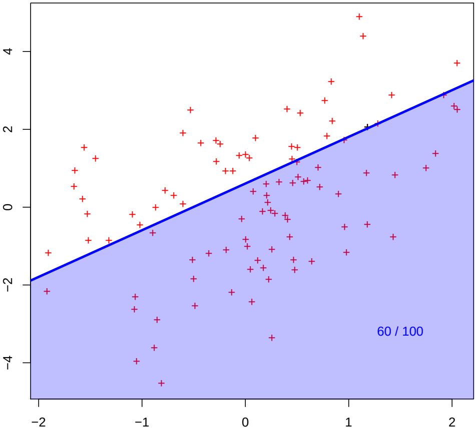

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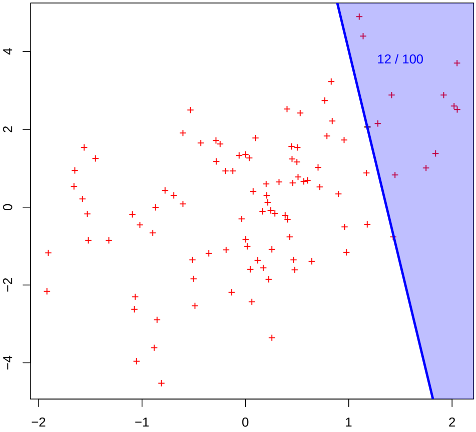

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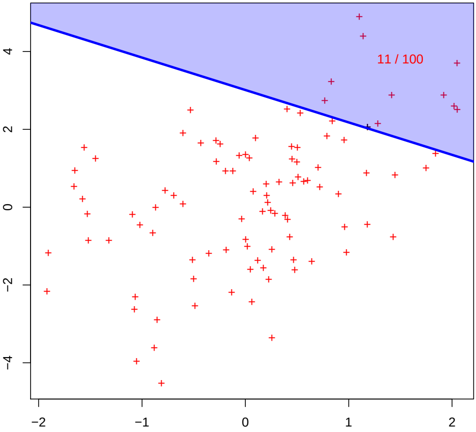

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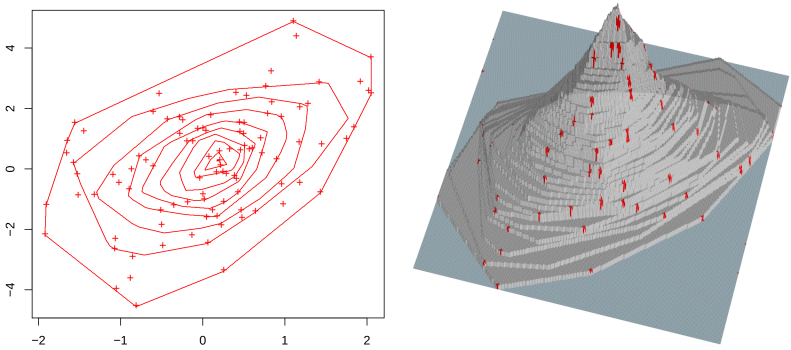

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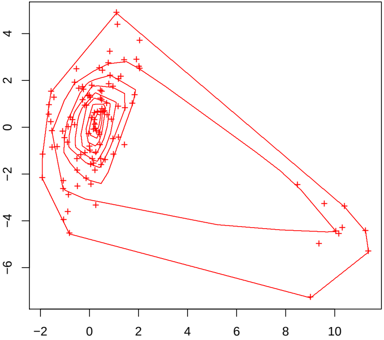

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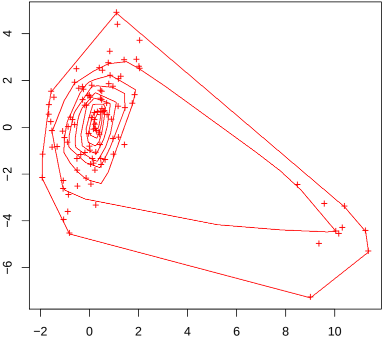

- The depth is entirely non-parametric since is based on the information about halfspaces only.

Contents

Zonoid depth (Koshevoy & Mosler, 1997; Mosler, 2002)

Koshevoy & Mosler (1997) and Mosler (2002) define the **zonoid trimmed region** as:

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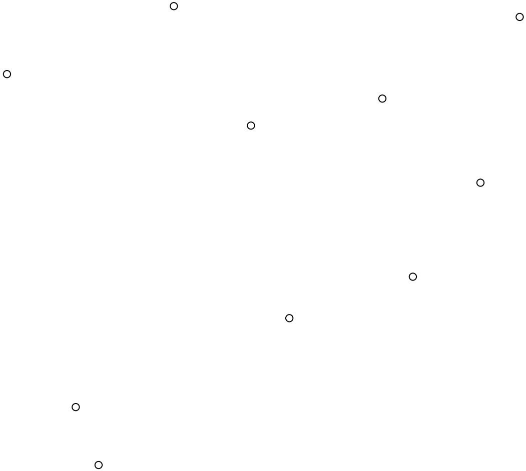

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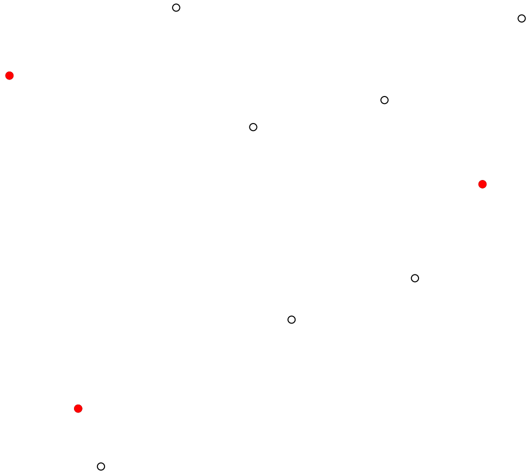

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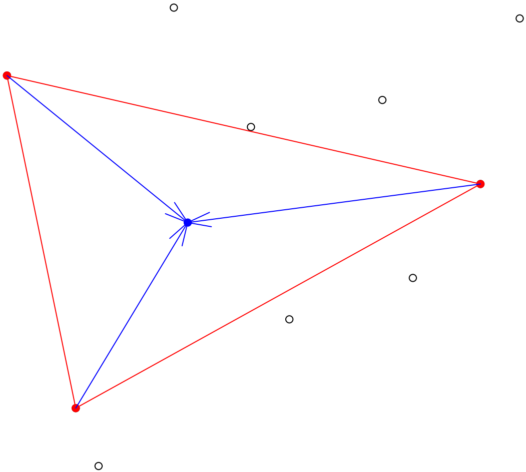

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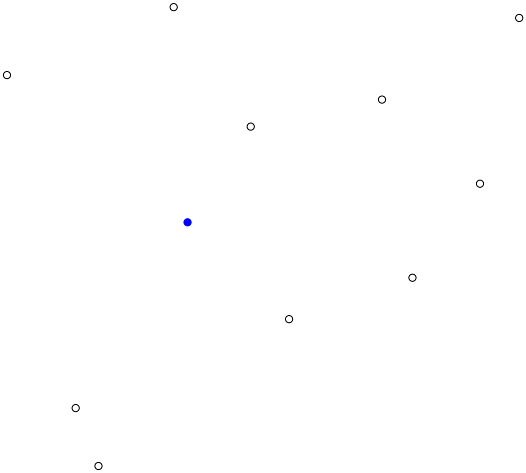

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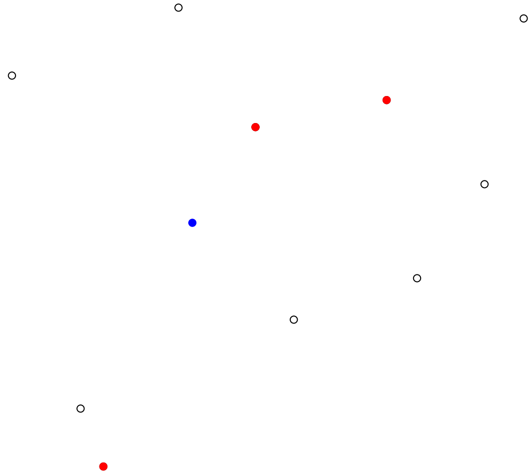

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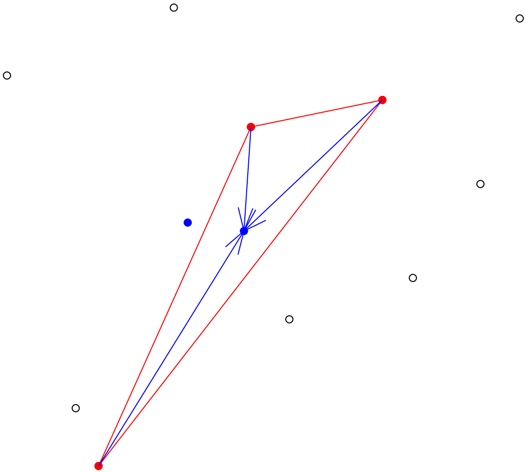

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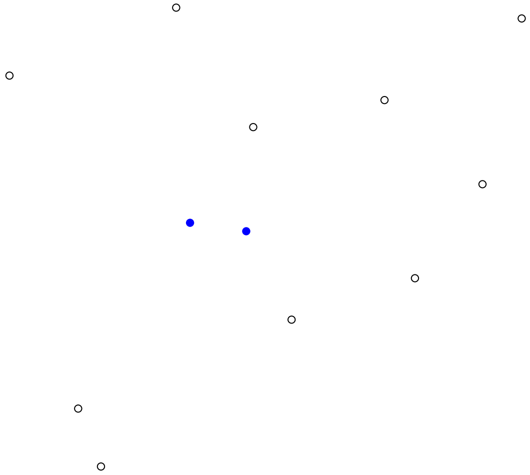

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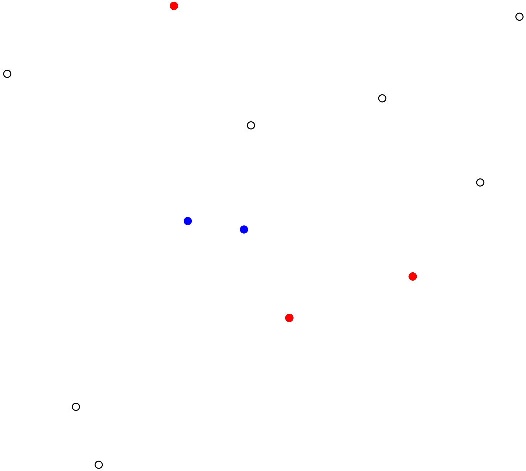

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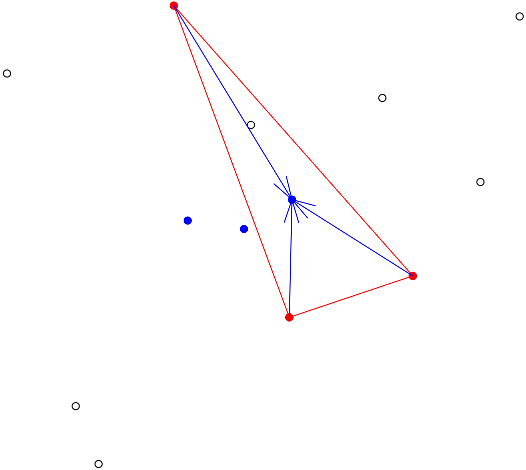

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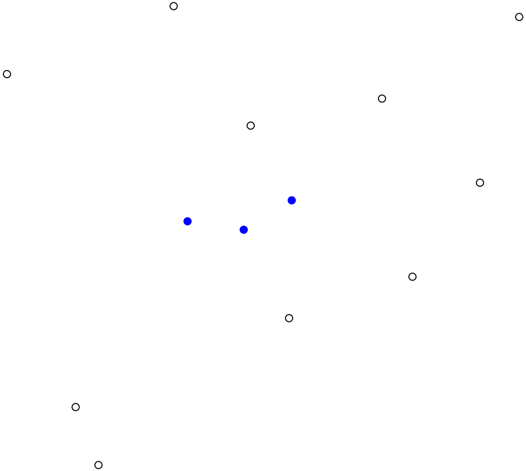

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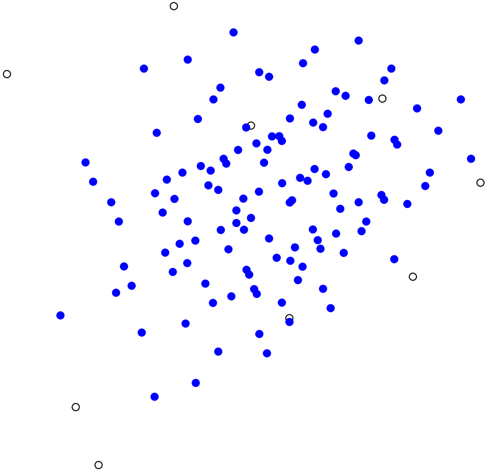

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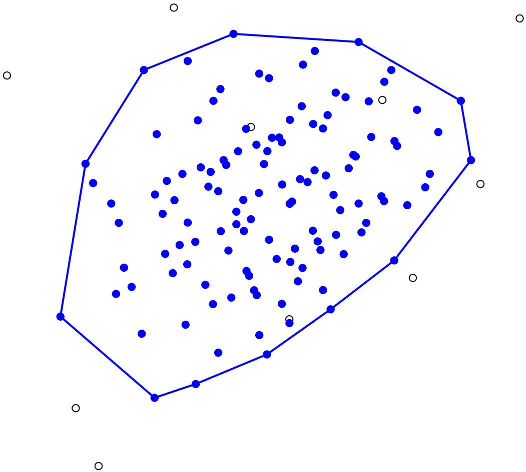

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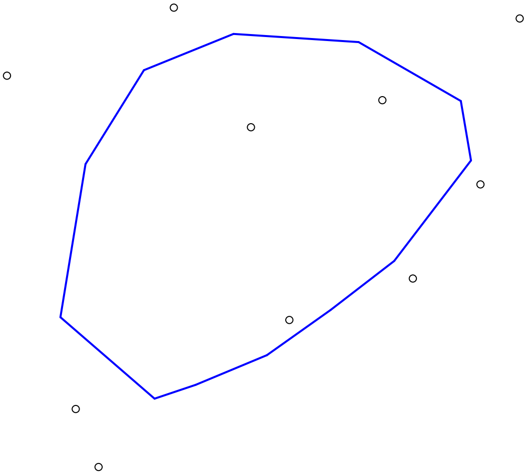

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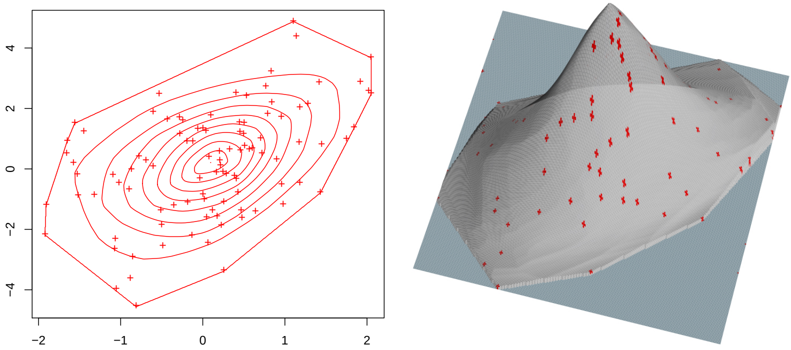

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$$\begin{aligned} \min \gamma \quad \text{s. t.} \quad \boldsymbol{X}^T\boldsymbol{\lambda} &= \boldsymbol{x}, \\ \boldsymbol{\lambda}^T\mathbf{1}_n &= 1, \\ \gamma\mathbf{1}_n - \boldsymbol{\lambda} &\ge \mathbf{0}_n, \\ \boldsymbol{\lambda} &\ge \mathbf{0}_n. \end{aligned}$$

(Notation: $\boldsymbol{X} = (\boldsymbol{x}_1, ..., \boldsymbol{x}_n)^T$, $\boldsymbol{\lambda} = (\lambda_1, ..., \lambda_n)^T$.)

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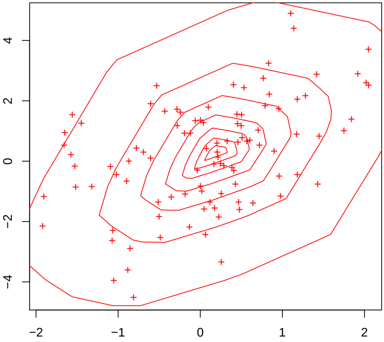

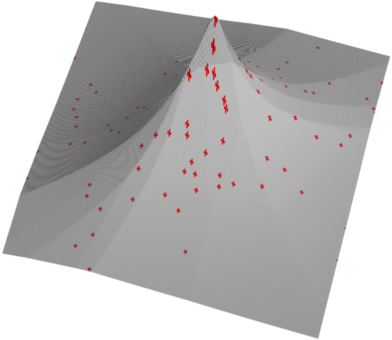

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A **data depth** measures how "close" a given point is located to the "center" of a distribution. For $\boldsymbol{x} \in \mathbb{R}^d$ and a d-variate random vector X distributed as $P \in \mathcal{P}$, a data depth is a function

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D4 **monotone on rays:** for any $\boldsymbol{x}^* \in \arg\max_{\boldsymbol{x} \in \mathbb{R}^d} D(\boldsymbol{x}|X)$, any $\boldsymbol{x} \in \mathbb{R}^d$, and any $0 \leq \alpha \leq 1$ it holds: $D(\boldsymbol{x}|X) \leq D(\boldsymbol{x}^* + \alpha(\boldsymbol{x} - \boldsymbol{x}^*)|X)$;

D5 **upper semicontinuous in $\boldsymbol{x}$:** the upper-level sets $D_\alpha(X) = \{\boldsymbol{x} \in \mathbb{R}^d : D(\boldsymbol{x}|X) \geq \alpha\}$ are closed for all α.

Statistical data depth (Mosler, 2013)

Some remarks:

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  If X is centrally symmetric about $\boldsymbol{x}^*$, then any depth function satisfying D1 – D5 $D(\cdot|X)$ is maximal at $\boldsymbol{x}^*$.

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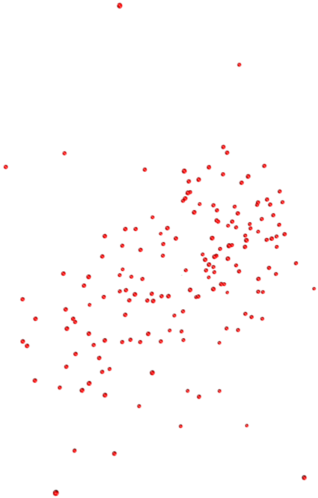
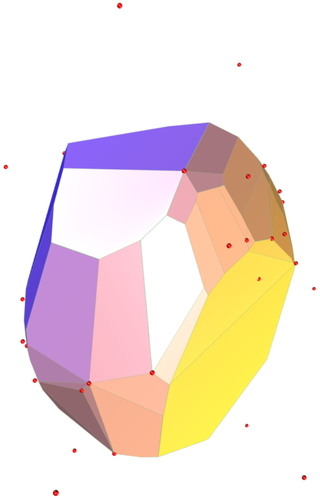
  - Due to **D5** $D_\alpha(X)$ is closed.

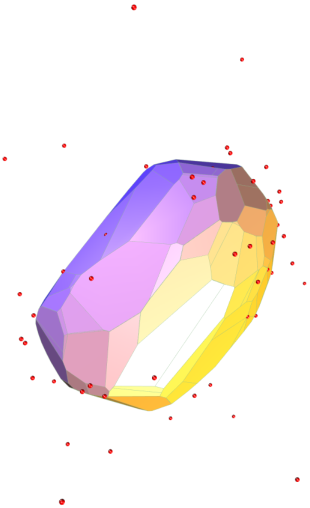
Tukey (halfspace, location) depth region



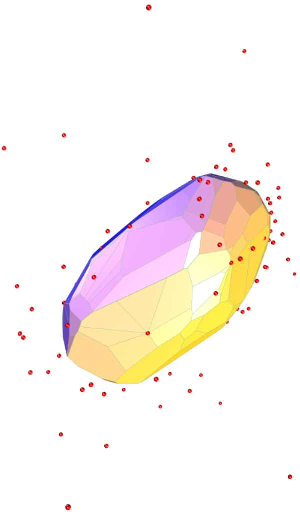
Tukey (halfspace, location) depth region: $\alpha = 2/161$



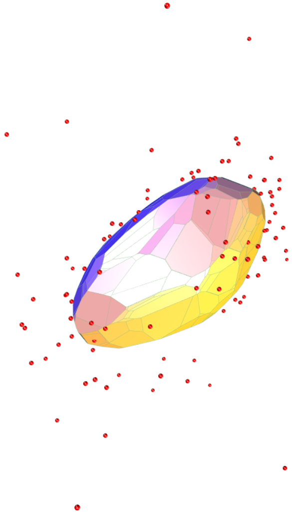
Tukey (halfspace, location) depth region: $\alpha = 5/161$



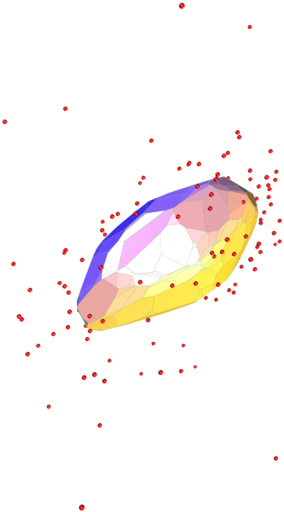
Tukey (halfspace, location) depth region: $\alpha = 9/161$



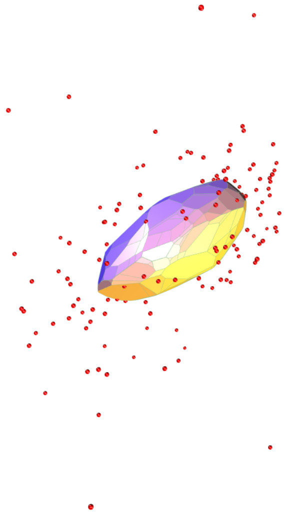
Tukey (halfspace, location) depth region: $\alpha = 13/161$



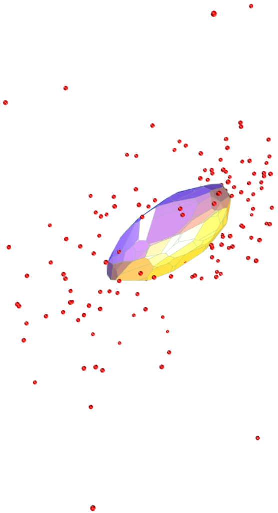
Tukey (halfspace, location) depth region: $\alpha = 17/161$



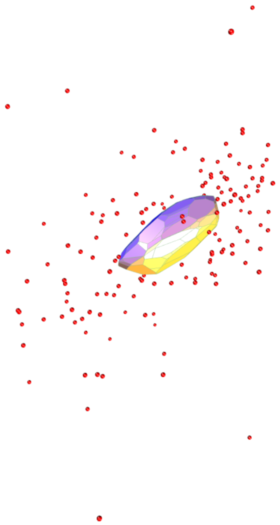
Tukey (halfspace, location) depth region: $\alpha = 25/161$



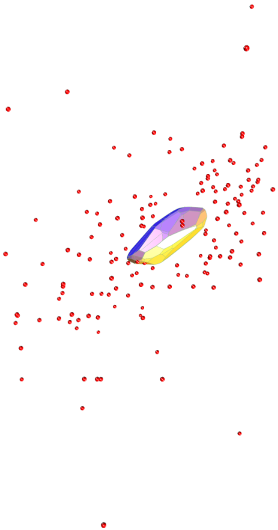
Tukey (halfspace, location) depth region: $\alpha = 33/161$



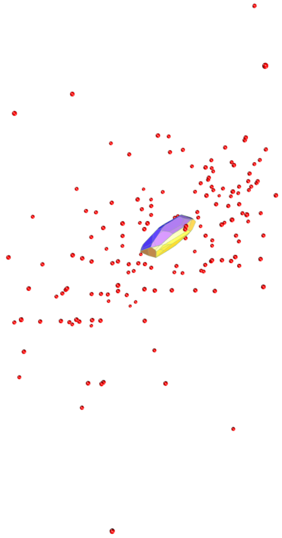
Tukey (halfspace, location) depth region: $\alpha = 41/161$



Tukey (halfspace, location) depth region: $\alpha = 49/161$



Tukey (halfspace, location) depth region: $\alpha = 57/161$



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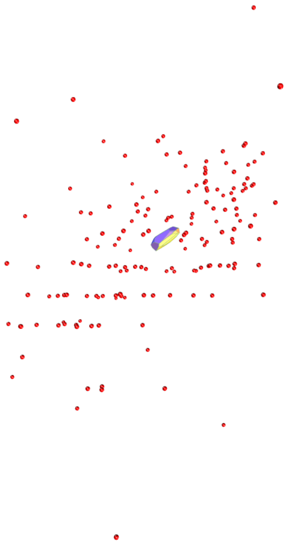

Tukey (halfspace, location) depth region: $\alpha = 68/161$

Applications

- **Multivariate data analysis** (Liu, Parelius, Singh '99);
- **Statistical quality control** (Liu, Singh '93);
- **Cluster analysis and classification** (Mosler, Hoberg '06; Li, Cuesta-Albertos, Liu '12; Mozharovskyi, Mosler, Lange '15);
- **Tests for multivariate location, scale, symmetry** (Liu '92; Dyckerhoff '02; Dyckerhoff, Ley, Paindaveine '15);
- **Outlier/anomaly detection** (Hubert, Rousseeuw, Segaert '15);
- **Multivariate risk measurement** (Cascos, Mochalov '07);
- **Robust linear programming** (Bazovkin, Mosler '15);
- **Missing data imputation** (Mozharovskyi, Josse, Husson '18);
- etc.

R-package **ddalpha** (Pokotylo, Mozharovskyi, Dyckerhoff, Nagy):
calculates a number of multivariate and functional depths;
performs depth-based classification of multivariate and functional data;
contains 50 multivariate and 5 functional data sets.

Contents

Projection property (Dyckerhoff, 2004)

- Let D be a depth. D satisfies the (**weak**) **projection property**, if for each point $\boldsymbol{x} \in \mathbb{R}^d$ and each random vector X it holds:

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Maximum depth classifier (Ghosh and Chaudhuri, 2005)

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DD-plot (Li, Cuesta-Albertos, Liu, 2012)

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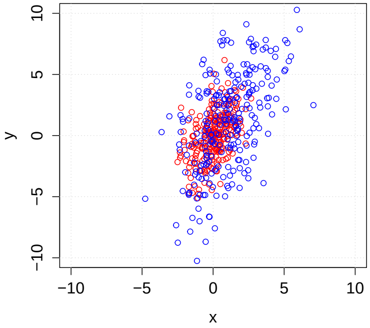

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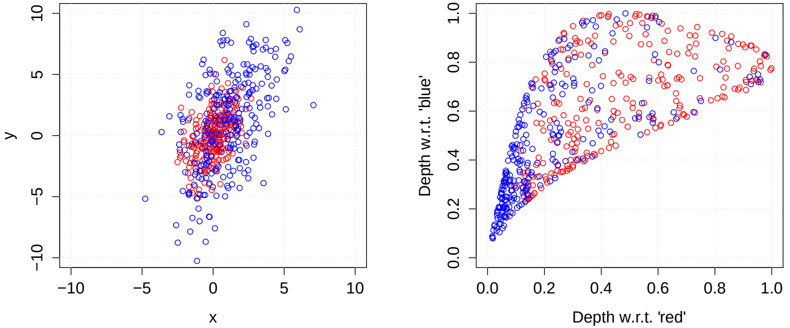

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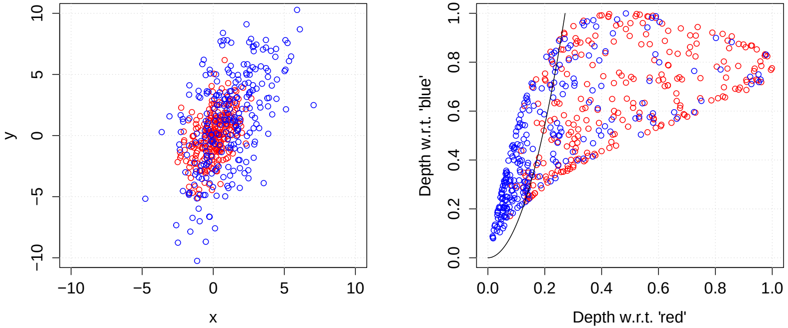

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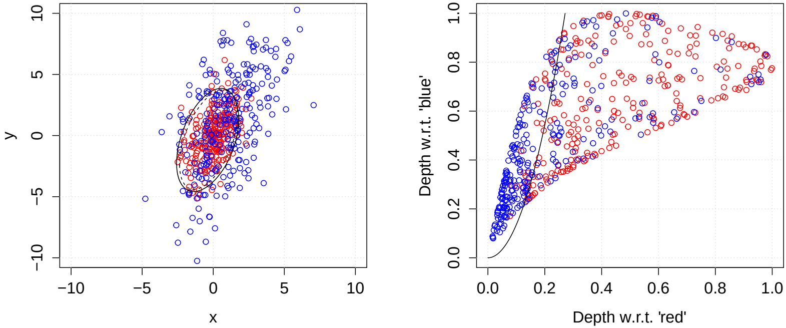
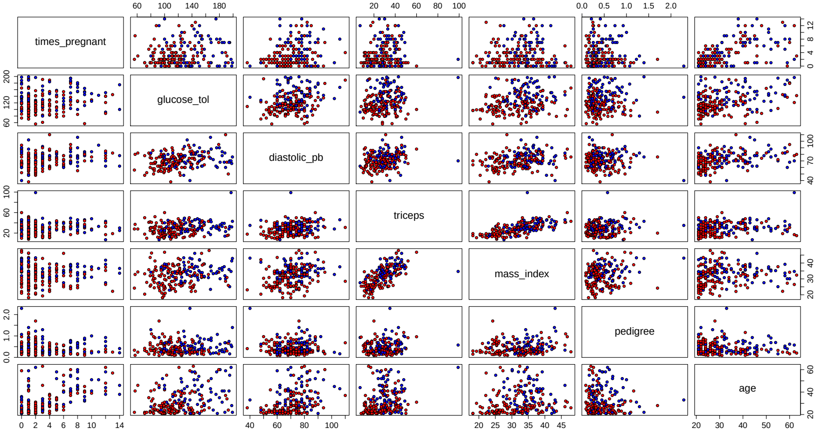
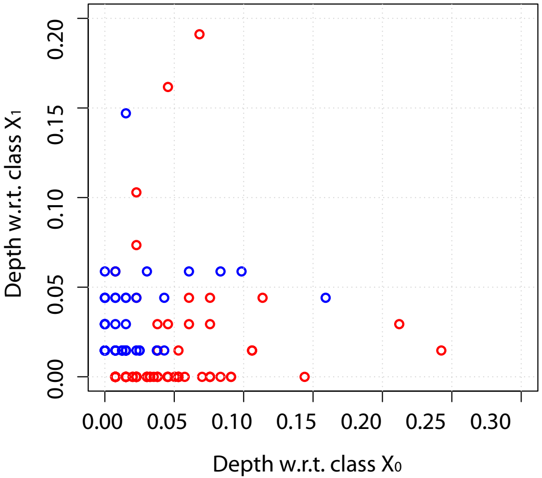


Pima Indians Diabetes (Subset: $m + n = 200$, $d = 7$)



Pima Indians Diabetes: *DD*-Plot



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Object number	Extended properties				
	p_1 $D_{\boldsymbol{X}_0}(x_i)$	p_2 $D_{\boldsymbol{X}_1}(x_i)$	p_3 $D_{\boldsymbol{X}_0}(x_i) \cdot D_{\boldsymbol{X}_1}(x_i)$	p_4 $D^2_{\boldsymbol{X}_0}(x_i)$	p_5 $D^2_{\boldsymbol{X}_1}(x_i)$
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2	$D_{\boldsymbol{X}_0}(x_2)$	$D_{\boldsymbol{X}_1}(x_2)$	$D_{\boldsymbol{X}_0}(x_2) \cdot D_{\boldsymbol{X}_1}(x_2)$	$D^2_{\boldsymbol{X}_0}(x_2)$	$D^2_{\boldsymbol{X}_1}(x_2)$
...					
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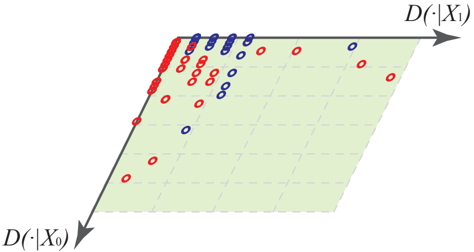

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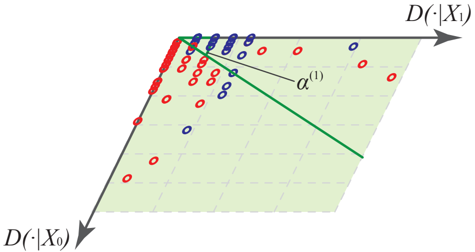

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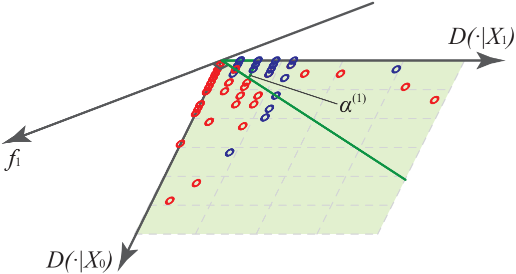

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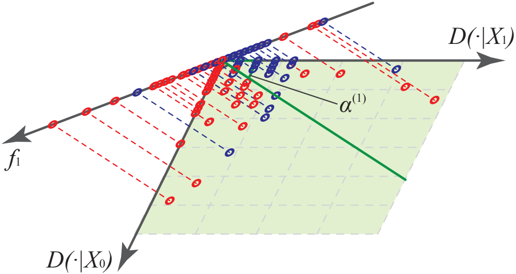

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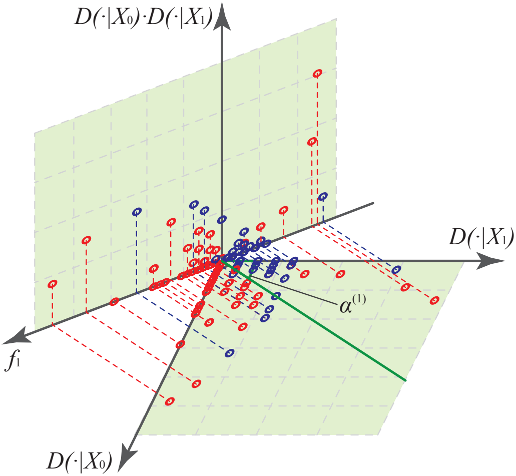

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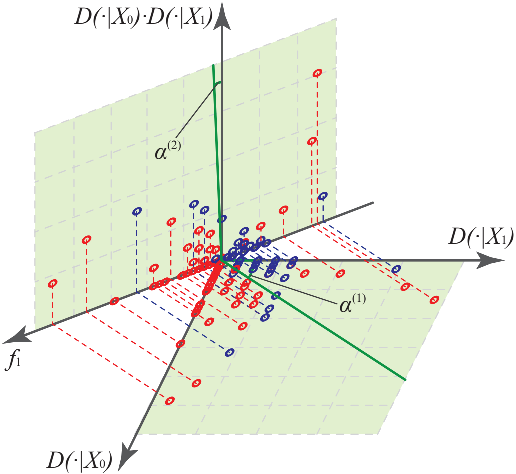

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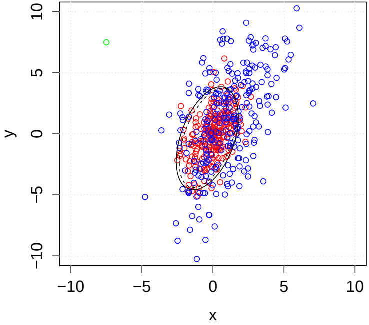
  - **fast**, as its complexity in each plane is of quick-sorting: $O\big((m+n)\log(m+n)\big)$.

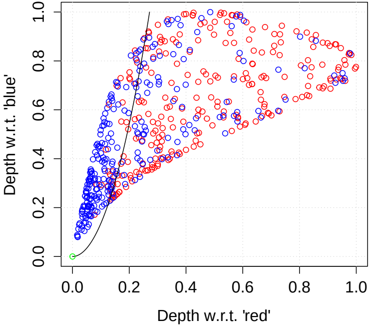
Contents

Outsiders

In the classification phase, an **outsider** is a point that have zero depth in all classes, and thus lies in the origin of the *DD*-plot.

These points need an additional **outsider treatment**.





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- Approximate decision boundary:
  - **SVM-simplified**.

Outsider treatments: SVM-simplified. Two SVMs

Optimal hyperplane

$\min_{\boldsymbol{w}} \frac{1}{2}\|\boldsymbol{w}\|^2$ s.t.

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Maximize:

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$$L_{ij} = y_i y_j K_\gamma(\boldsymbol{x}_i, \boldsymbol{x}_j),\ \ i, j = 1, ..., m+n;$$
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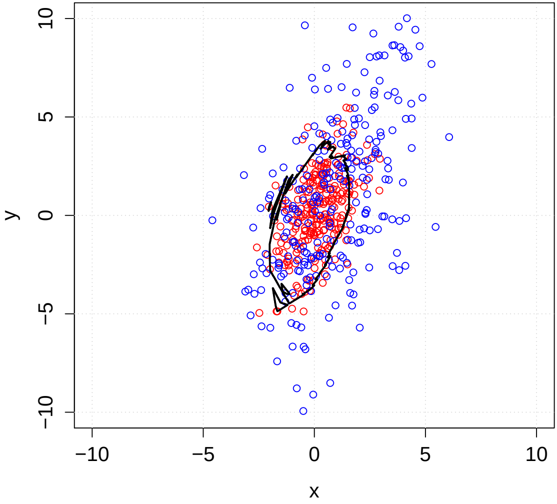

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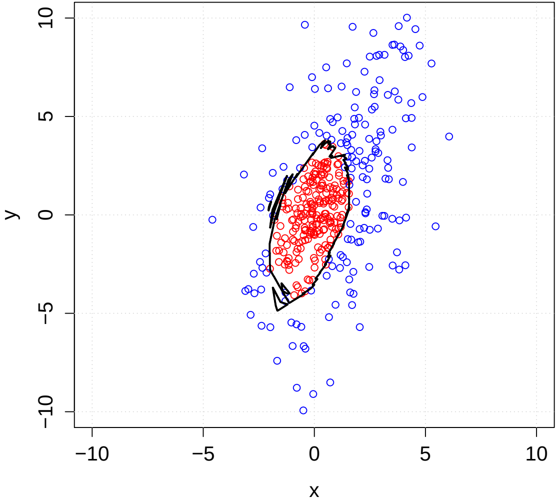

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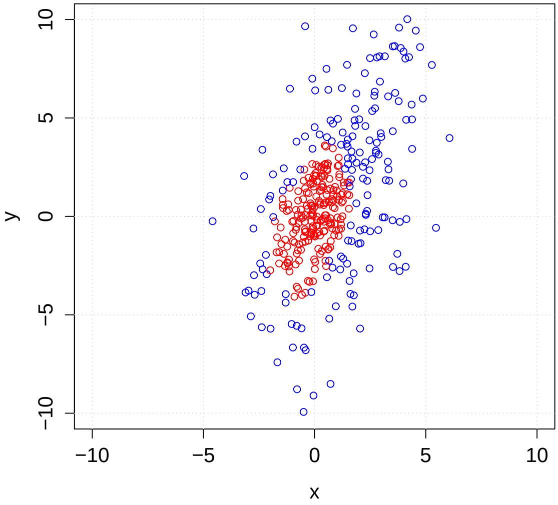

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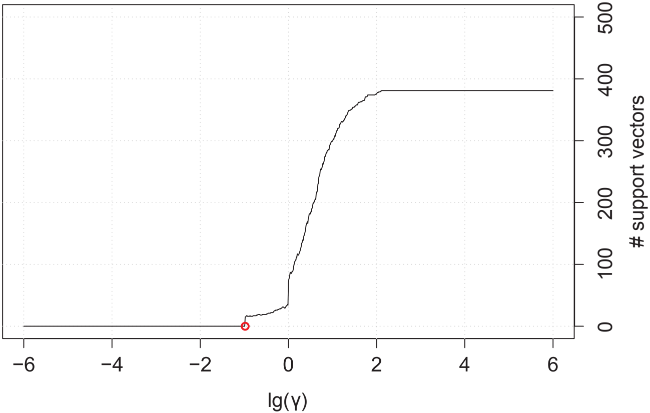

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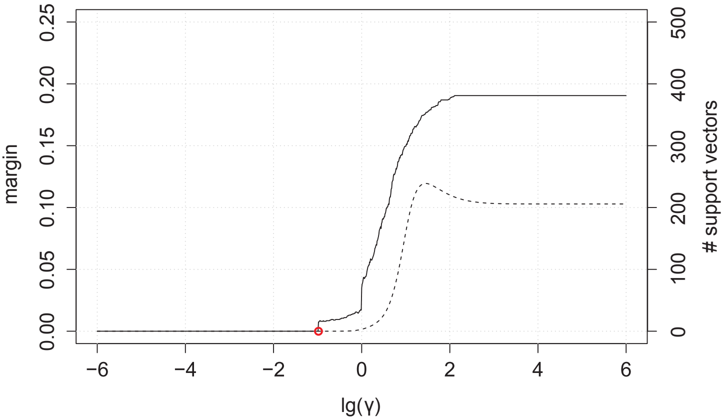

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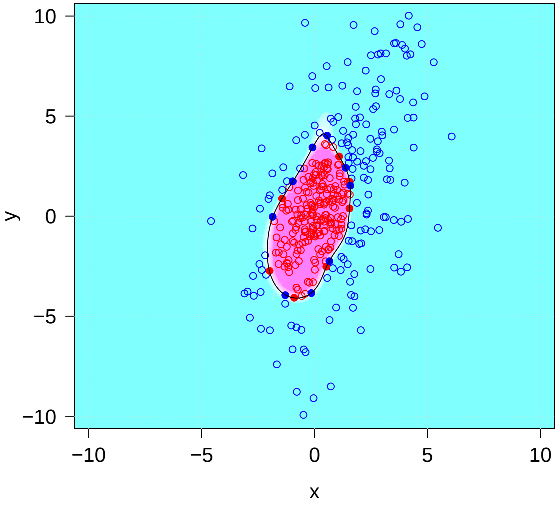

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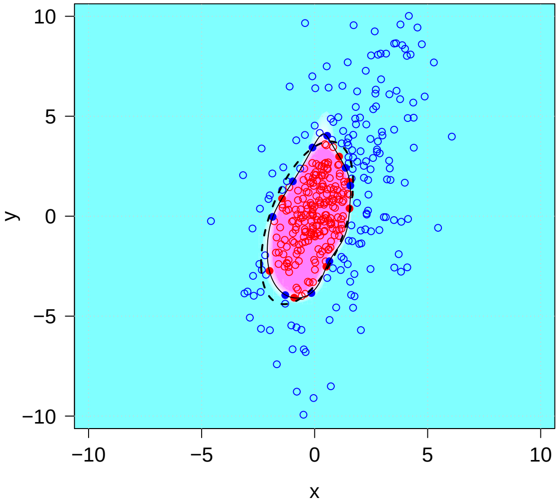

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- Parameter k should be tuned,
  e.g. chosen through cross-validation.

Contents

Thank you for your attention! Questions?

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