

# Machine learning for multivariate and functional anomaly detection: orderings and data depth

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Datacraft Seminar

Paris, October 12, 2020

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## Introduction

## Non-parametric approaches

- One-class support vector machines

- Local outlier factor

- Isolation forest

## Systematic orderings: data depth

- The notion of depth and the Tukey depth

- Central regions

- Further depth notions

## Functional anomaly detection

- Integrated data depth

- Functional isolation forest

- Depth for curve data

## Practical session

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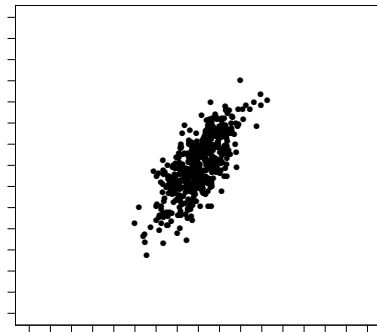
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## A real task

Regard two measurements during a test in a production process:



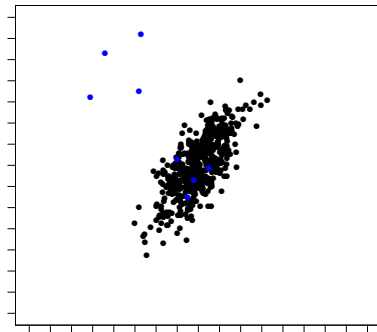
Given **training data**, polluted or not with anomalies:

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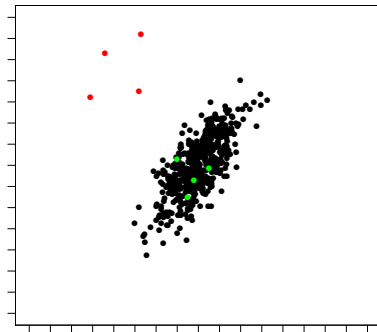
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# Multivariate framework

- ▶ A training data set:

$$\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset \mathbb{R}^d$$

of observations in the  $d$ -dimensional Euclidean space.

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- ▶ Construct a decision function:

$$\mathbb{R}^d \rightarrow \{-1, +1\} : \mathbf{x} \mapsto g(\mathbf{x}),$$

which attributes to any (possible)  $\mathbf{x} \in \mathbb{R}^d$  a label whether it is an anomaly (e.g.,  $+1$ ) or a normal observation (e.g.,  $-1$ ).

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- ▶ It is more useful to provide an ordering on  $\mathbb{R}^d$ :

$$\mathbb{R}^d \rightarrow \mathbb{R} : \mathbf{x} \mapsto g(\mathbf{x}),$$

such that abnormal observations obtain higher anomaly score.

# Practical session

## Notebooks:

- ▶ `anomdet_simulation1.Rmd`,
- ▶ `anomdet_hurricanes.Rmd`,
- ▶ `anomdet_brainimaging.Rmd`,
- ▶ `anomdet_cars.ipynb`,
- ▶ `anomdet_airbus.ipynb`.

## Data sets:

- ▶ `carsanom.csv`: Data set on anomaly detection for cars.
- ▶ `airbus_data.csv`: Data set from Airbus.
- ▶ `hurdat2-1851-2019-052520.txt`: Historical hurricane data.
- ▶ `101_1_dwi_fa.nii`: Anatomical brain volume data.
- ▶ `101_1_dwi.voxelcoordsL.txt`: Left brain fiber's bundle.
- ▶ `101_1_dwi.voxelcoordsR.txt`: Right brain fiber's bundle.

## Supplementary scripts:

- ▶ `depth_routines.py`: Routines for data depth calculation.
- ▶ `FIF.py`: Implementation of the functional isolation forest.
- ▶ `depth_routines.R`: Routines for curves' parametrization.
- ▶ `DTI.R`: Routines for input of brain imaging data.

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# One-class support vector machines

(Schölkopf, Platt, Shawe-Taylor, Smola, Williamson; 1999)

## Generalized portrait:

- ▶ The method of the **generalized portrait** was introduced by Vapnik & Lerner (1963) and Vapnik & Chervonenkis (1974).

# One-class support vector machines

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## Generalized portrait:

- ▶ The method of the **generalized portrait** was introduced by Vapnik & Lerner (1963) and Vapnik & Chervonenkis (1974).
- ▶ Generalized portrait is the vector:

$$\psi = \frac{\varphi}{\min_{\mathbf{x} \in \mathbf{X}} \langle \mathbf{x}, \varphi \rangle} \quad \text{with } \varphi \text{ from } \max_{\|\varphi\|=1} \min_{\mathbf{x} \in \mathbf{X}} \langle \mathbf{x}, \varphi \rangle.$$

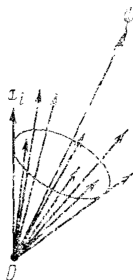


Рис. 24.

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**Kernel trick** (Boser, Guyon, Vapnik; 1992):

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- ▶ Allow for a portion of points from  $\mathbf{X}$  to be beyond the margin, label points far from the origin by “1”, those close by “-1”.

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- ▶ Controlled by a parameter  $\nu \in (0, 1)$   
(Schölkopf, Platt, Shawe-Taylor, Smola, Williamson; 1999).



# One-class support vector machines

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This can be formulated as a quadratic programming problem

$$\begin{aligned} \min_{\psi \in \mathcal{H}, \xi \in \mathbb{R}^n, \rho \in \mathbb{R}} \quad & \frac{1}{2} \|\psi\|^2 + \frac{1}{\nu n} \sum_{i=1}^n \xi_i - \rho \\ \text{subject to} \quad & \langle \xi, \Phi(\mathbf{x}_i) \rangle \geq \rho - \xi_i, \quad \xi_i \geq 0 \text{ for } i = 1, \dots, n, \end{aligned}$$

with  $\xi = (\xi_1, \dots, \xi_n)^\top$ .

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The solution  $(\psi^*, \xi^*, \rho^*)$  yields the following **decision function**:

$$g_{OCSVM}(\mathbf{x}) = \text{sgn}(\langle \xi^*, \Phi(\mathbf{x}) \rangle - \rho^*).$$

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One can reformulate the optimization problem to employ the **kernel trick**.

# One-class support vector machines (Schölkopf *et al.*, 1999)

In dual formulation, using the Lagrangian, one can restate the optimization problem as follows:

$$\min_{\alpha} \quad \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{subject to} \quad 0 \leq \alpha_i \leq \frac{1}{\nu n} \text{ for } i = 1, \dots, n, \quad \sum_{i=1}^n \alpha_i = 1,$$

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The **decision function** is then:

$$g_{\text{OC SVM}}(\mathbf{x}) = \text{sgn} \left( \sum_{i=1}^n \alpha_i K(\mathbf{x}_i, \mathbf{x}) - \rho \right),$$

where  $\rho$  can be recovered from any  $\mathbf{x}_j$  such that  $0 < \alpha_j < \frac{1}{\nu n}$ :

$$\rho = \langle \psi, \Phi(\mathbf{x}_j) \rangle = \sum_{i=1}^n \alpha_i K(\mathbf{x}_i, \mathbf{x}_j).$$

# One-class support vector machines (Schölkopf *et al.*, 1999)

**Idea 2:** Put points into a small ball.

$$\begin{aligned} \min_{R \in \mathbb{R}, \xi \in \mathbb{R}^n, \mathbf{c} \in \mathcal{H},} \quad & R^2 + \frac{1}{\nu n} \sum_{i=1}^n \xi_i \\ \text{subject to} \quad & \|\Phi(\mathbf{x}_i) - \mathbf{c}\| \leq R^2 + \xi_i, \quad \xi_i \geq 0 \text{ for } i = 1, \dots, n. \end{aligned}$$

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This leads to the dual:

$$\begin{aligned} \min_{\alpha} \quad & \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) - \sum_{i=1}^n \alpha_i K(\mathbf{x}_i, \mathbf{x}_i) \\ \text{subject to} \quad & 0 \leq \alpha_i \leq \frac{1}{\nu n}, \text{ for } i = 1, \dots, n, \quad \sum_{i=1}^n \alpha_i = 1. \end{aligned}$$



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which leads to the **decision function**:

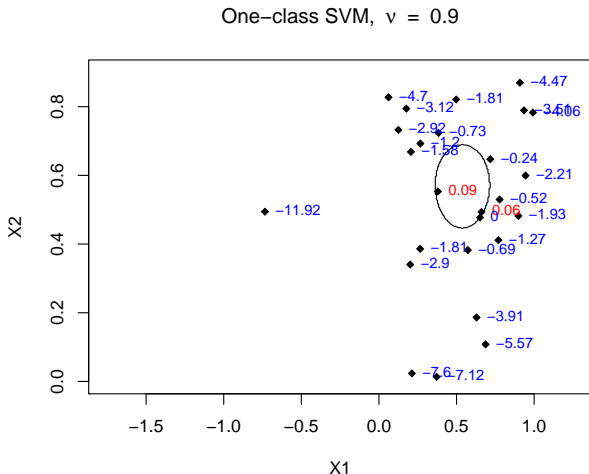
$$g_{OCSVM}(\mathbf{x}) = \left( R^2 - \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) + 2 \sum_{i=1}^n \alpha_i K(\mathbf{x}_i, \mathbf{x}) - K(\mathbf{x}, \mathbf{x}) \right),$$

with  $R^2 = \sum_{i,j} \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) - 2 \sum_i \alpha_i K(\mathbf{x}_i, \mathbf{x}_k) + K(\mathbf{x}_k, \mathbf{x}_k)$  for any  $\mathbf{x}_k$  such that  $0 < \alpha_k < 1/(\nu n)$ .

# One-class support vector machines

(Schölkopf, Platt, Shawe-Taylor, Smola, Williamson; 1999)

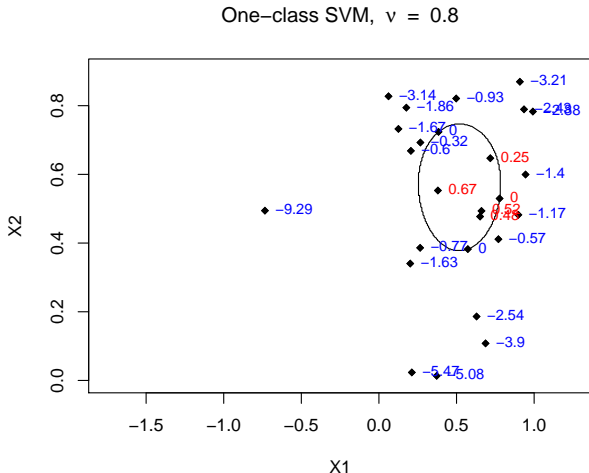
## Illustration: Case 1



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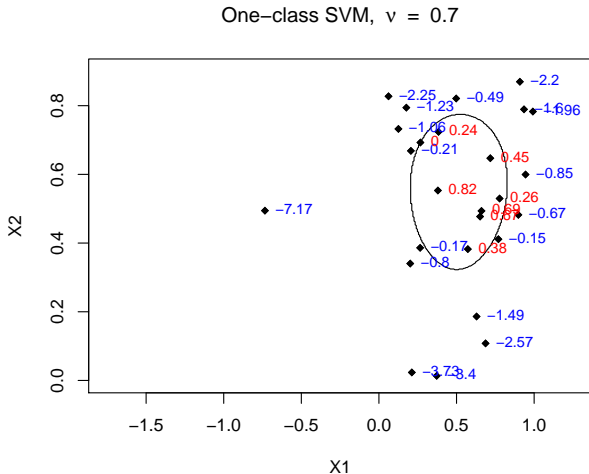
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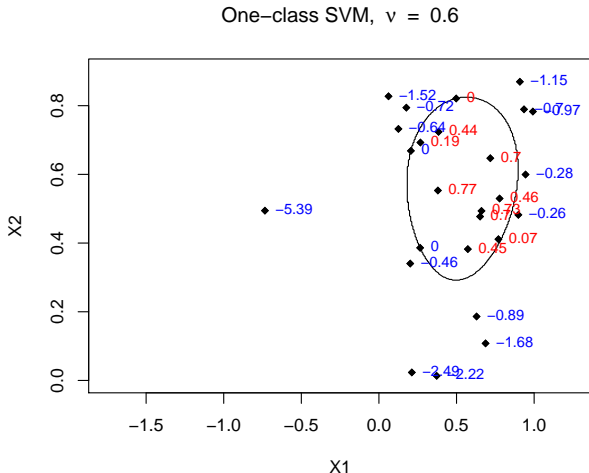
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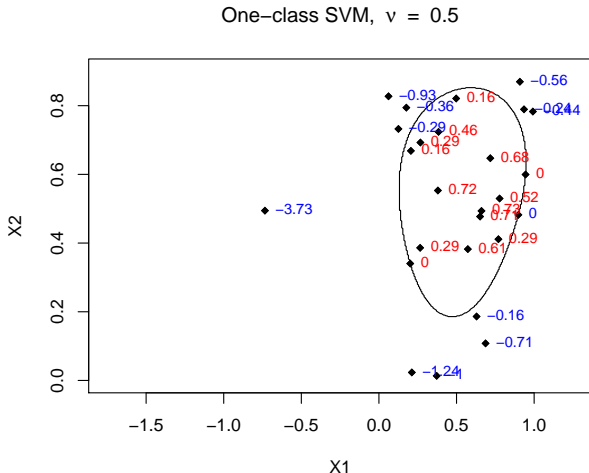
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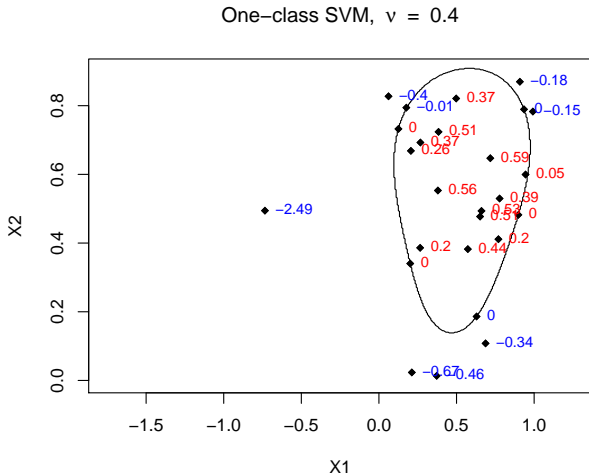
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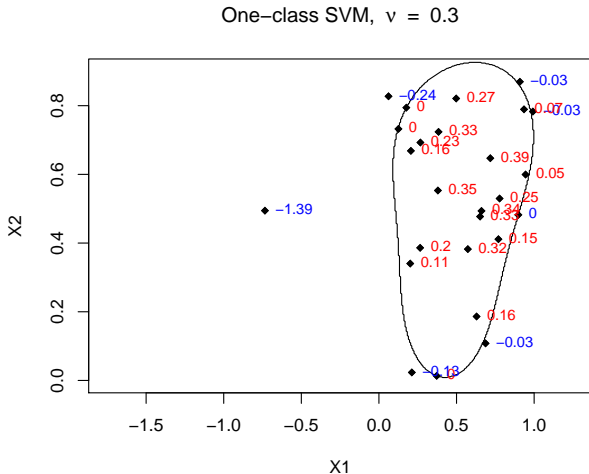
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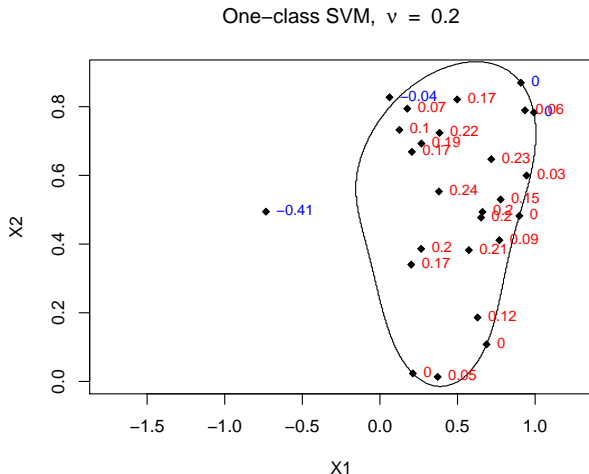




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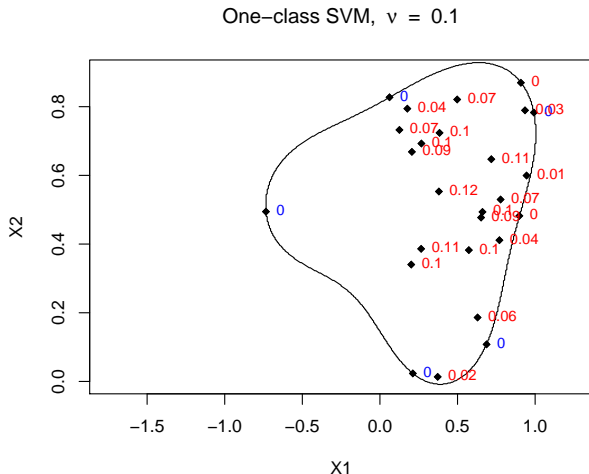
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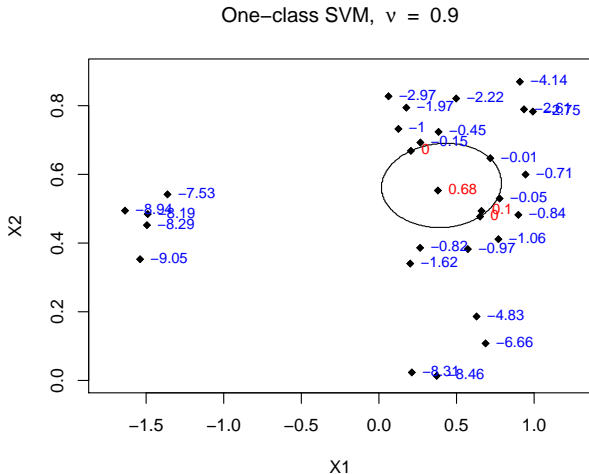
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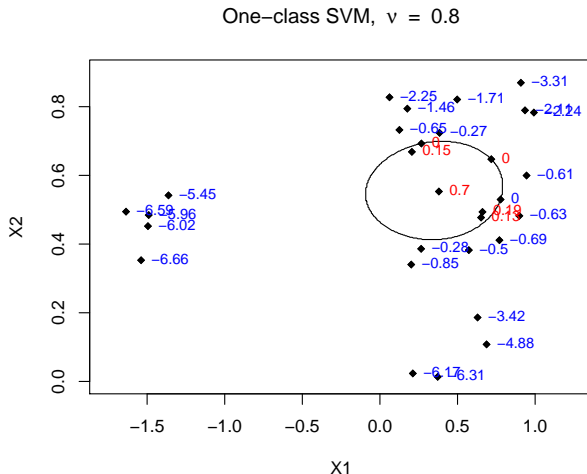
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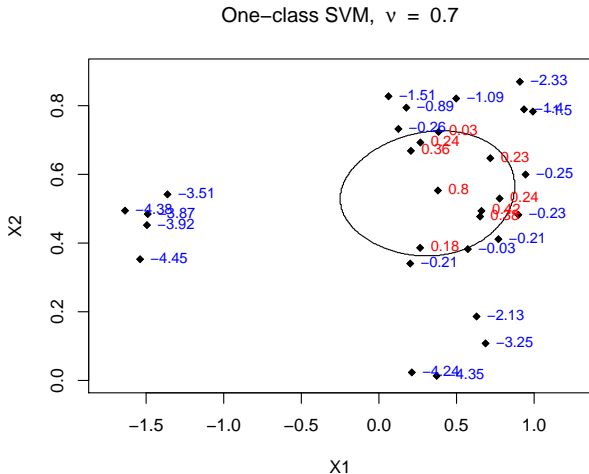
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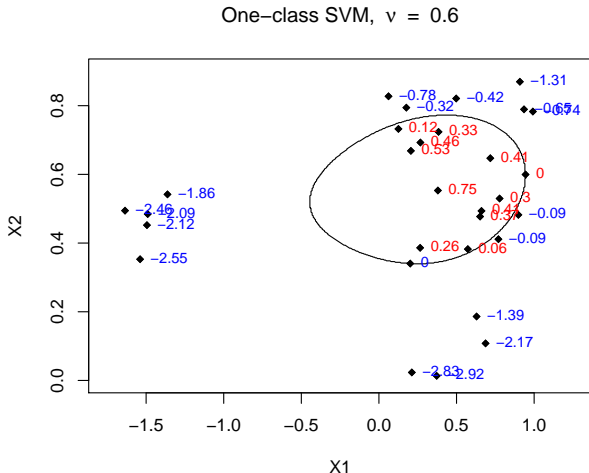
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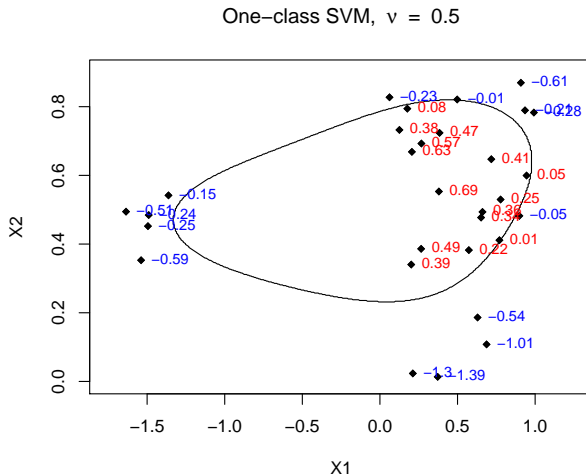
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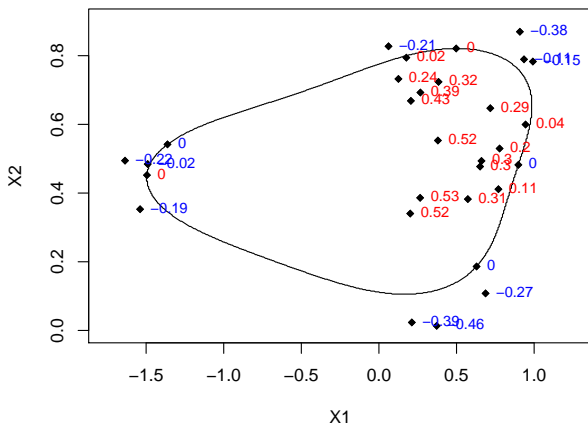
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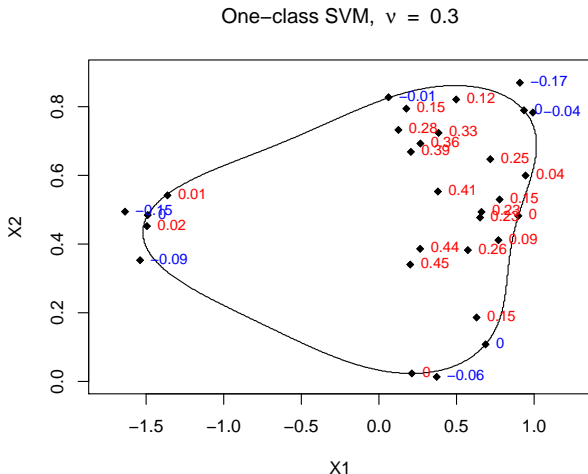




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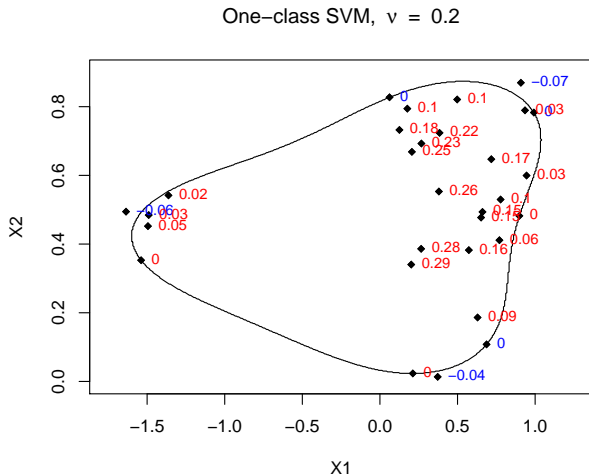
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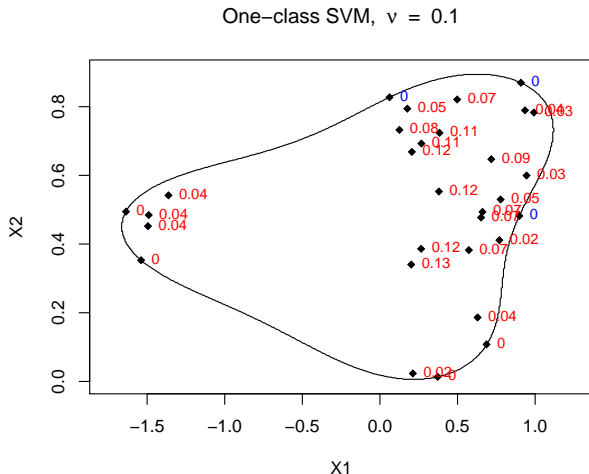
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# Local outlier factor (Breunig, Kriegel, Ng, Sander; 2000)

**$k$ -distance** of a point  $\mathbf{x}$ :

For any integer  $k > 0$ , the  $k$ -distance of point  $\mathbf{x}$ , denoted as  $k\text{-dist}(\mathbf{x})$ , is defined as the distance  $d(\mathbf{x}, \mathbf{o})$  between  $\mathbf{x}$  and a point  $\mathbf{o} \in \mathbf{X}$  such that:

- ▶ for at least  $k$  points  $\mathbf{o}' \in \mathbf{X} \setminus \{\mathbf{x}\}$  it holds that  $d(\mathbf{x}, \mathbf{o}') \leq d(\mathbf{x}, \mathbf{o})$ , and
- ▶ for at most  $k - 1$  points  $\mathbf{o}' \in \mathbf{X} \setminus \{\mathbf{x}\}$  it holds that  $d(\mathbf{x}, \mathbf{o}') < d(\mathbf{x}, \mathbf{o})$ .

# Local outlier factor (Breunig, Kriegel, Ng, Sander; 2000)

**$k$ -distance** of a point  $\mathbf{x}$ :

For any integer  $k > 0$ , the  $k$ -distance of point  $\mathbf{x}$ , denoted as  $k\text{-dist}(\mathbf{x})$ , is defined as the distance  $d(\mathbf{x}, \mathbf{o})$  between  $\mathbf{x}$  and a point  $\mathbf{o} \in \mathbf{X}$  such that:

- ▶ for at least  $k$  points  $\mathbf{o}' \in \mathbf{X} \setminus \{\mathbf{x}\}$  it holds that  $d(\mathbf{x}, \mathbf{o}') \leq d(\mathbf{x}, \mathbf{o})$ , and
- ▶ for at most  $k - 1$  points  $\mathbf{o}' \in \mathbf{X} \setminus \{\mathbf{x}\}$  it holds that  $d(\mathbf{x}, \mathbf{o}') < d(\mathbf{x}, \mathbf{o})$ .

(=Distance from  $\mathbf{x}$  to its  $k$ th neighbor.)

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**$k$ -neighborhood** of a point  $\mathbf{x}$ :

Given the  $k\text{-dist}(\mathbf{x})$ , the  **$k$ -neighborhood** of  $\mathbf{x}$ , denoted  $N_k(\mathbf{x})$ , contains every point whose distance from  $\mathbf{x}$  is not greater than the  $k\text{-dist}(\mathbf{x})$ , i.e.:

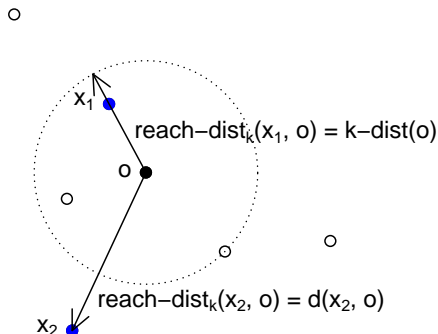
$$N_k(\mathbf{x}) = \{ \mathbf{q} \in \mathbf{X} \setminus \{\mathbf{x}\} \mid d(\mathbf{x}, \mathbf{q}) \leq k\text{-dist}(\mathbf{x}) \}.$$

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**Reachability distance** of order  $k$  of point  $\mathbf{x}$  w.r.t. point  $\mathbf{o}$ :

For  $k \in \mathbb{N}$ , the **reachability distance** of order  $k$  of point  $\mathbf{x}$  with respect to point  $\mathbf{o}$  is defined as:

$$\text{reach-dist}_k(\mathbf{x}, \mathbf{o}) = \max\{k\text{-dist}(\mathbf{o}), d(\mathbf{x}, \mathbf{o})\}.$$





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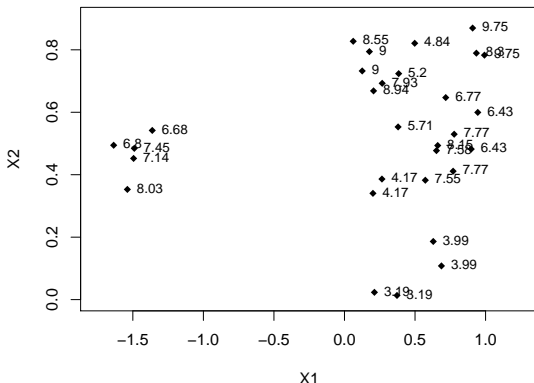
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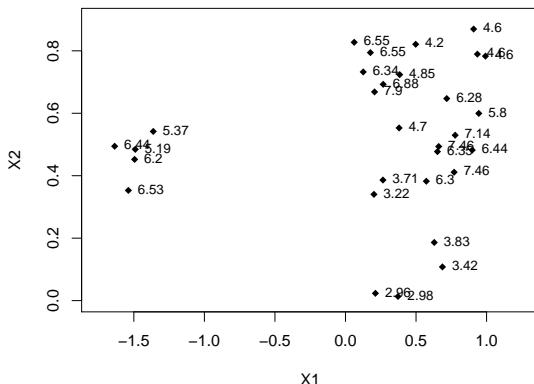
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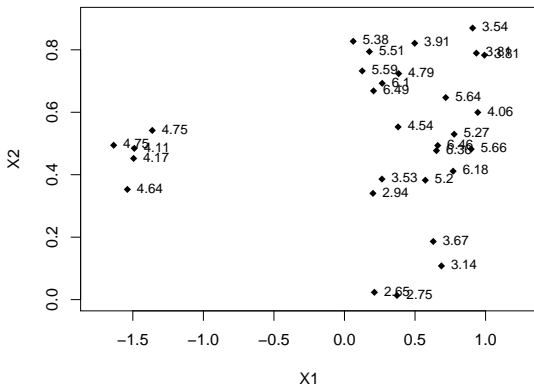
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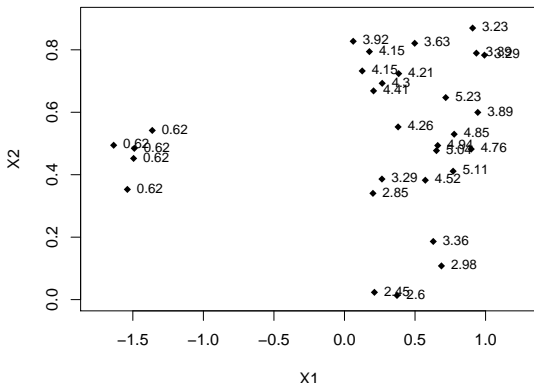
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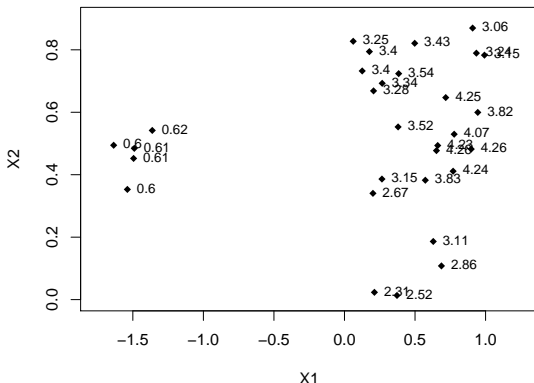
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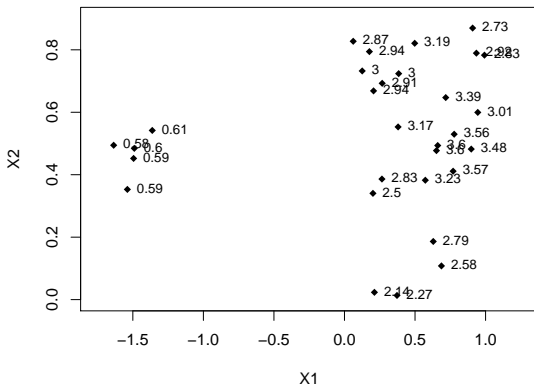
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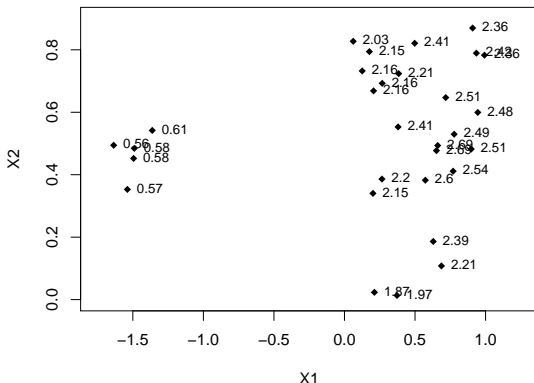
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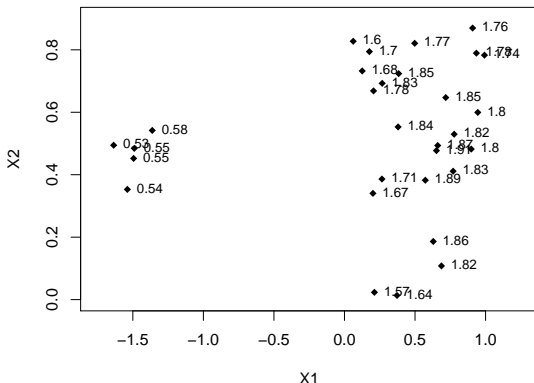
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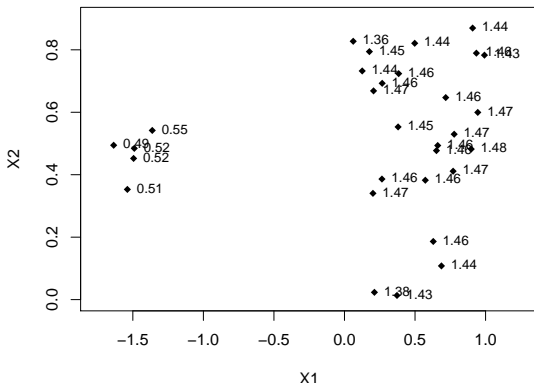
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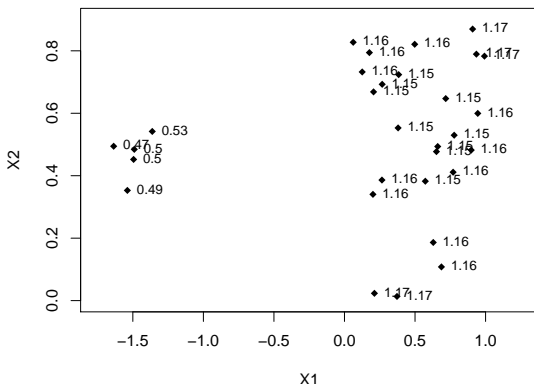
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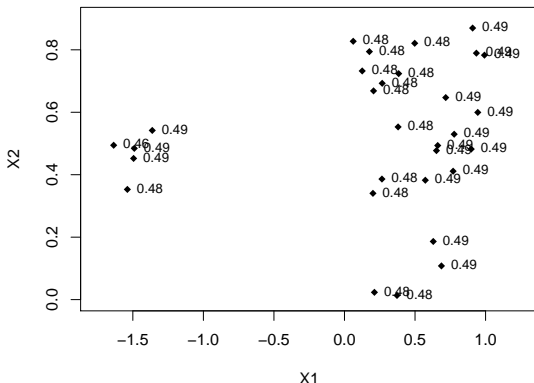
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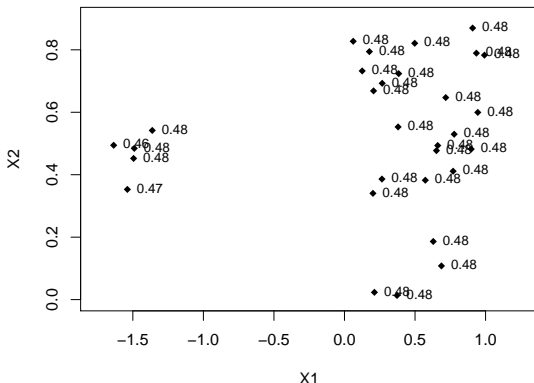
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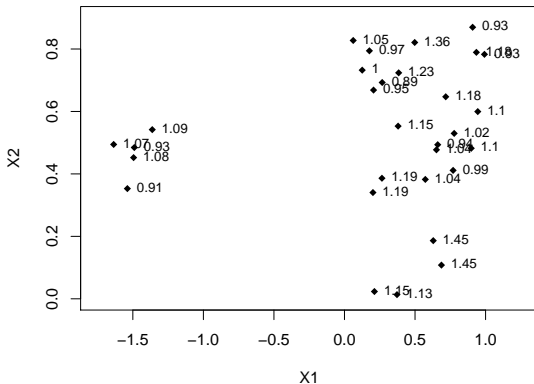
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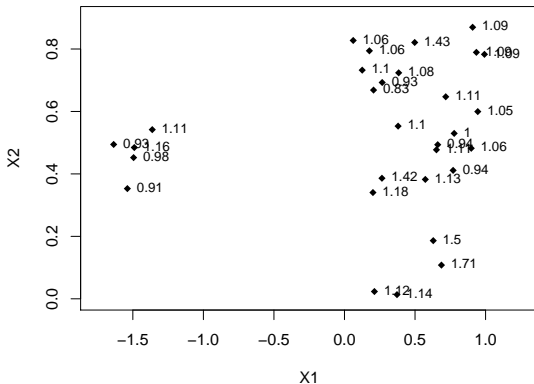
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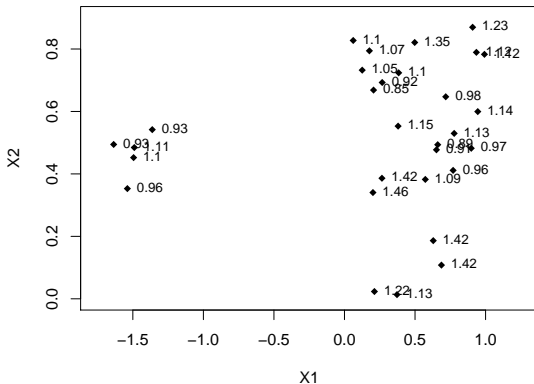
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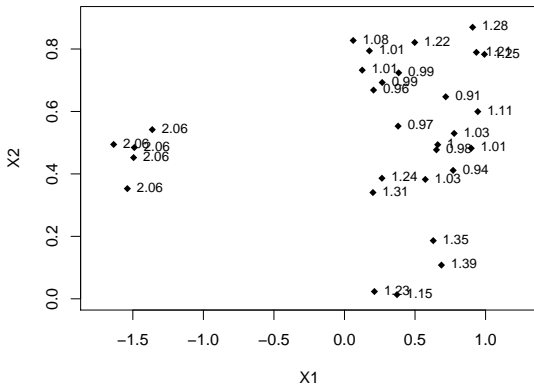
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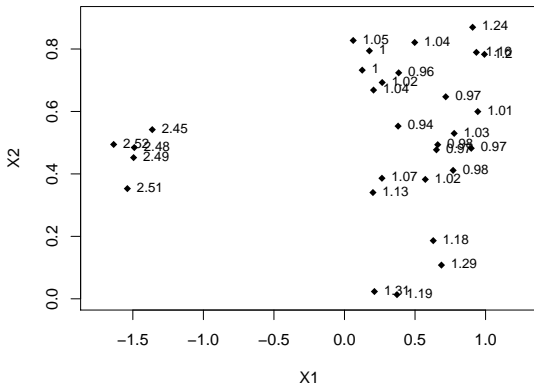
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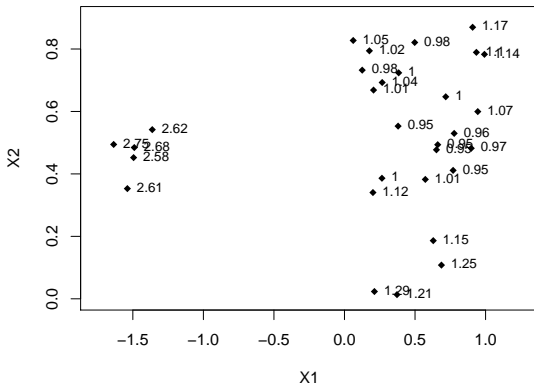
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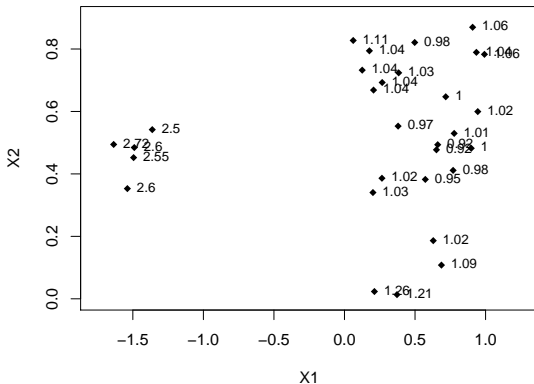
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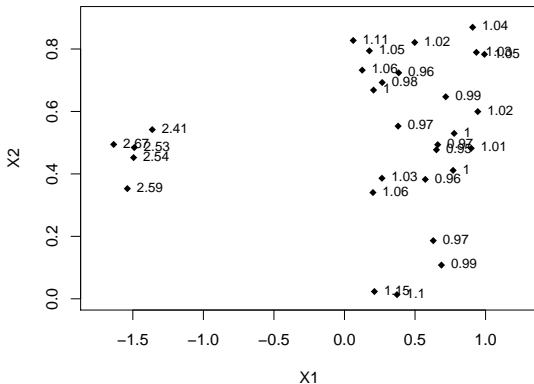
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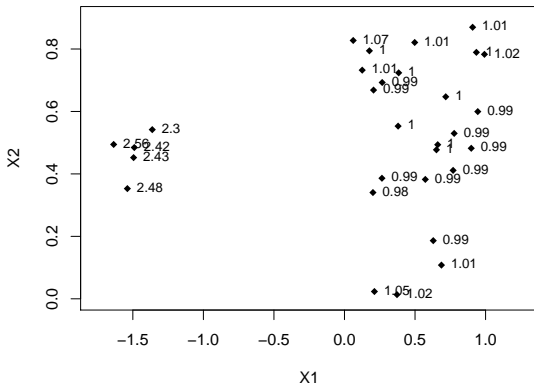
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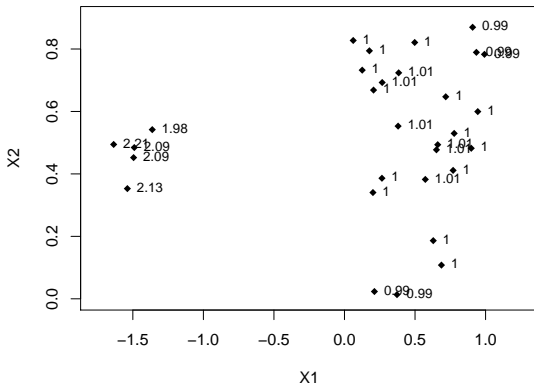
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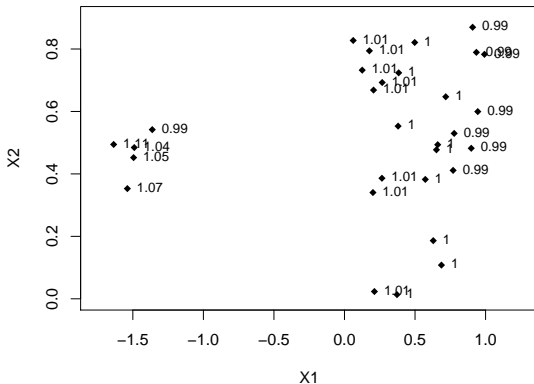
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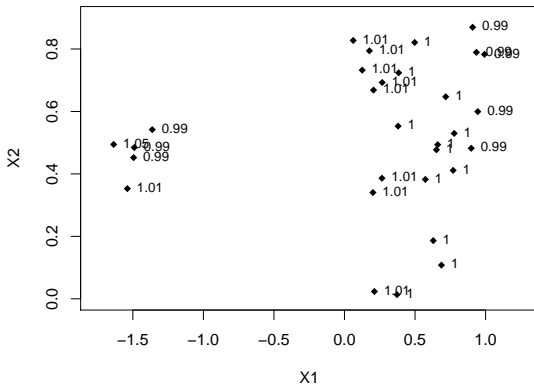
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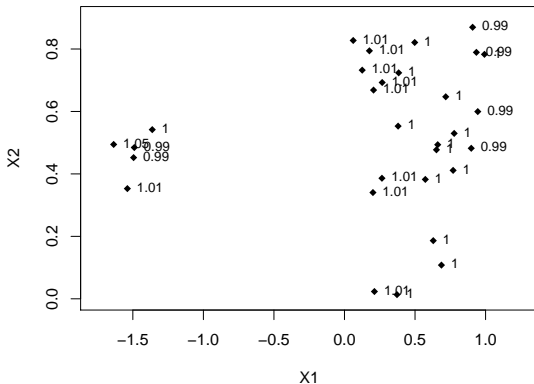
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Integrated data depth

Functional isolation forest

Depth for curve data

## Practical session

# Isolation forest (Liu, Ting, Zhou; 2008)

- ▶ **Isolation forest** (Liu, Ting, Zhou; 2008) is an anomaly detection method inherited from the famous **random forest** algorithm (Breiman, 2001).
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- ▶ **Main idea:** **Outlying observations are isolated faster.**
- ▶ Tree-kind partitioning is done until “full isolation”: **outlying observations will have smaller depth** (on an average) in the **isolation tree**.
- ▶ A **monotone transform** is usually applied to the aggregated estimate.
- ▶ To reduce both **masking effect** and **computation cost**, small-size sub-sampling is used instead of bootstrap.



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$$\left[ \min_{\mathbf{x} \in \mathcal{S}_{j,k}} \langle \mathbf{x}, \mathbf{e}_l \rangle, \max_{\mathbf{x} \in \mathcal{S}_{j,k}} \langle \mathbf{x}, \mathbf{e}_l \rangle \right].$$

3. Form the children subsets

$$\begin{aligned} \mathcal{C}_{j+1,2k} &= \mathcal{C}_{j,k} \cap \{\mathbf{x} \in \mathbb{R}^d : \langle \mathbf{x}, \mathbf{e}_l \rangle \leq \kappa\}, \\ \mathcal{C}_{j+1,2k+1} &= \mathcal{C}_{j,k} \cap \{\mathbf{x} \in \mathbb{R}^d : \langle \mathbf{x}, \mathbf{e}_l \rangle > \kappa\}. \end{aligned}$$

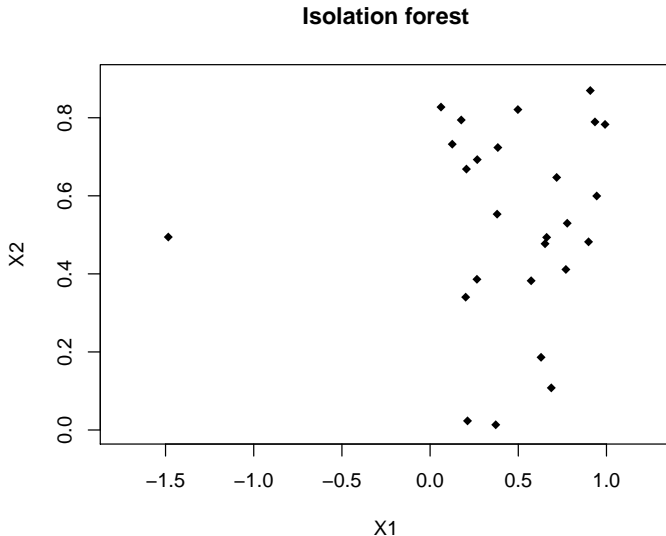
as well as the children training datasets

$$\mathcal{S}_{j+1,2k} = \mathcal{S}_{j,k} \cap \mathcal{C}_{j+1,2k} \text{ and } \mathcal{S}_{j+1,2k+1} = \mathcal{S}_{j,k} \cap \mathcal{C}_{j+1,2k+1}.$$

**Stop** when only one observation is in each node: **isolation**.

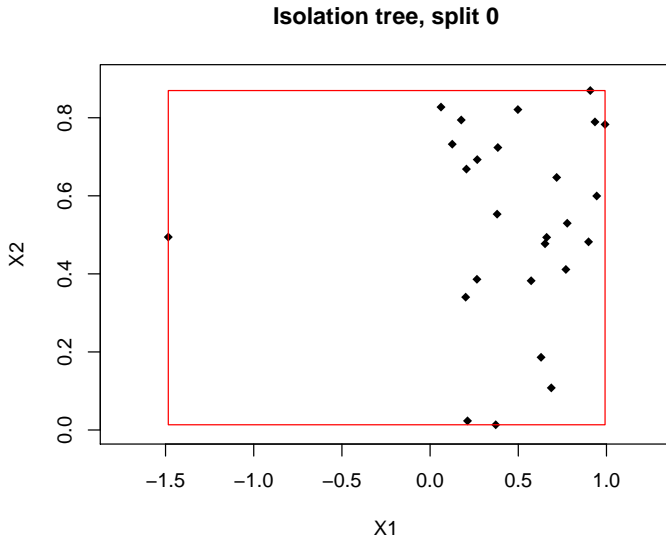
# Isolation forest (Liu, Ting, Zhou; 2008)

## Illustration: Isolation tree



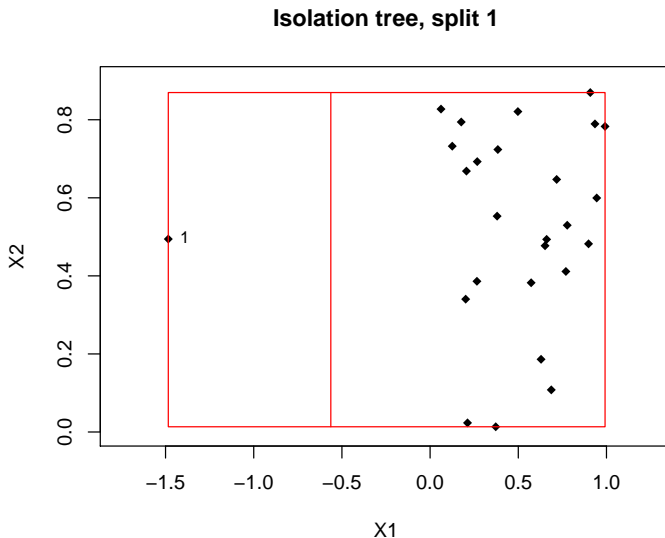
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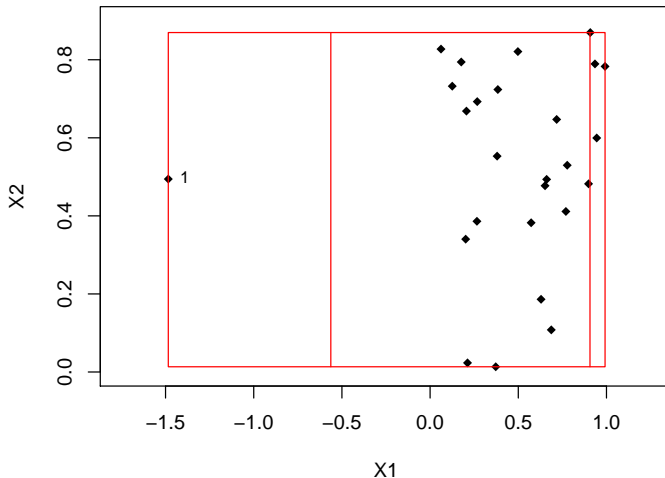




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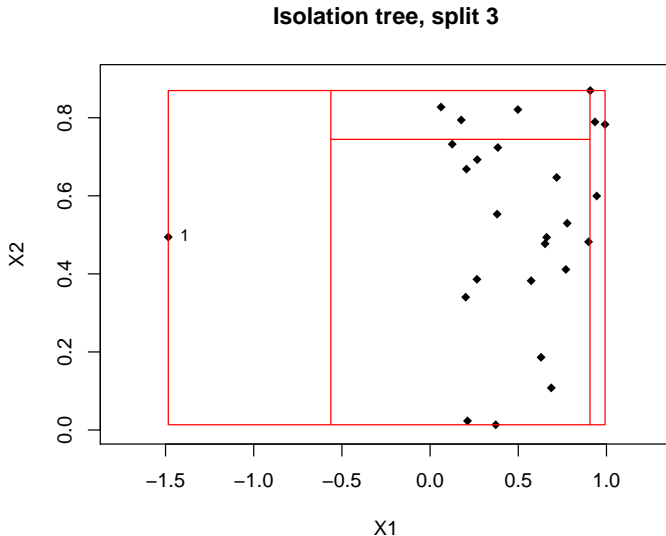
## Illustration: Isolation tree

Isolation tree, split 2



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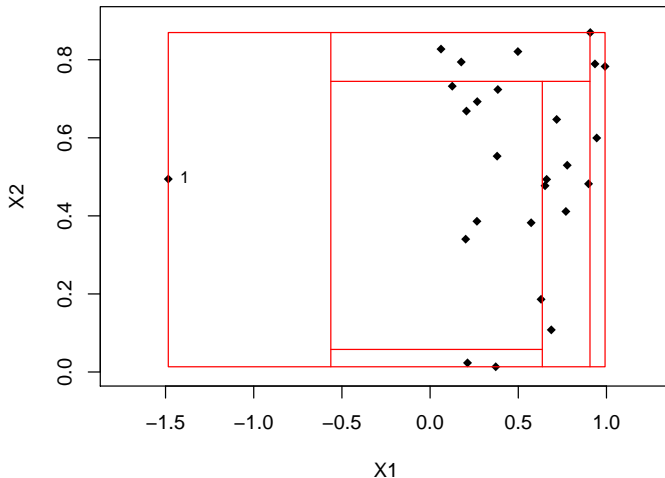




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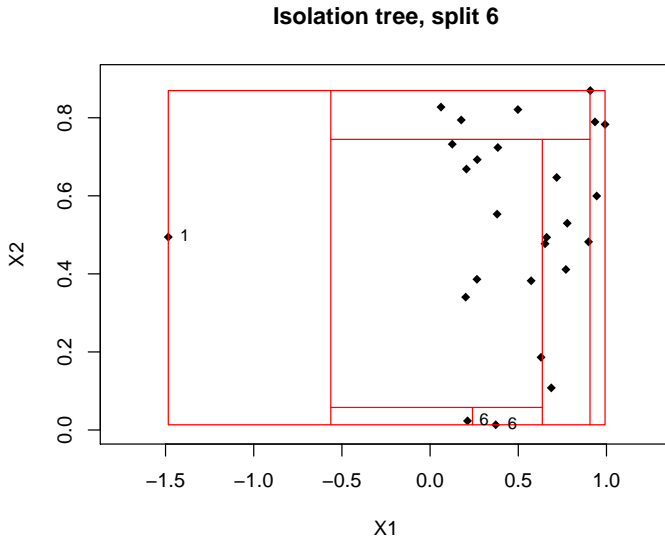
## Illustration: Isolation tree

Isolation tree, split 5



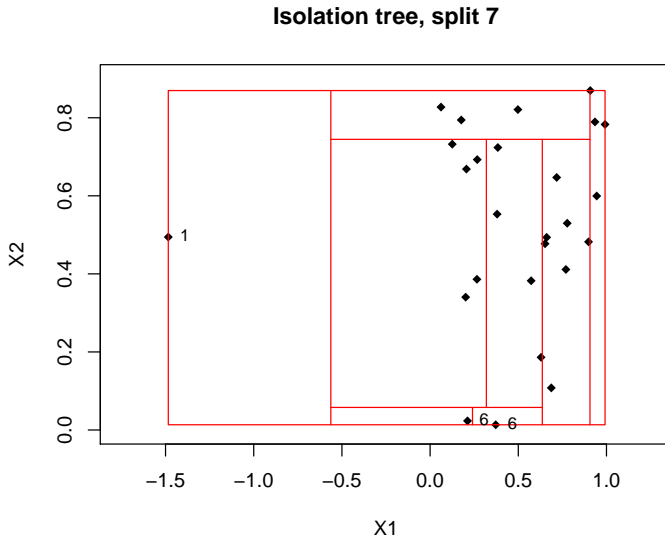
# Isolation forest (Liu, Ting, Zhou; 2008)

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# Isolation forest (Liu, Ting, Zhou; 2008)

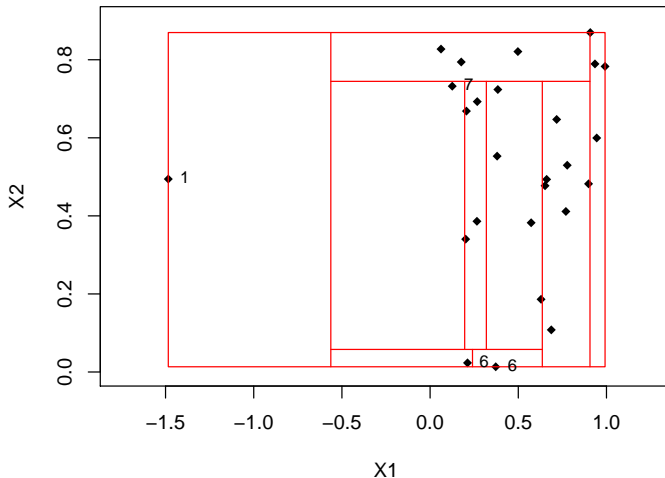
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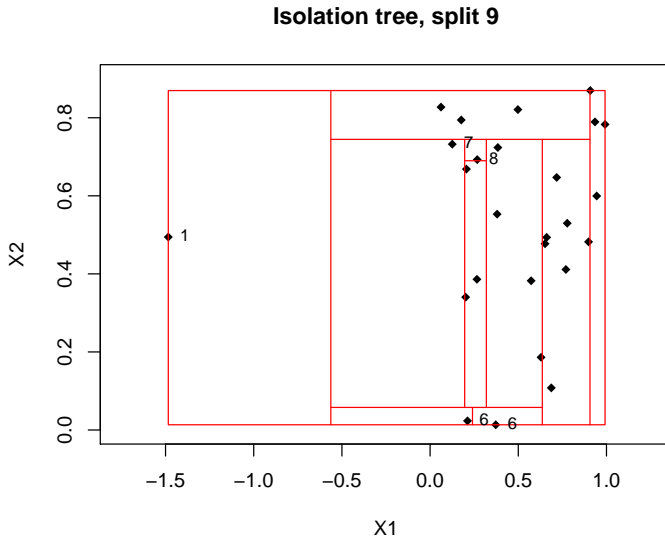
## Illustration: Isolation tree

Isolation tree, split 8



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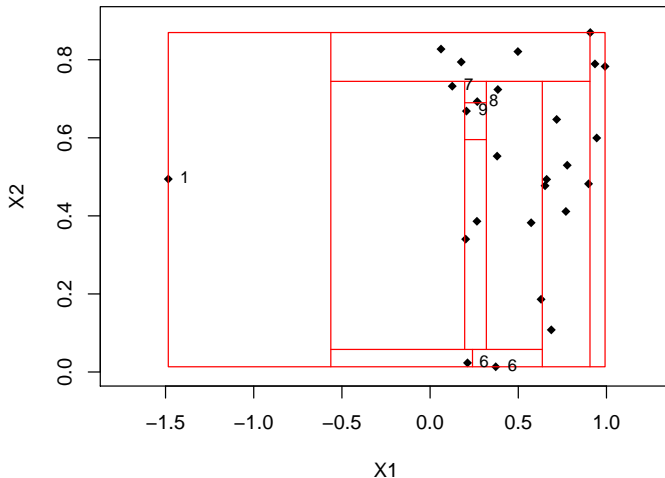




# Isolation forest (Liu, Ting, Zhou; 2008)

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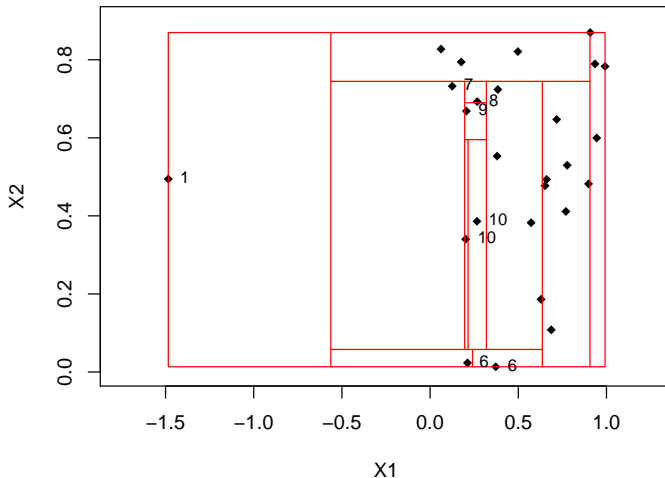
Isolation tree, split 10



# Isolation forest (Liu, Ting, Zhou; 2008)

## Illustration: Isolation tree

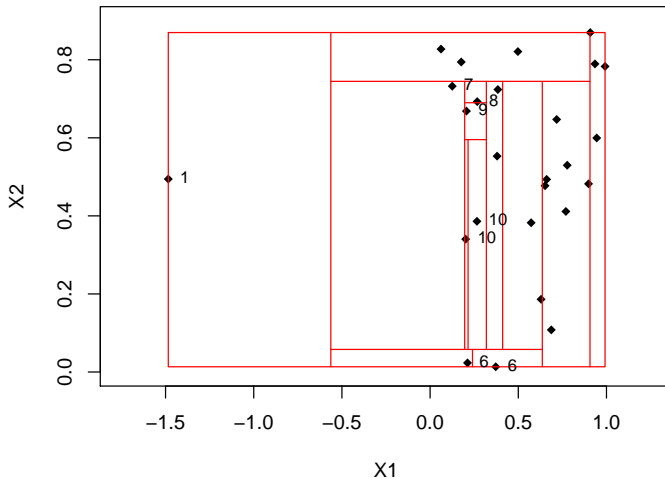
Isolation tree, split 11



# Isolation forest (Liu, Ting, Zhou; 2008)

## Illustration: Isolation tree

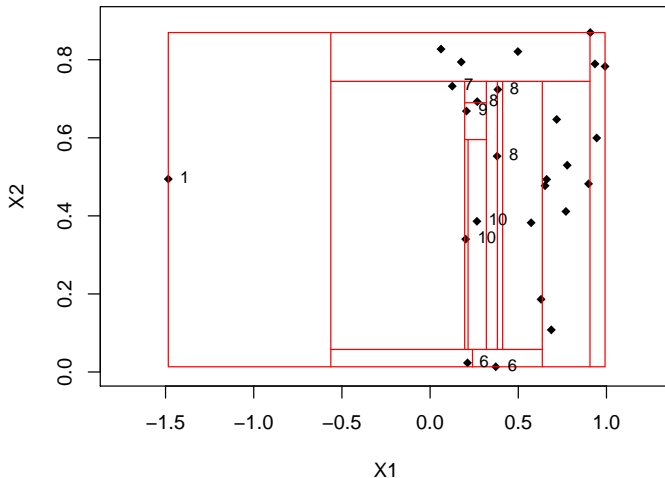
Isolation tree, split 12



# Isolation forest (Liu, Ting, Zhou; 2008)

## Illustration: Isolation tree

Isolation tree, split 13

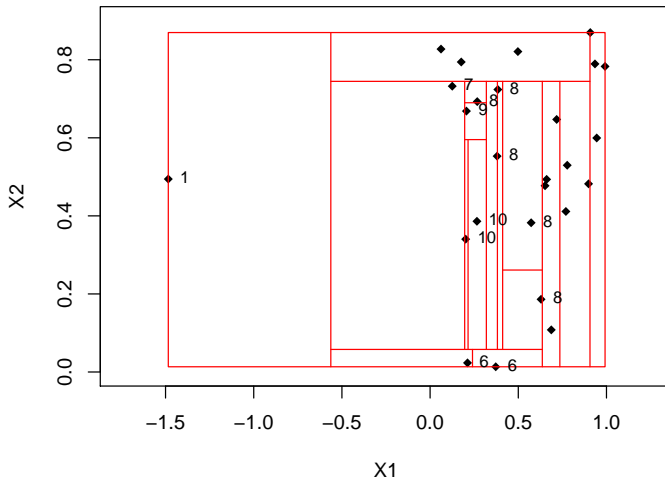




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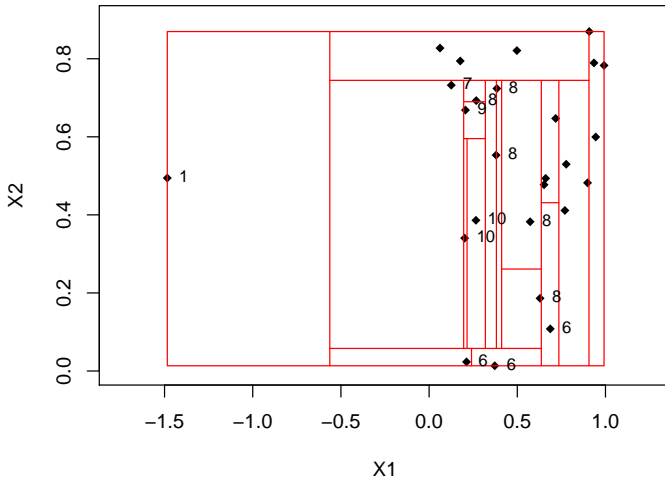
Isolation tree, split 15



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## Illustration: Isolation tree

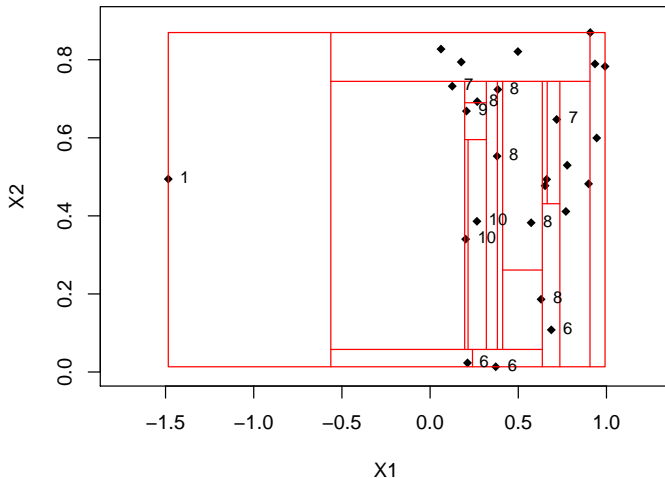
Isolation tree, split 16



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## Illustration: Isolation tree

Isolation tree, split 17

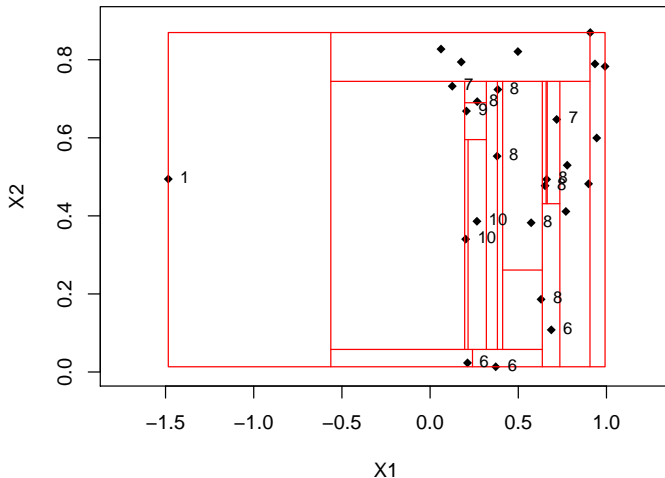




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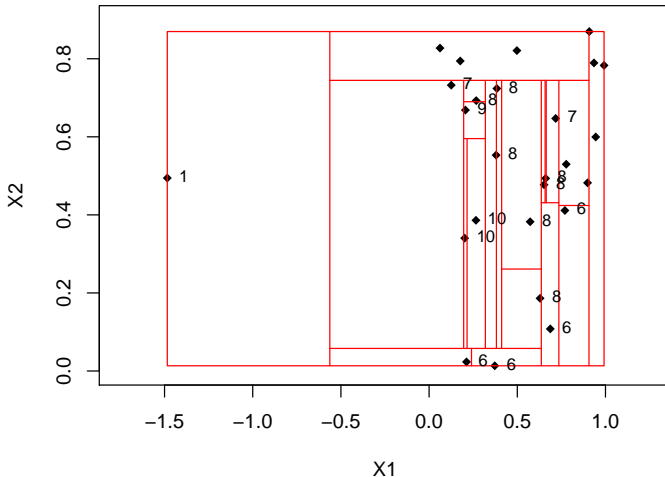
Isolation tree, split 18



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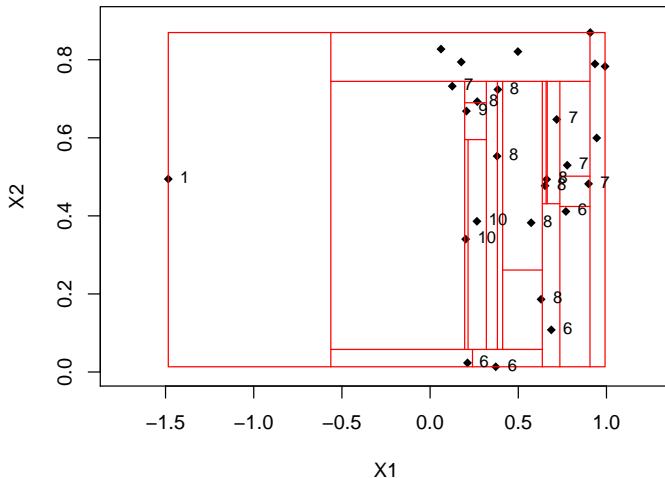
Isolation tree, split 19



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## Illustration: Isolation tree

Isolation tree, split 20

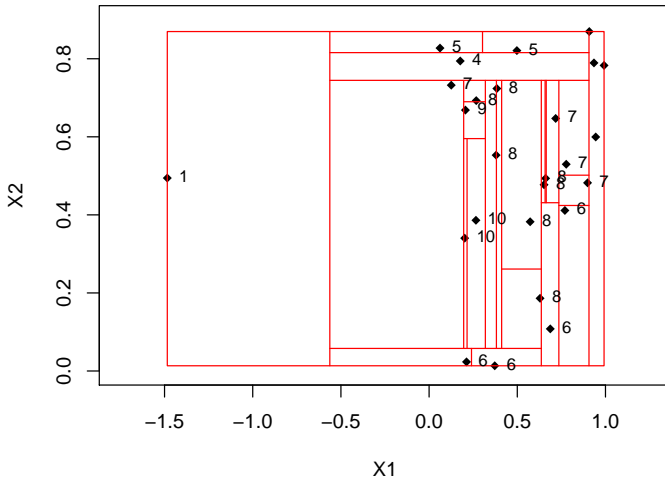




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## Illustration: Isolation tree

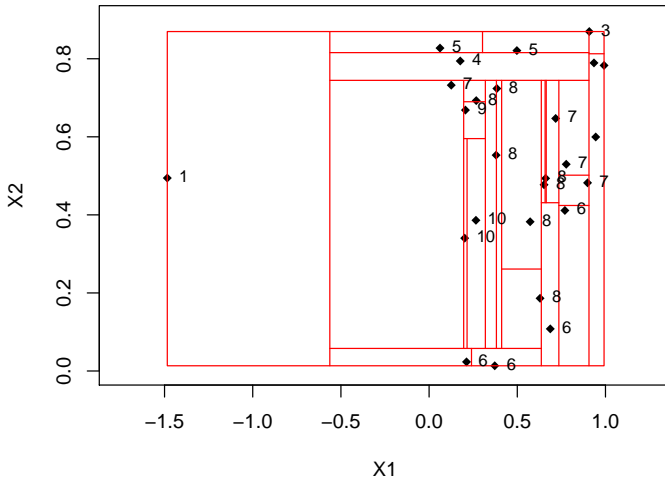
Isolation tree, split 22



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## Illustration: Isolation tree

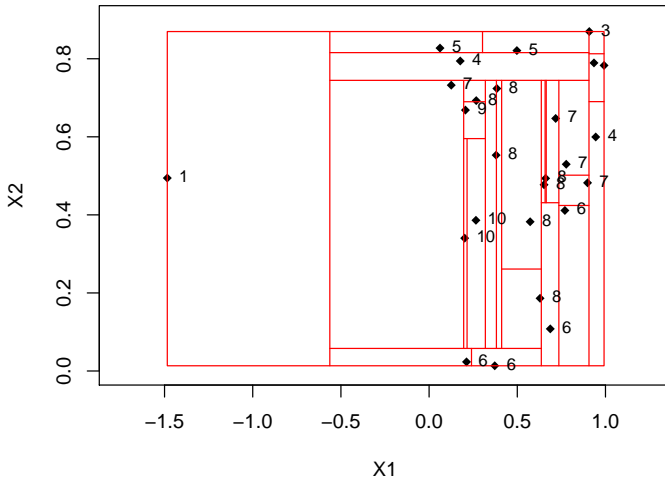
Isolation tree, split 23



# Isolation forest (Liu, Ting, Zhou; 2008)

## Illustration: Isolation tree

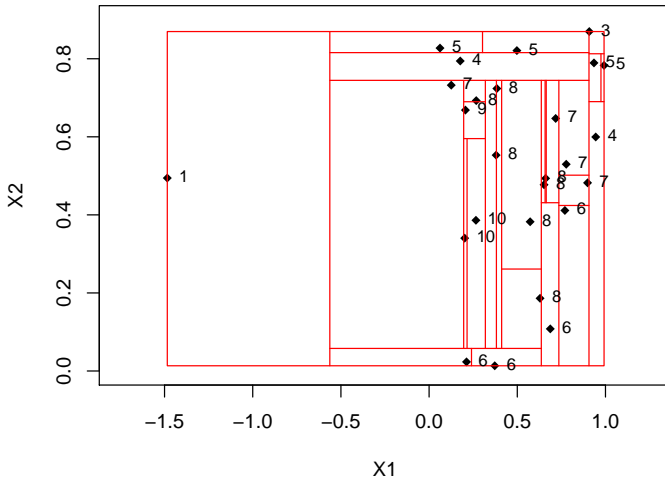
Isolation tree, split 24



# Isolation forest (Liu, Ting, Zhou; 2008)

## Illustration: Isolation tree

Isolation tree, split 25





# Isolation forest (Liu, Ting, Zhou; 2008)

**Anomaly score calculation** for observation  $\mathbf{x}$ :

1. For each **isolation tree**  $i \in \{1, \dots, T\}$ , locate  $\mathbf{x}$  in a **terminal node** and calculate the **depth** of this node  $h_i(\mathbf{x})$ .
2. Attribute the **anomaly score**:

$$s(\mathbf{x}) = 2^{-\frac{\frac{1}{n} \sum_{i=1}^T h_i(\mathbf{x})}{c(n)}},$$

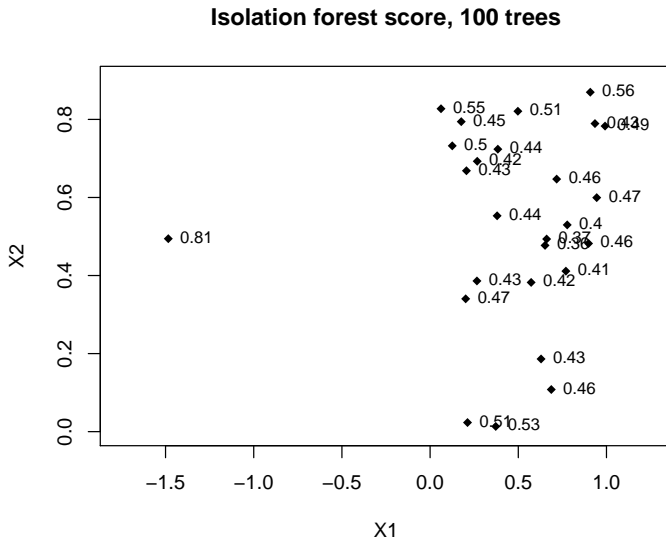
with  $c(n) = 2H(n-1) - \frac{2(n-1)}{n}$  where  $H(k)$  is the harmonic number and can be estimated by  $\ln(k) + 0.5772156649$ .

**Score behavior:**

- ▶ when  $\frac{1}{n} \sum_{i=1}^T h_i(\mathbf{x}) \rightarrow c(n)$ ,  $s(\mathbf{x}) \rightarrow 0.5$ ,
- ▶ when  $\frac{1}{n} \sum_{i=1}^T h_i(\mathbf{x}) \rightarrow 0$ ,  $s(\mathbf{x}) \rightarrow 1$ ,
- ▶ when  $\frac{1}{n} \sum_{i=1}^T h_i(\mathbf{x}) \rightarrow n-1$ ,  $s(\mathbf{x}) \rightarrow 0$ .

# Isolation forest (Liu, Ting, Zhou; 2008)

## Illustration: Anomaly score



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## Non-parametric approaches

- One-class support vector machines

- Local outlier factor

- Isolation forest

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- The notion of depth and the Tukey depth

- Central regions

- Further depth notions

## Functional anomaly detection

- Integrated data depth

- Functional isolation forest

- Depth for curve data

## Practical session

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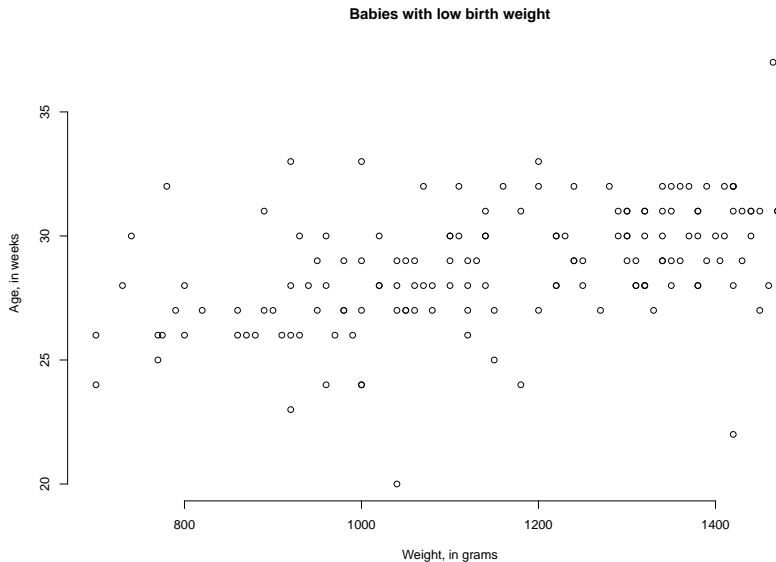
Integrated data depth

Functional isolation forest

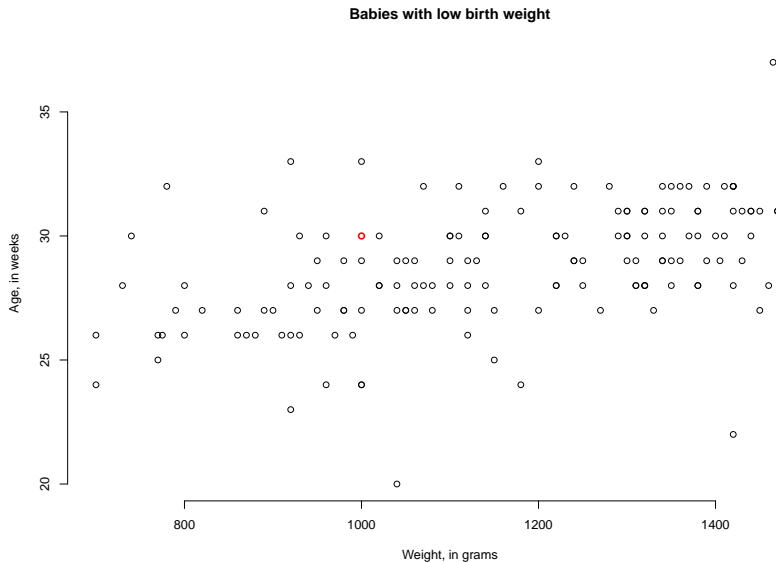
Depth for curve data

## Practical session

# Data depth



# Data depth



## Statistical data depth

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

$$D : \mathbb{R}^p \times \mathcal{P} \rightarrow [0, 1], (\mathbf{x}, P) \mapsto D(\mathbf{x}|P)$$

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

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Depth notions: **Mahalanobis** ('36), **projection** (Stahel, '81; Donoho, '82), **simplicial volume** (Oja, '83), **simplicial** (Liu, '90), **zonoid** (Koshevoy, Mosler, '97), **spatial** (Vardi, Zhang, '00; Serfling, '02), **lens** (Liu, Modarres, '11), ... depth.

## Applications of data depth:

- ▶ **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; M., Mosler, Lange '15);
- ▶ **Tests for multivariate location, scale, symmetry** (Liu '92; Dyckerhoff '02; Dyckerhoff, Ley, Paindaveine '15);
- ▶ **Outlier detection** (Hubert, Rousseeuw, Segaert '15);
- ▶ **Multivariate risk measurement** (Casco, Mochalov '07);
- ▶ **Robust linear programming** (Bazovkin, Mosler '15);
- ▶ **Missing data imputation** (M., Josse, Husson '20);
- ▶ etc.

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

## Tukey (=halfspace, location) depth

**Tukey (1975) — “Mathematics and the picturing of data”**

Tukey depth of  $\mathbf{x} \in \mathbb{R}^p$  w.r.t. a  $d$ -variate random vector  $X$  distributed as  $P$  is defined as the smallest probability mass of a closed halfspace containing  $\mathbf{x}$ :

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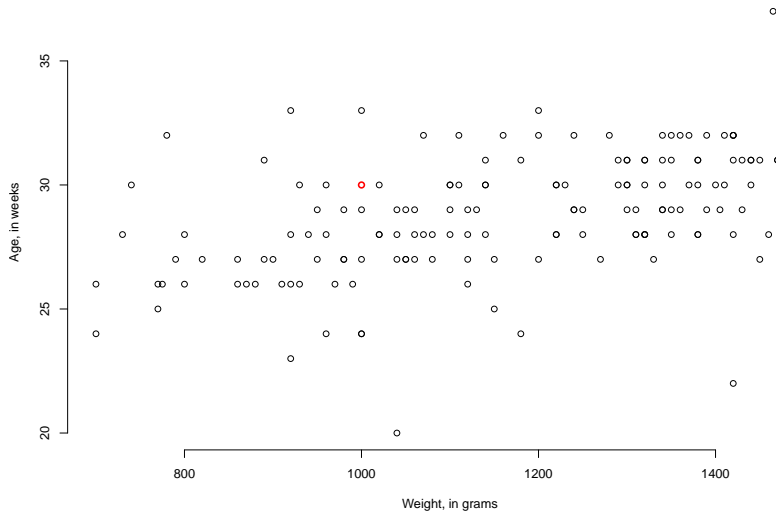
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## Tukey depth

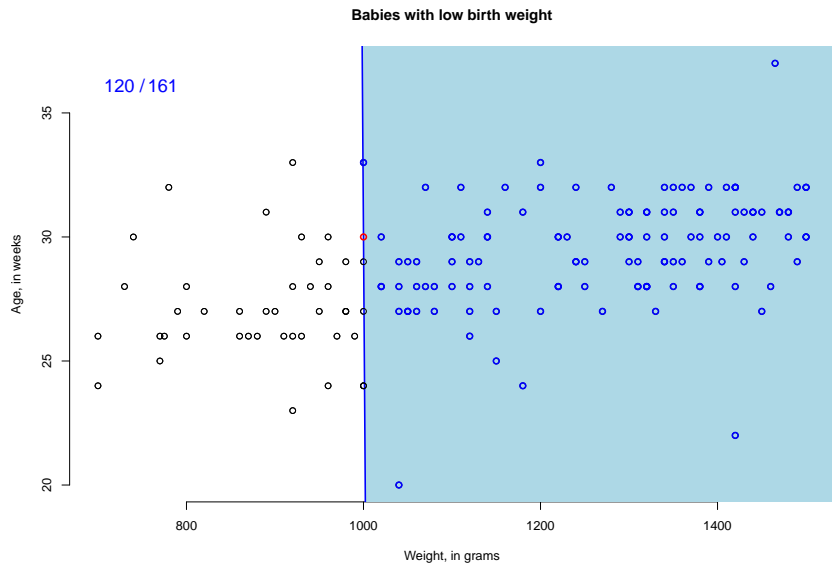
- ▶ satisfies all the above postulates,
- ▶ is purely non-parametric and robust,
- ▶ has direct connection to quantiles and many applications.

# Tukey (=halfspace, location) data depth

Babies with low birth weight

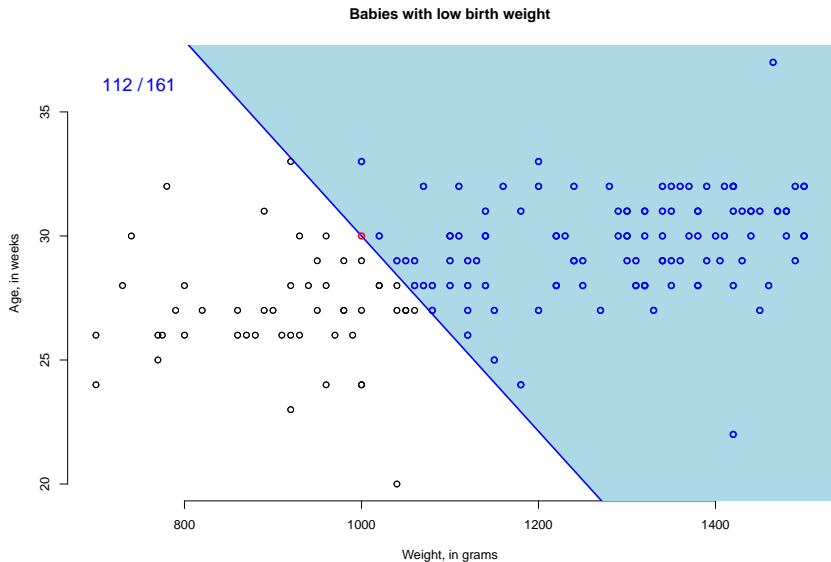


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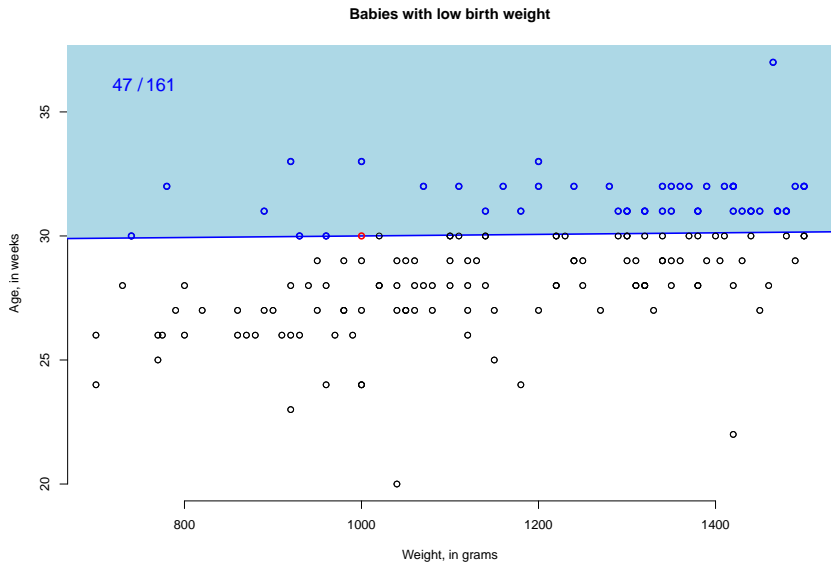




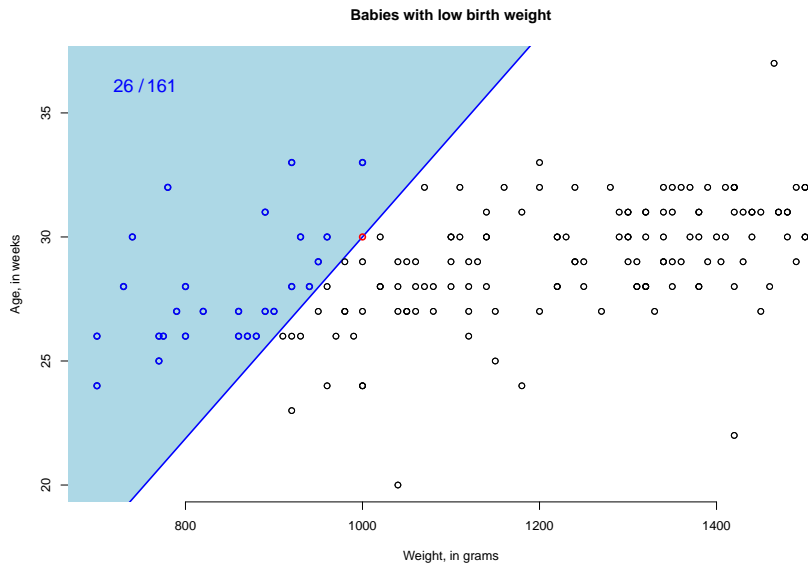
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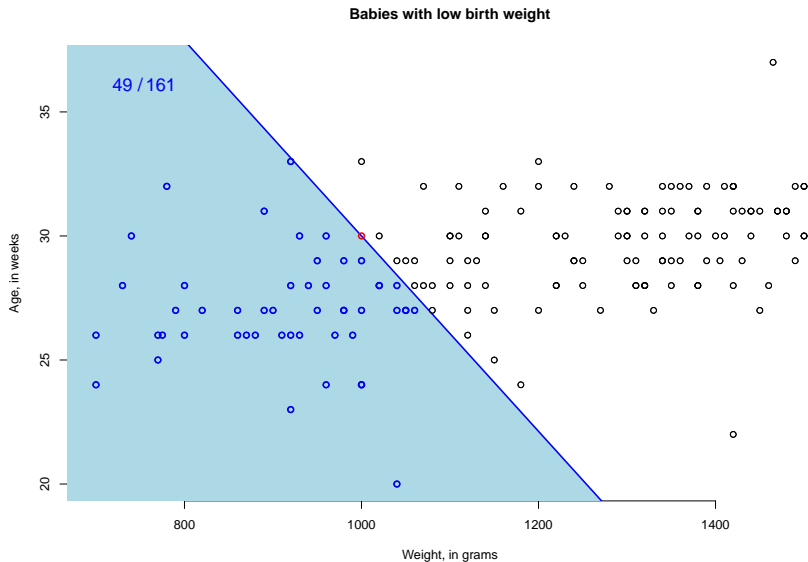
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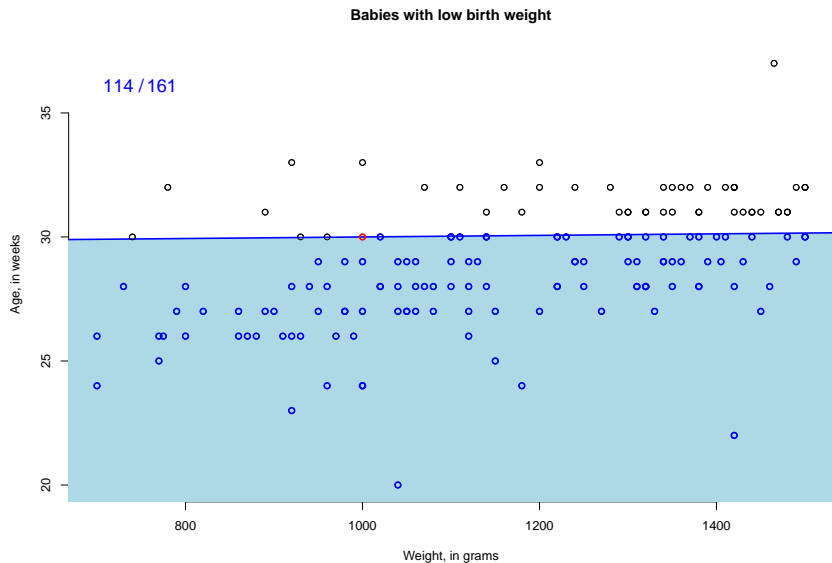
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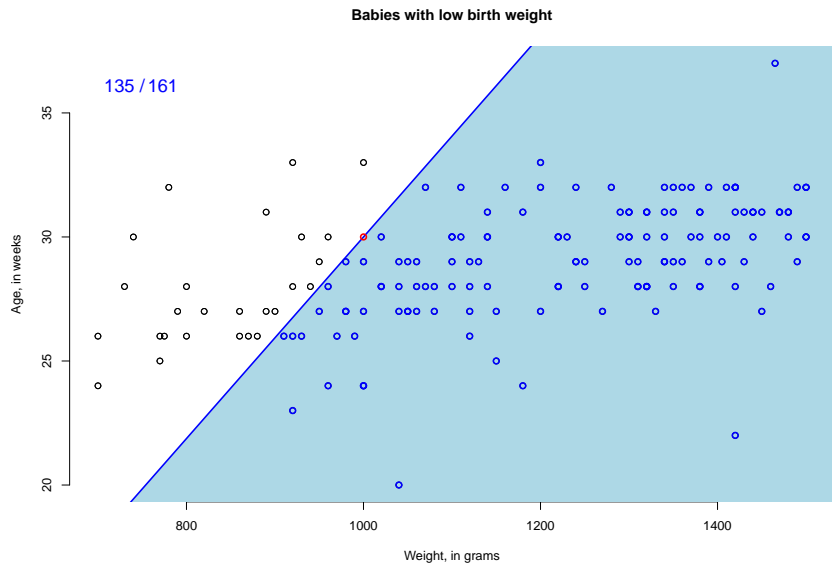
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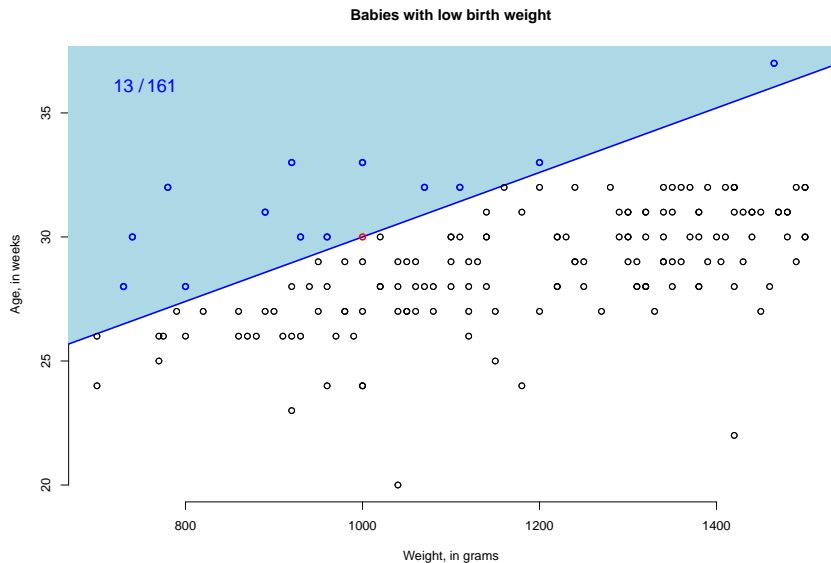
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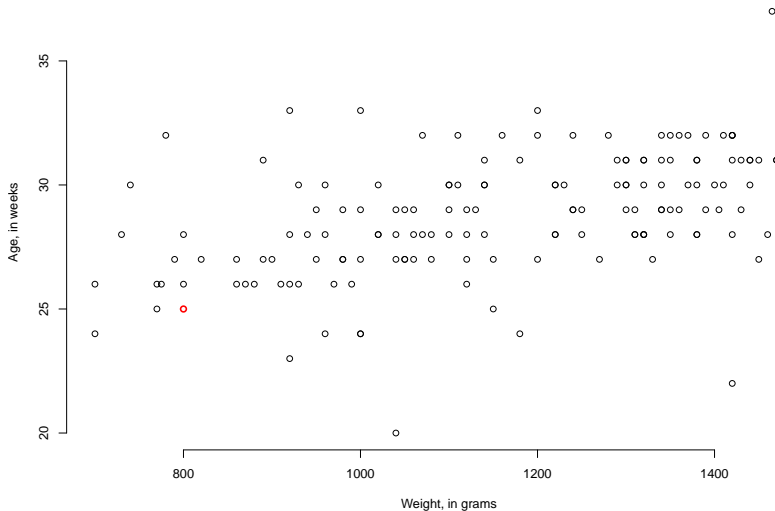
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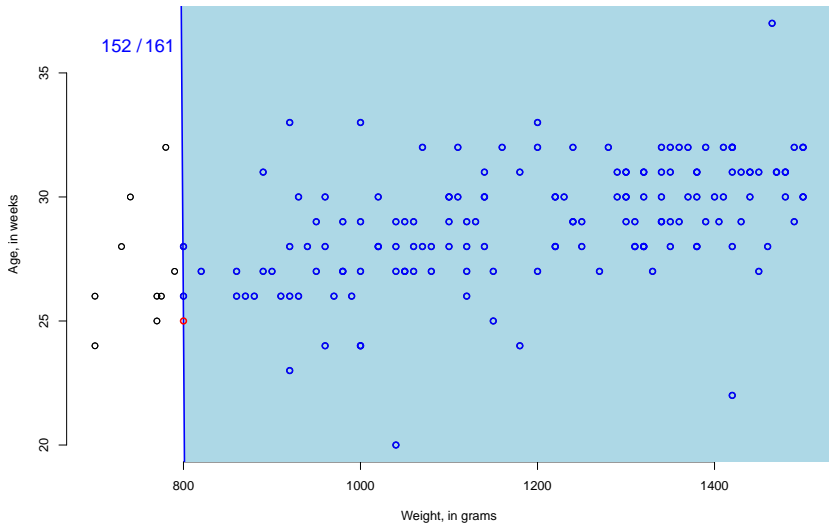
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Babies with low birth weight

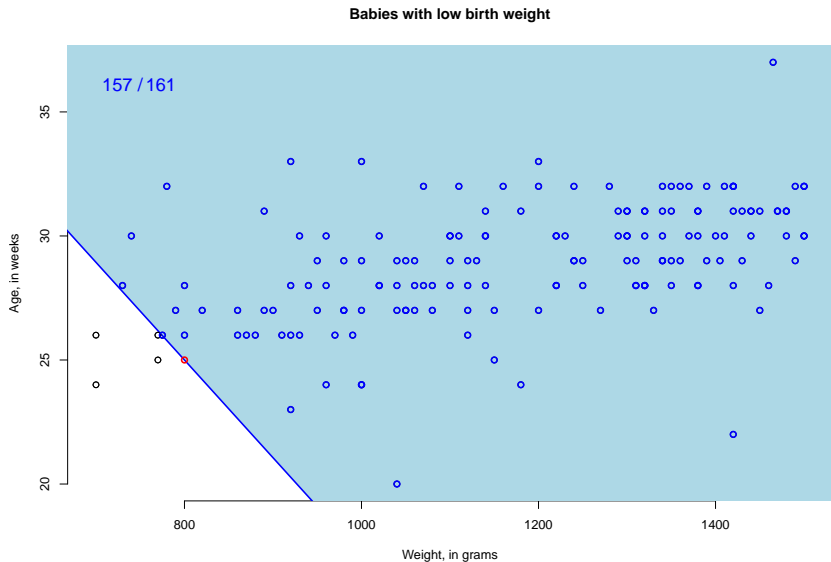


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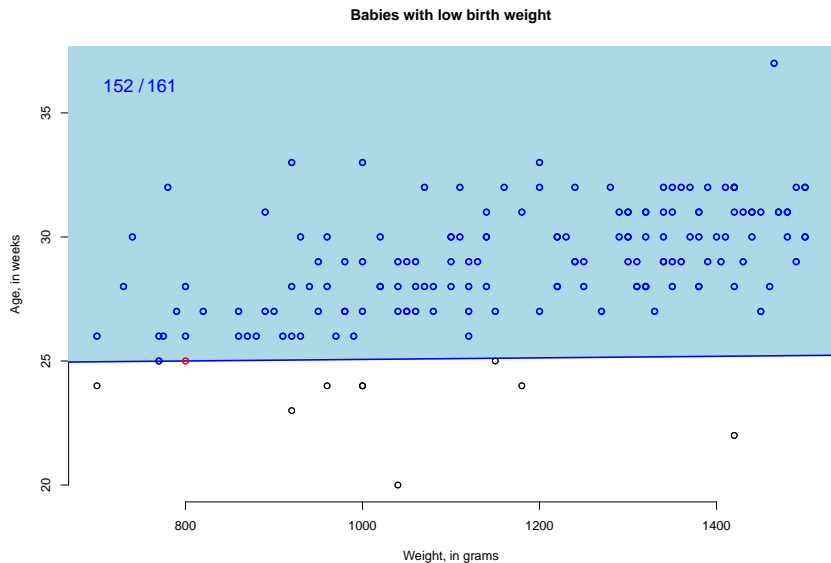
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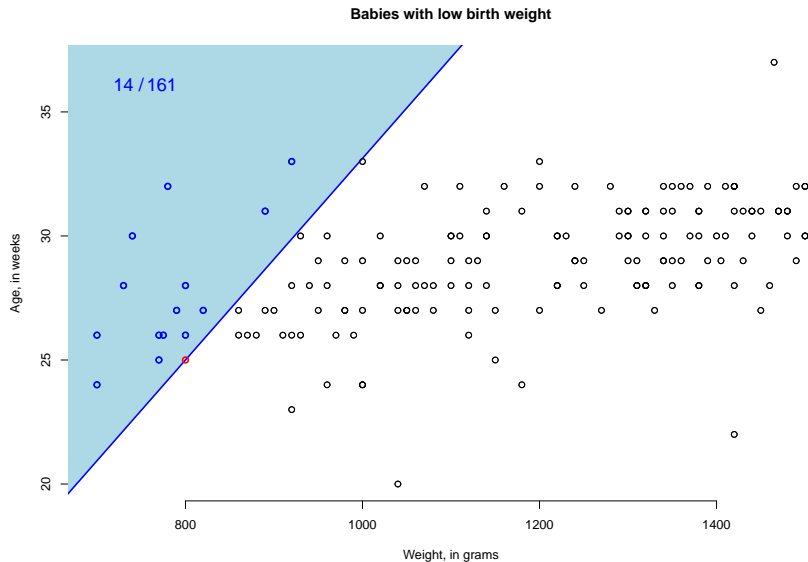
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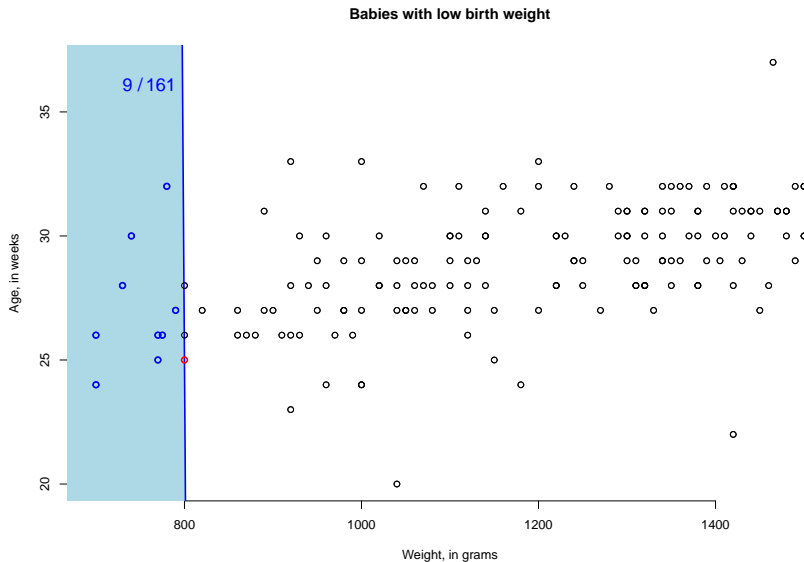
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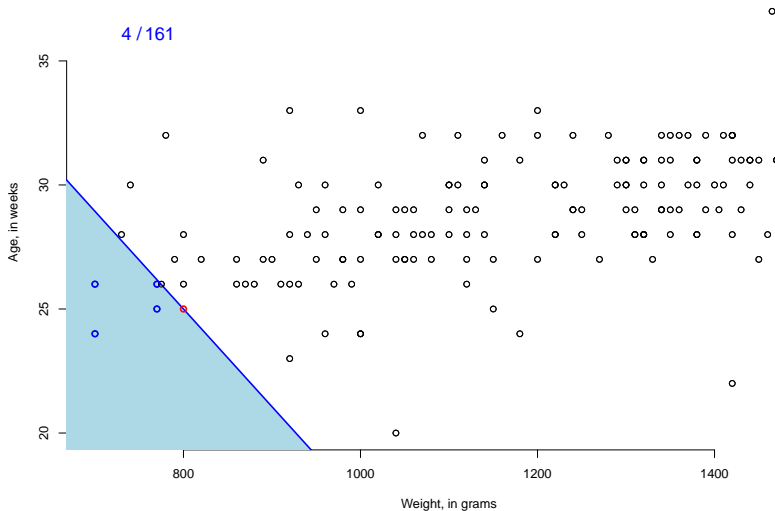


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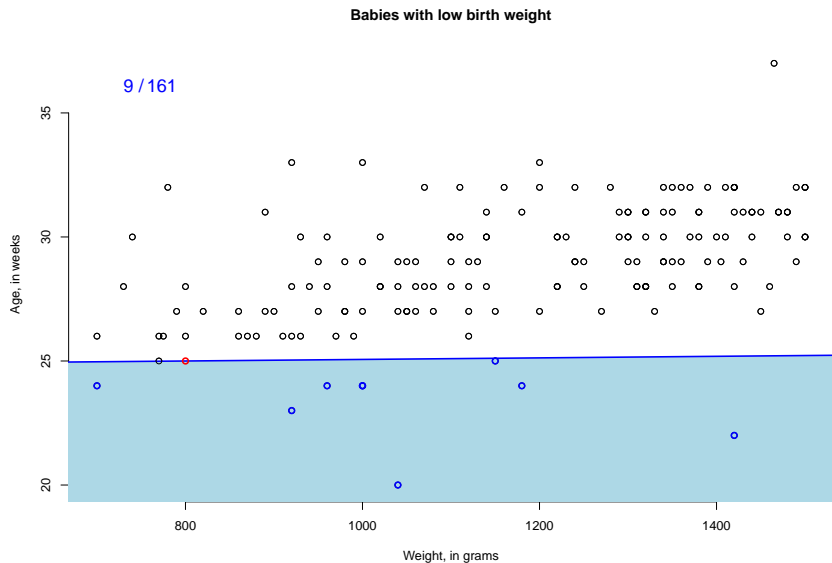


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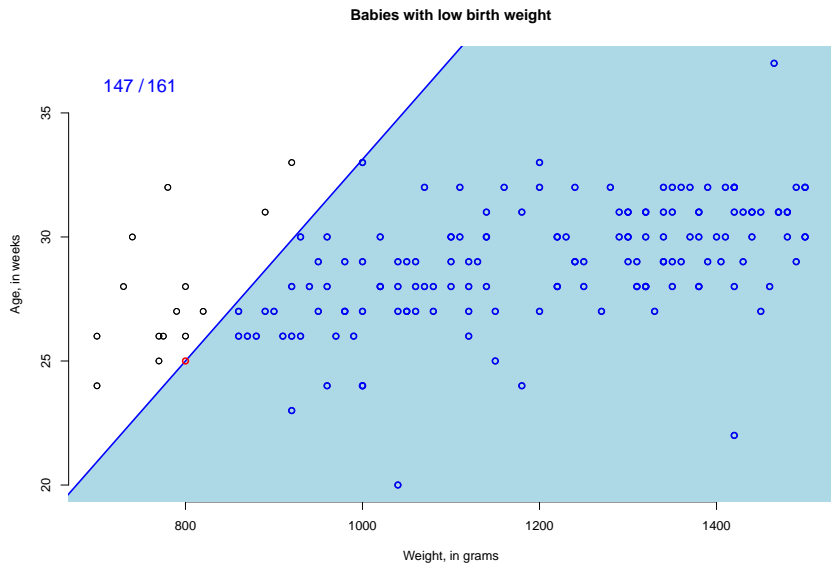


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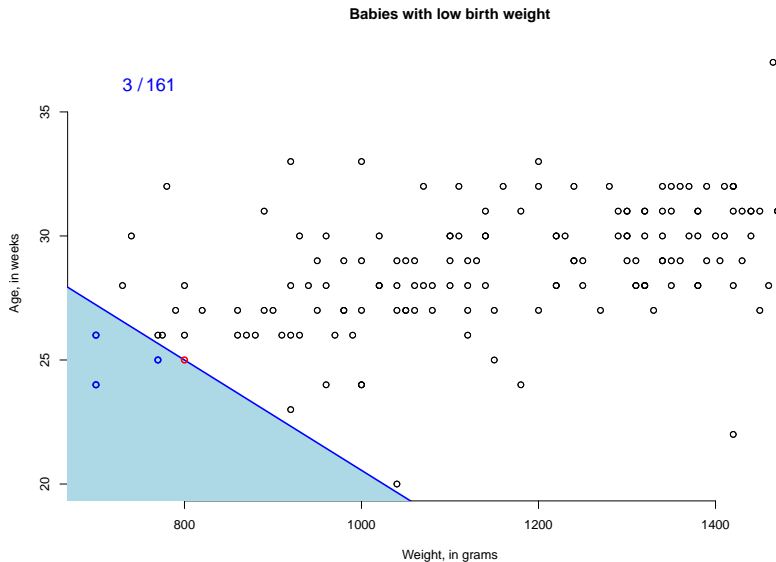




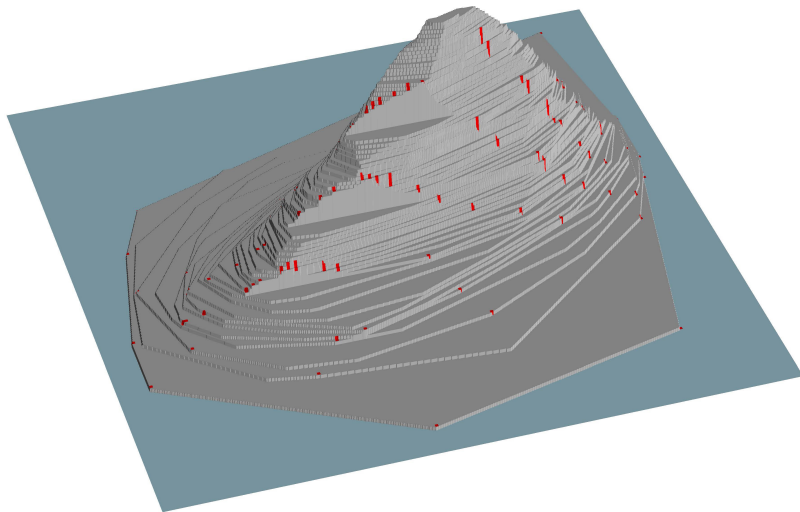
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Tukey depth defines a family of (depth-)trimmed (central) regions  $D_{\tau}^T(X)$ , the upper-level sets of the depth function:

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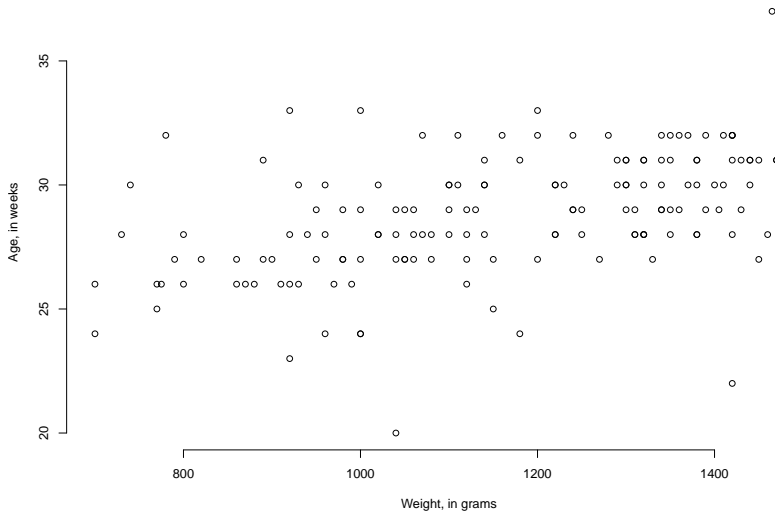
- ▶ Affine invariant;
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- ▶ Quasiconcave.

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Bounded;  
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Closed;  
Convex.

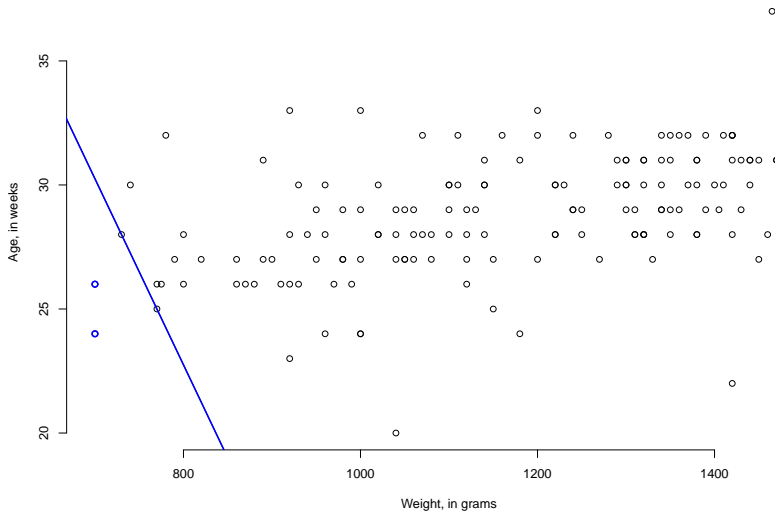
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Babies with low birth weight



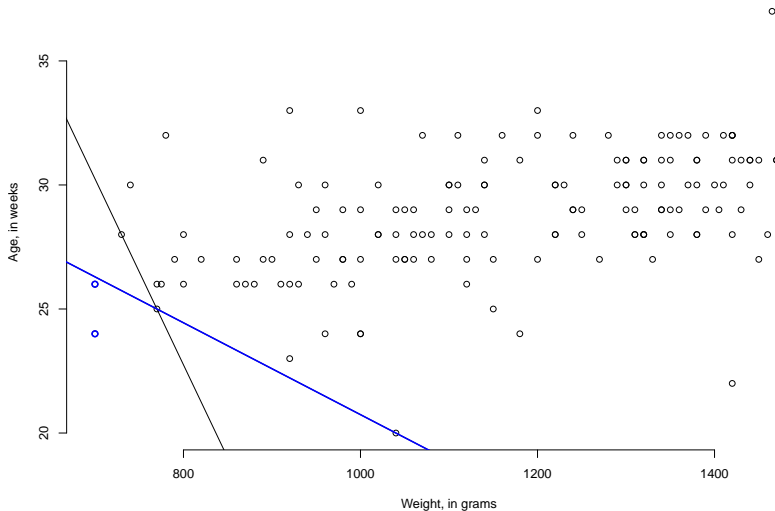
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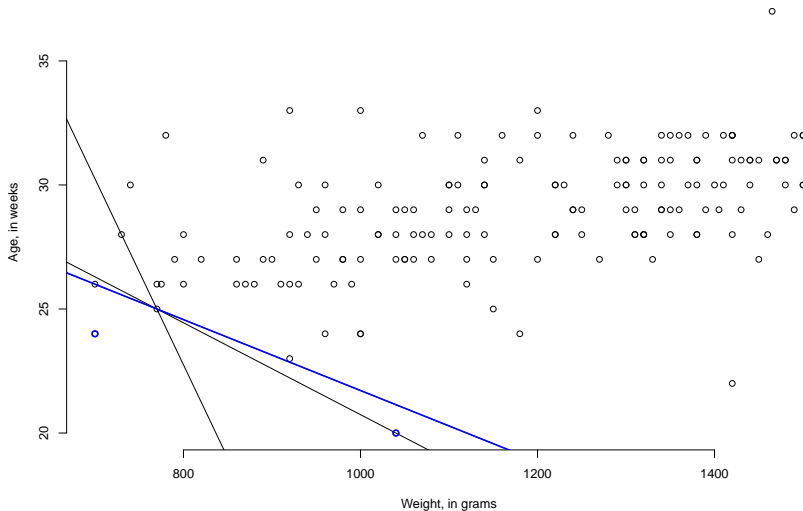
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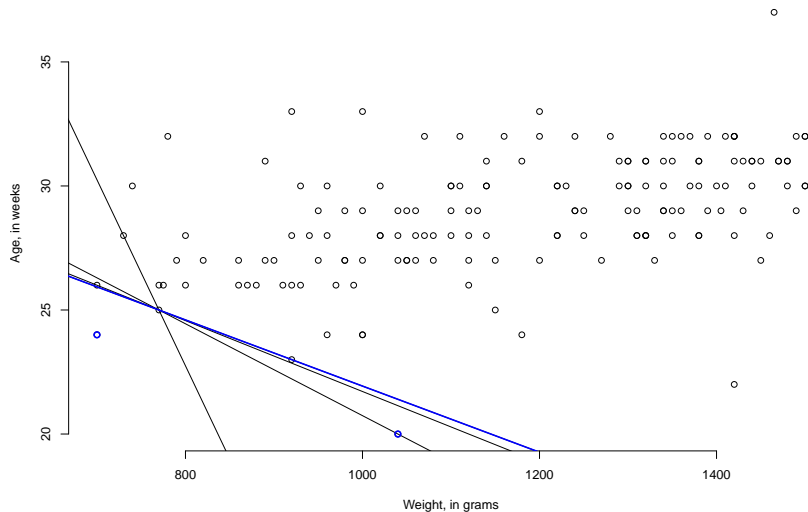
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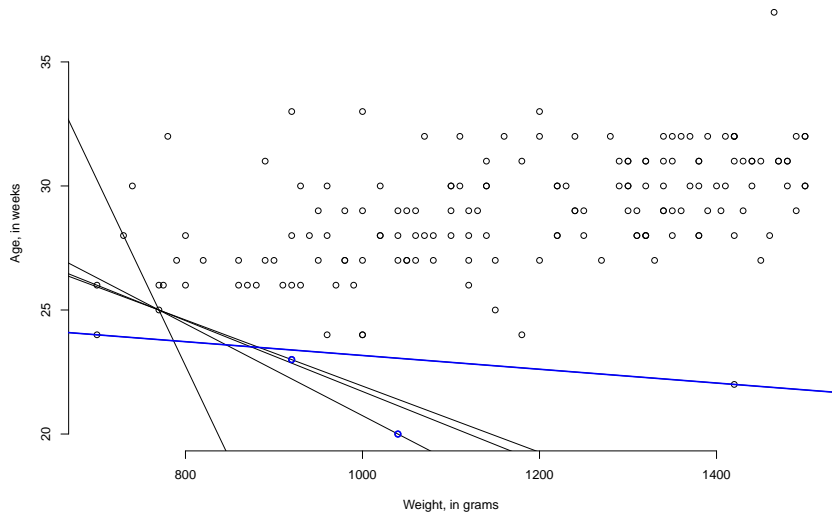
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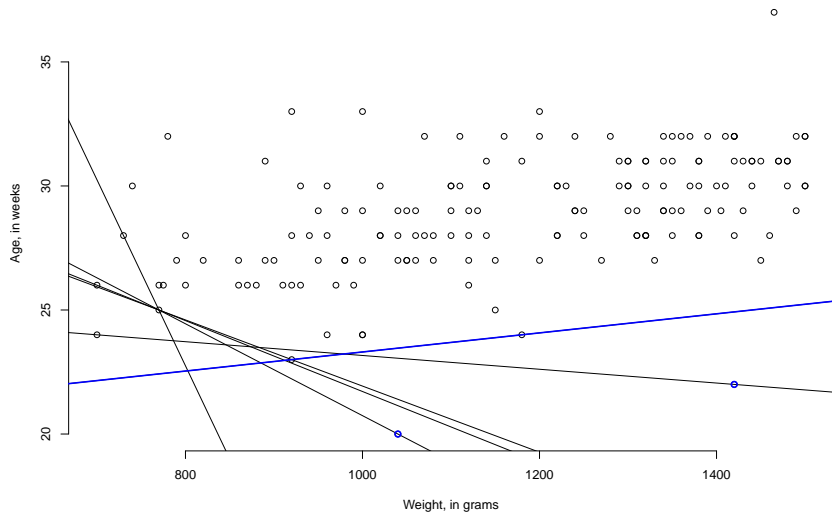
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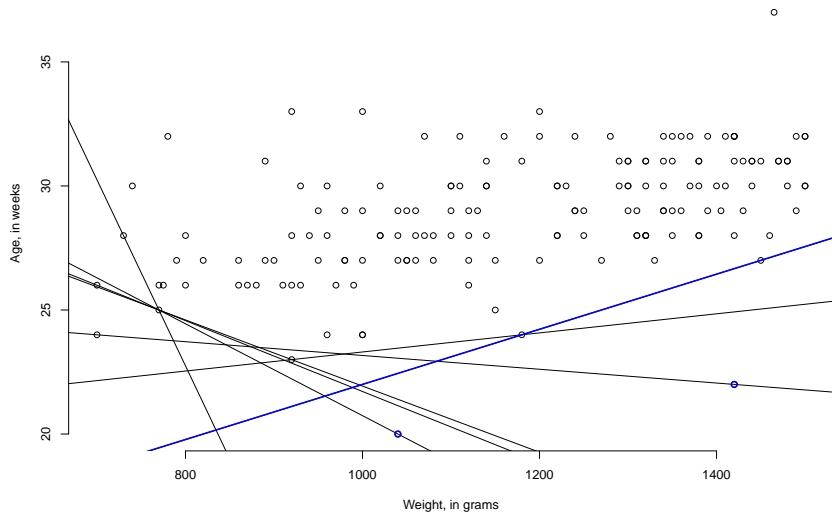
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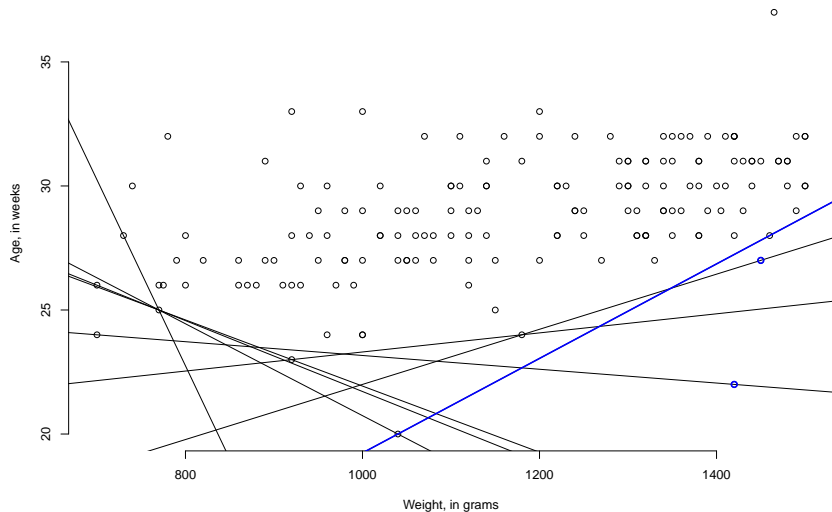
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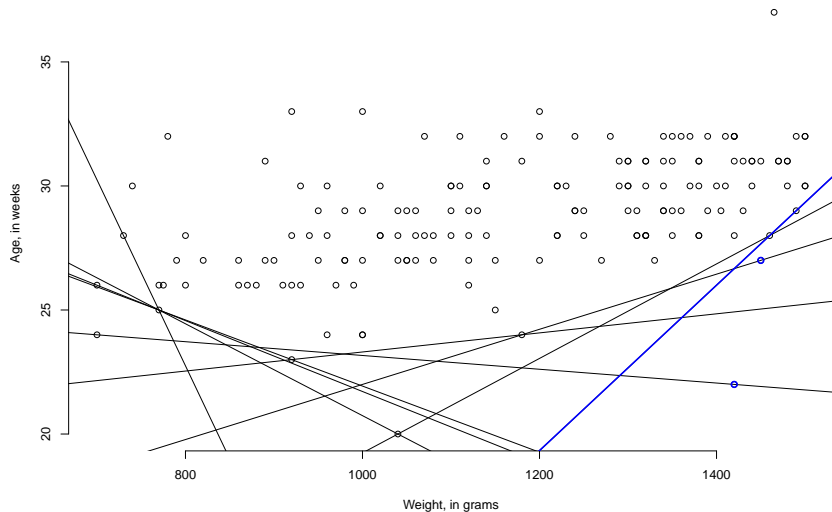
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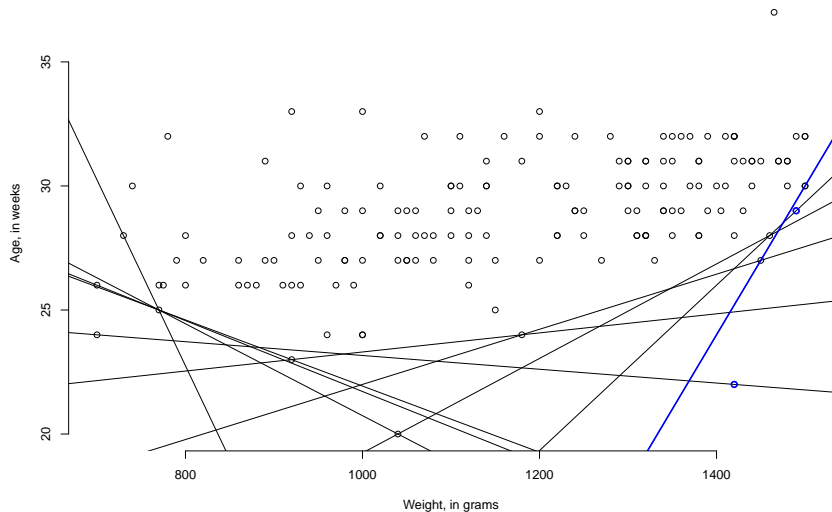
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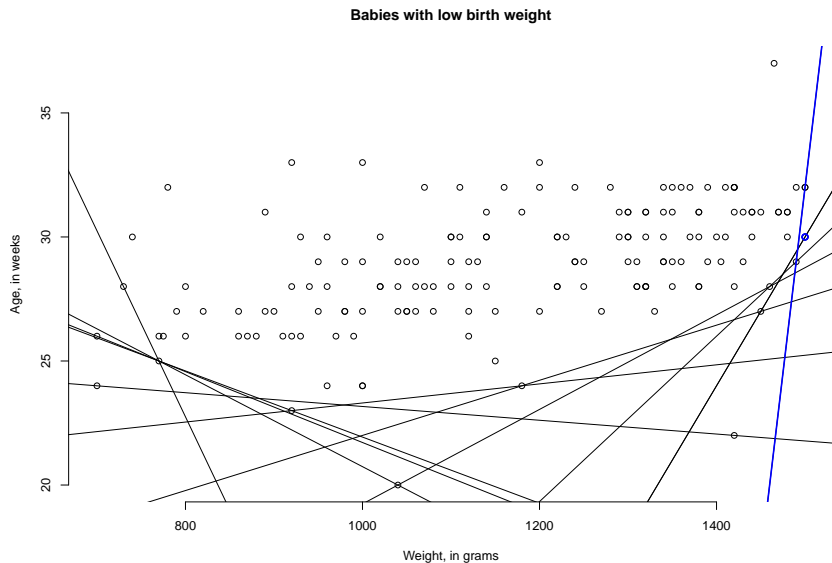


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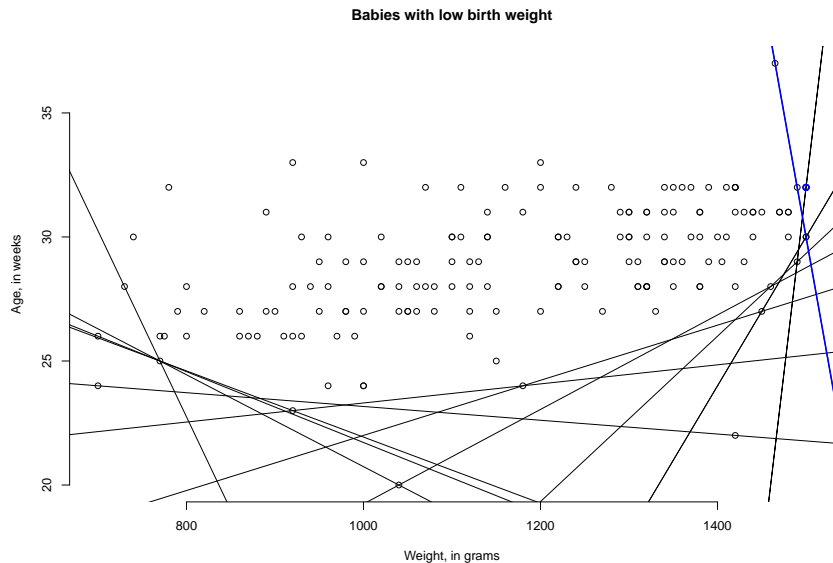
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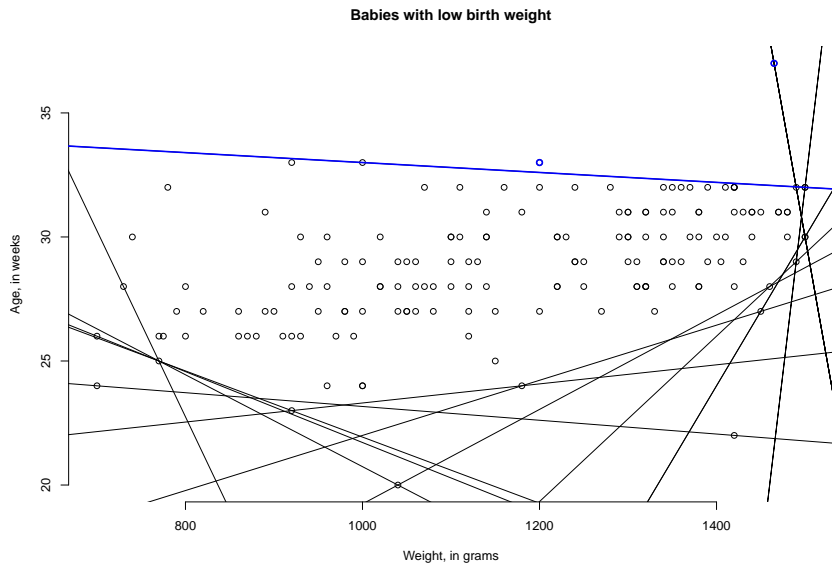
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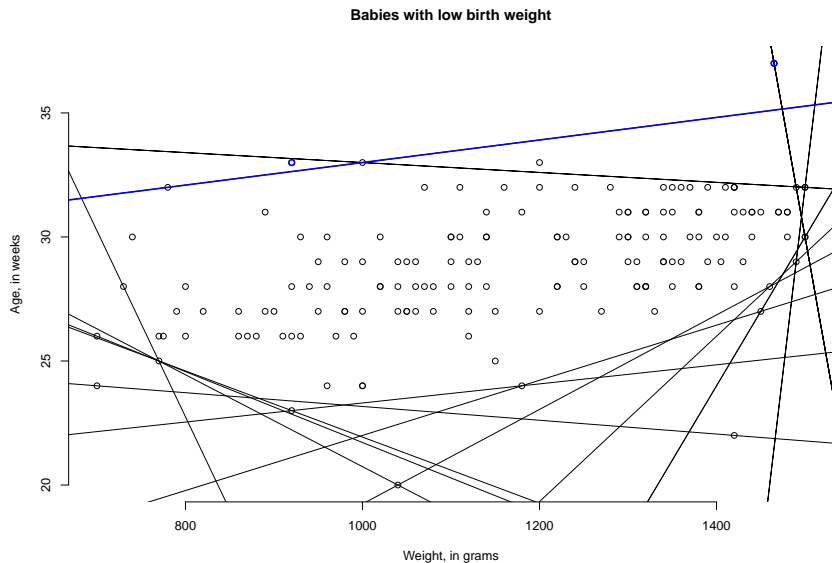


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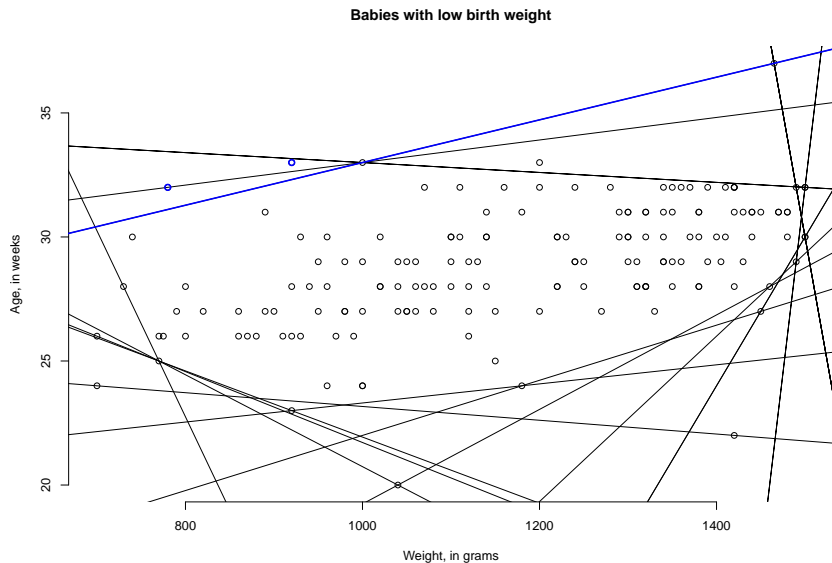




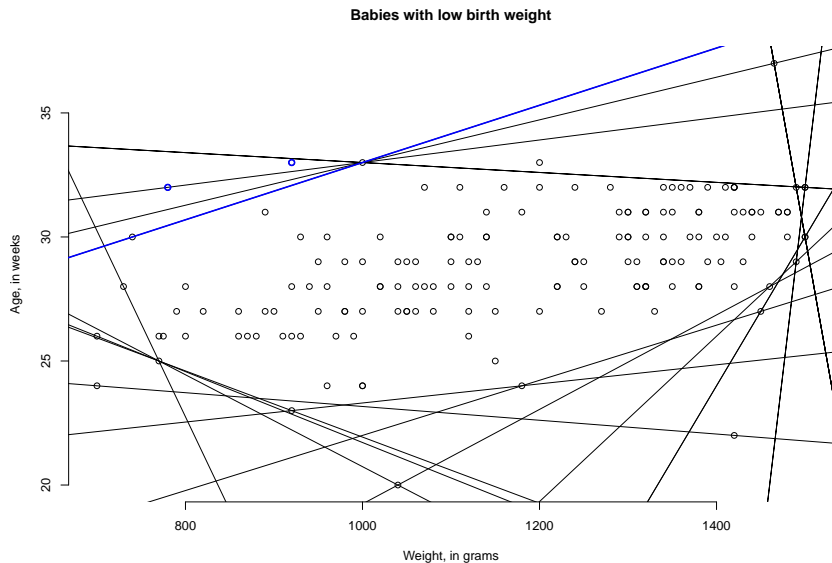
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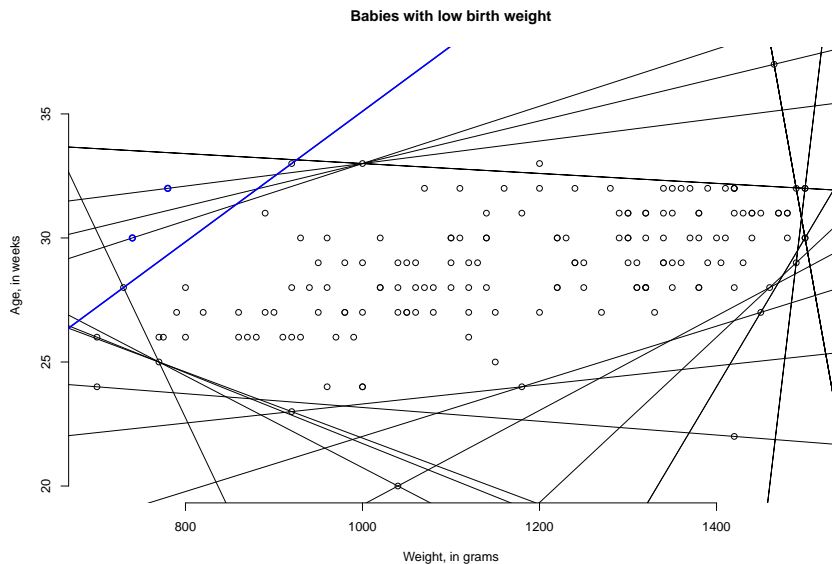
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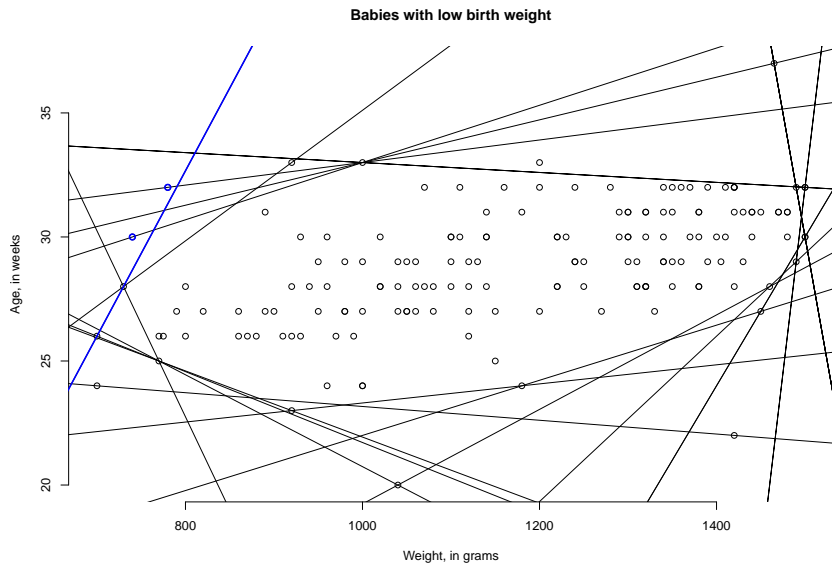
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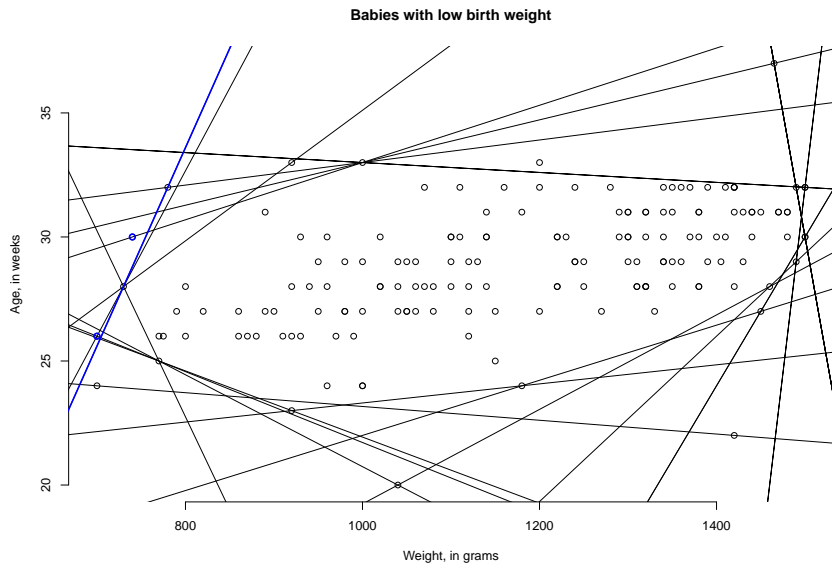
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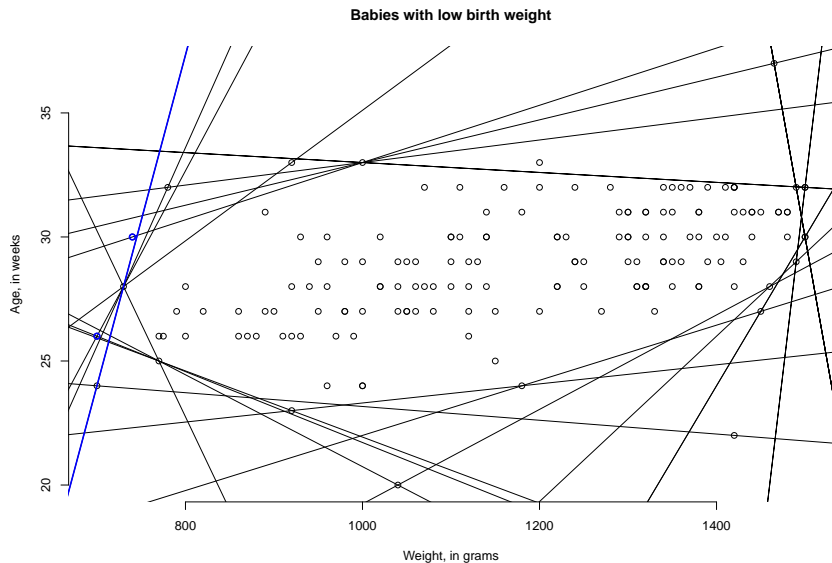
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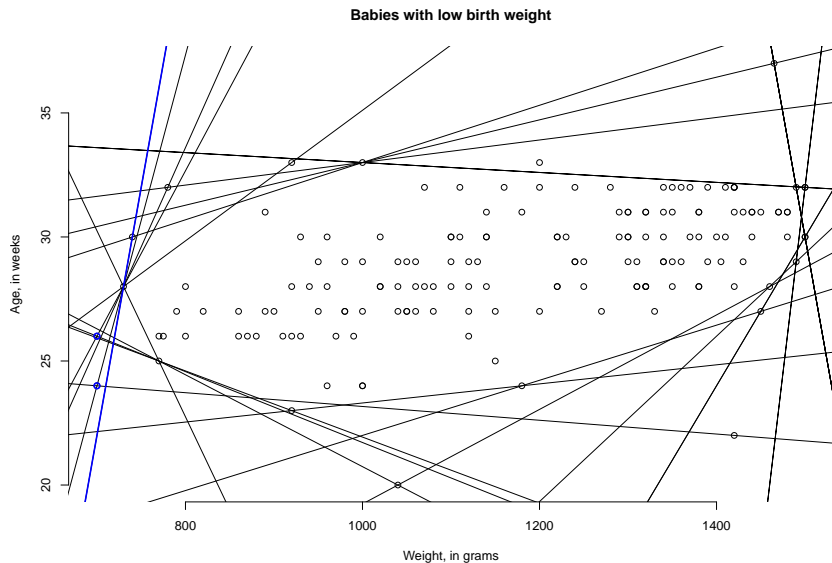
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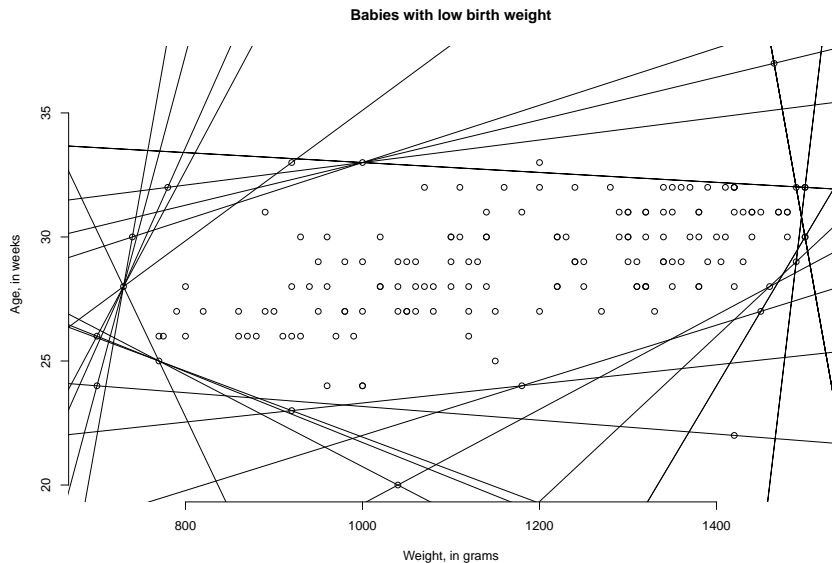


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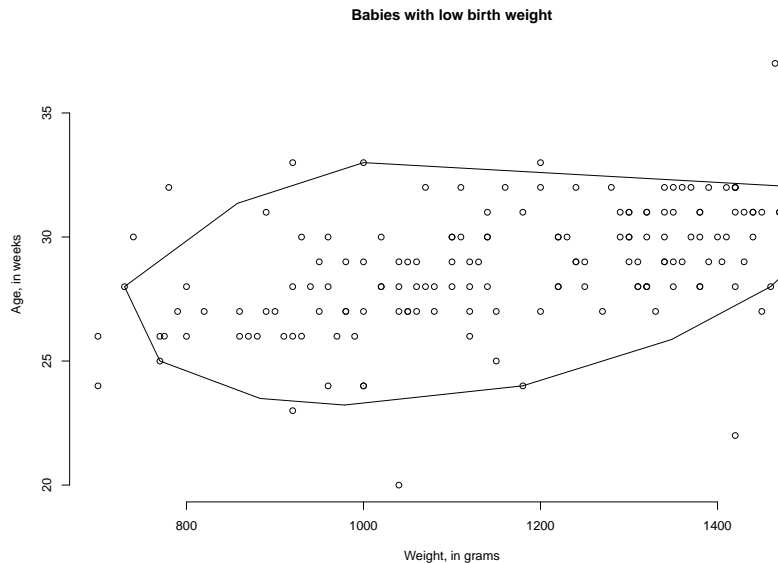




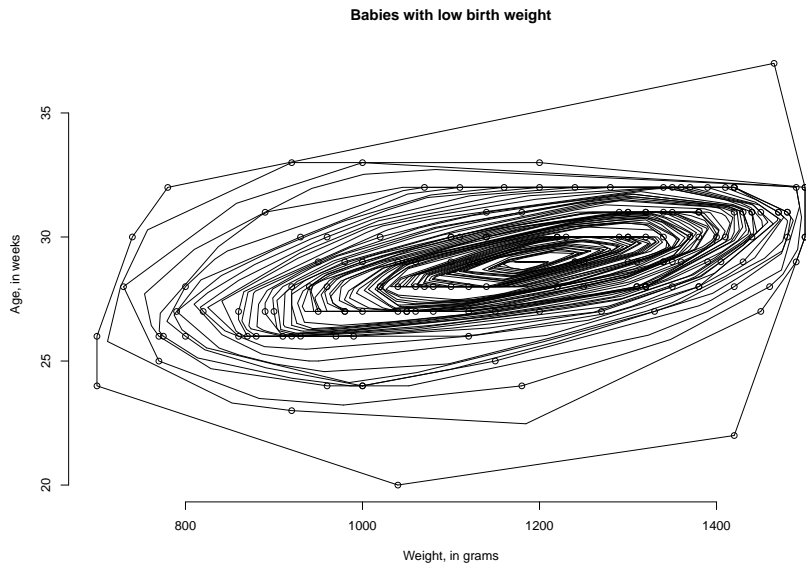
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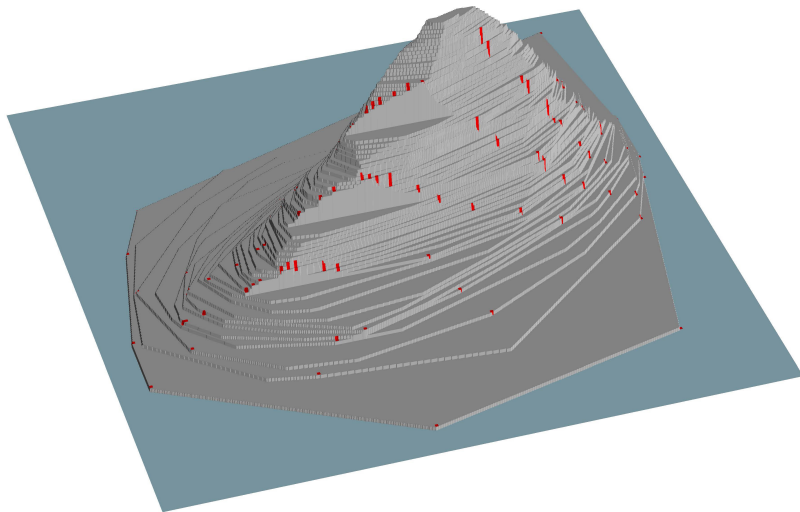
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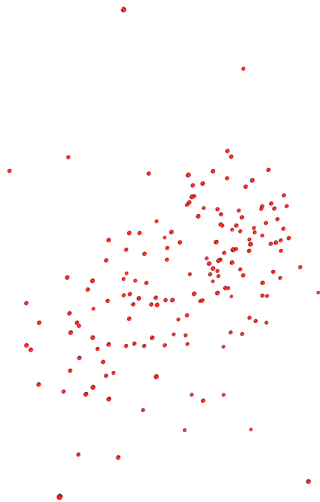
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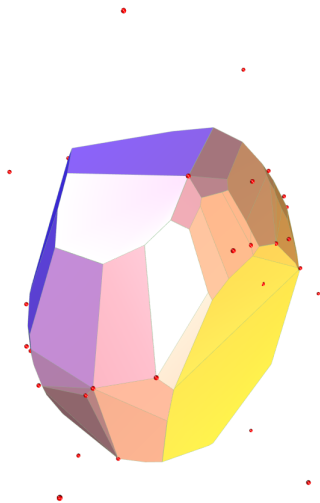
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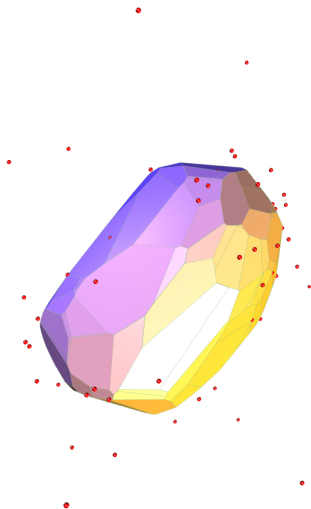
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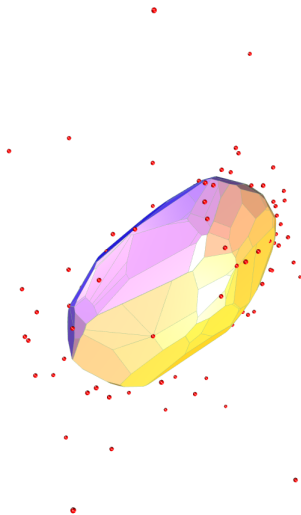
Tukey (=halfspace, location) depth region:  $\tau = 2/161$



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

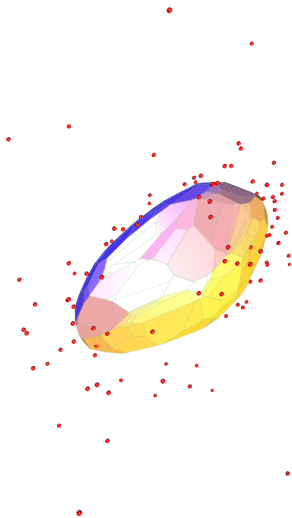


Tukey (=halfspace, location) depth region:  $\tau = 9/161$

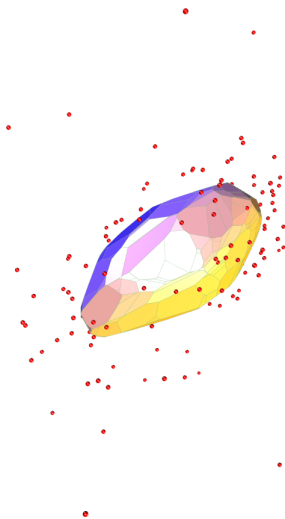




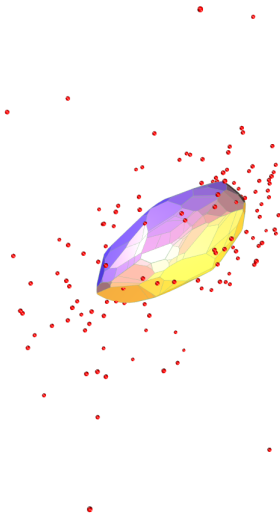
Tukey (=halfspace, location) depth region:  $\tau = 13/161$



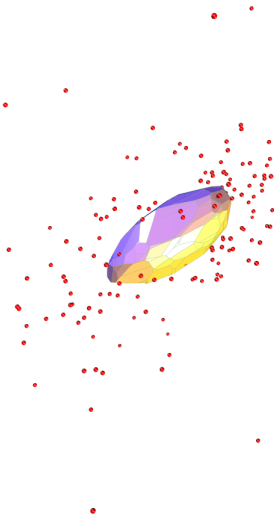
Tukey (=halfspace, location) depth region:  $\tau = 17/161$



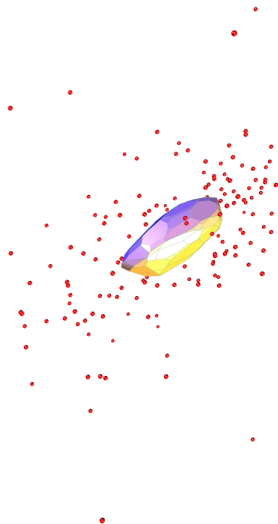
Tukey (=halfspace, location) depth region:  $\tau = 25/161$



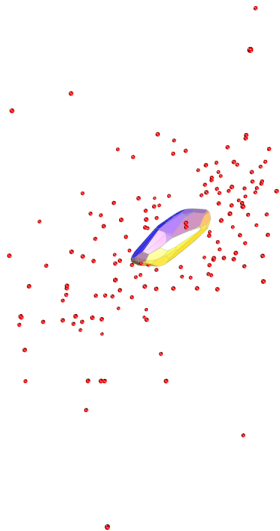
Tukey (=halfspace, location) depth region:  $\tau = 33/161$



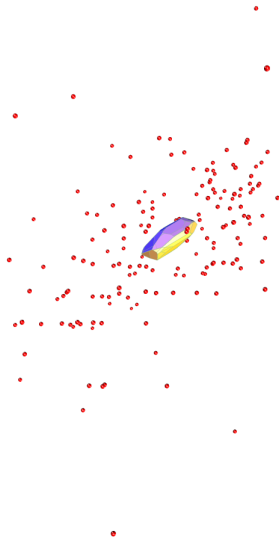
Tukey (=halfspace, location) depth region:  $\tau = 41/161$



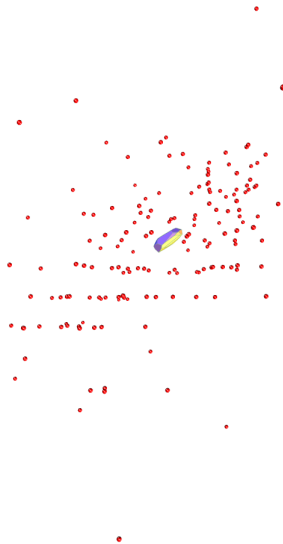
Tukey (=halfspace, location) depth region:  $\tau = 49/161$



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

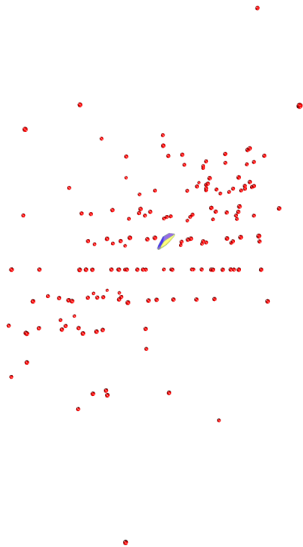


Tukey (=halfspace, location) depth region:  $\tau = 65/161$





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



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Depth for curve data

## Practical session

# Mahalanobis depth (Mahalanobis, 1936)

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based on Mahalanobis distance:

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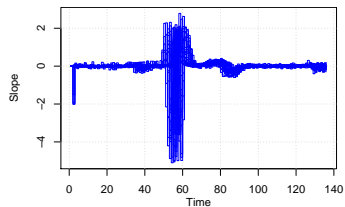
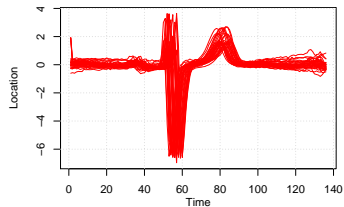
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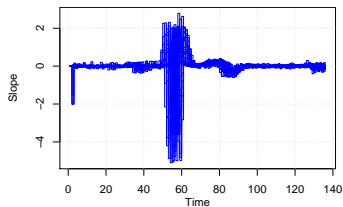
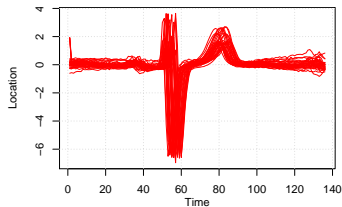
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  - ▶ by a single elliptical contour characterizes a multivariate **normal distribution** or one within an affine **family of non-degenerate elliptical distributions**.

# ECG five days data





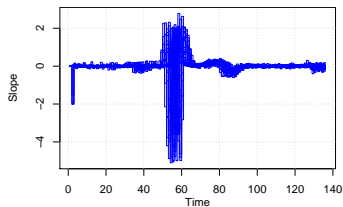
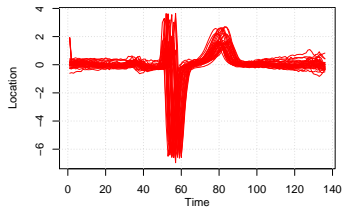
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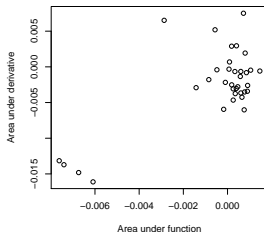
with  $\hat{f}_i(t)$  being the function obtained by connecting the points  $(t_{ij}, f_i(t_{ij}))$ ,  $j = 1, \dots, N_i$  with line segments,  $\hat{f}'_i(t)$  its derivative.

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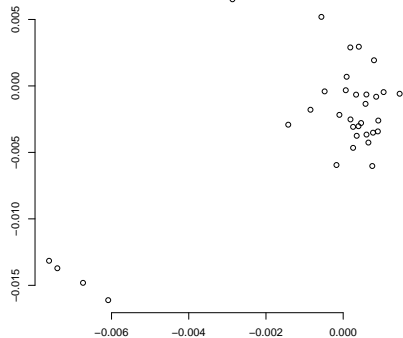


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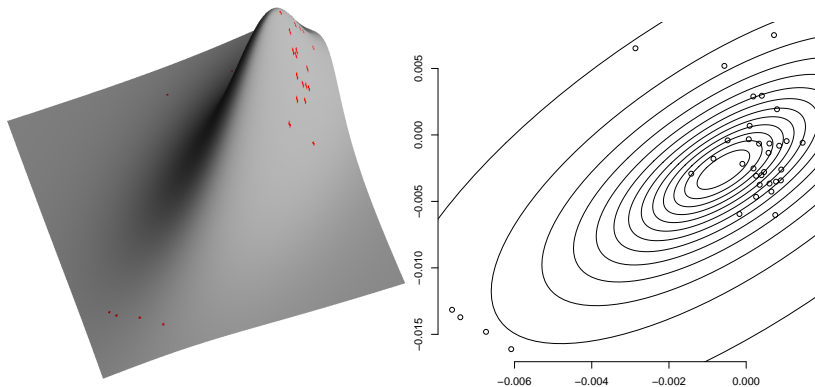
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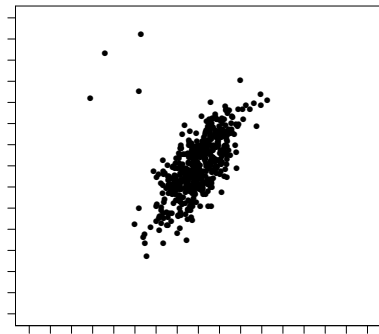
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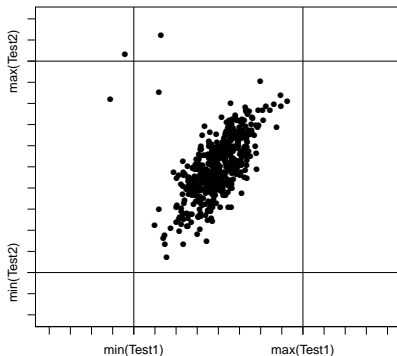
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## Multivariate anomaly detection: an example

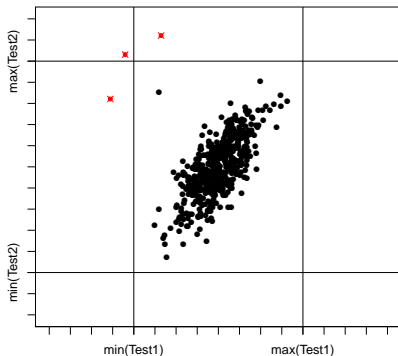


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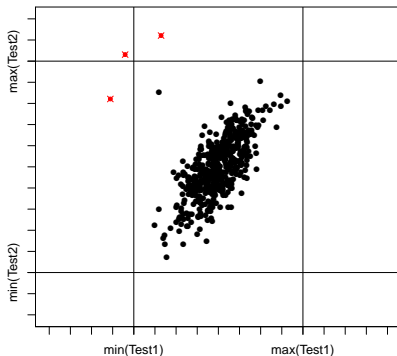
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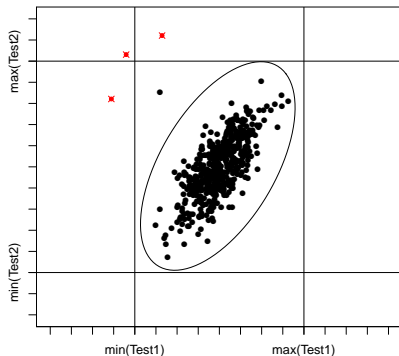
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- ▶ **Not all** anomalies can be detected.



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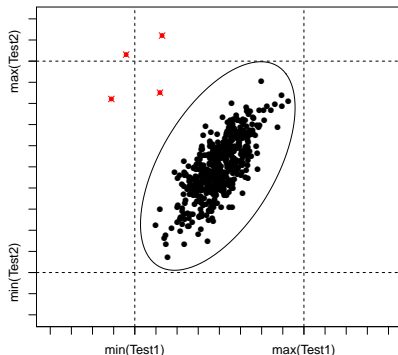


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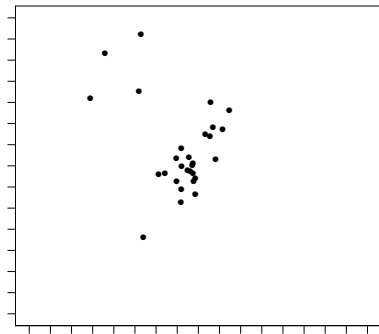
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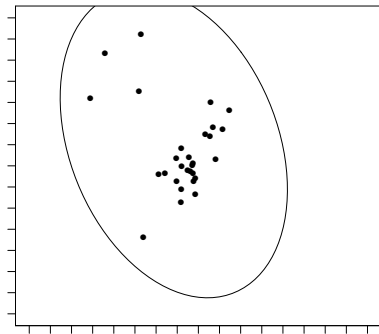
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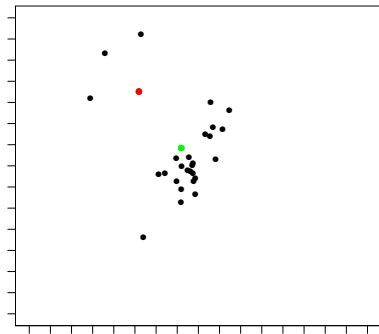


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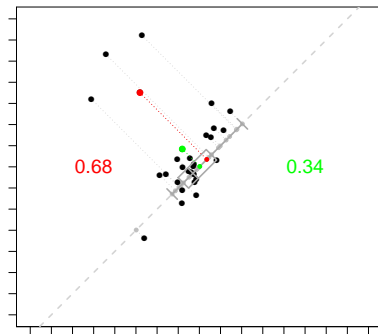
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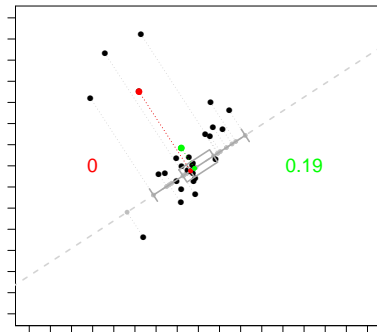
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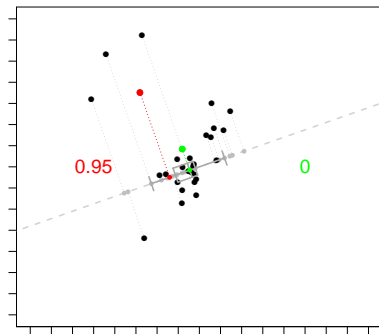
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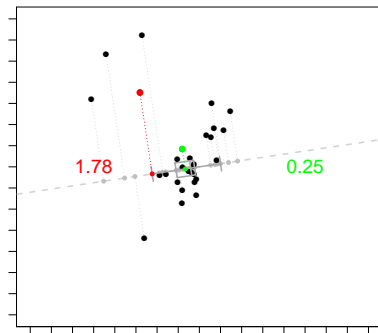


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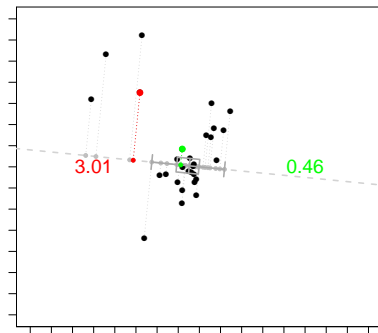
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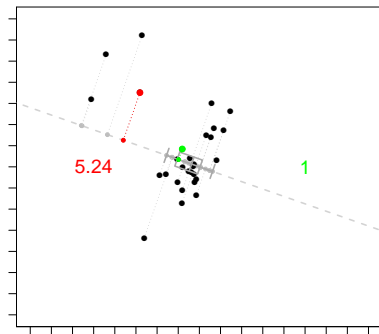
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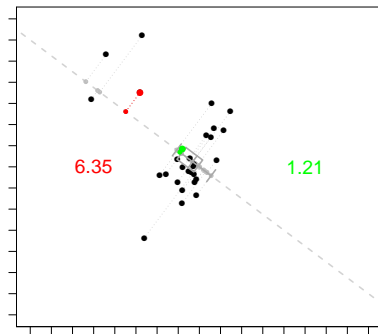
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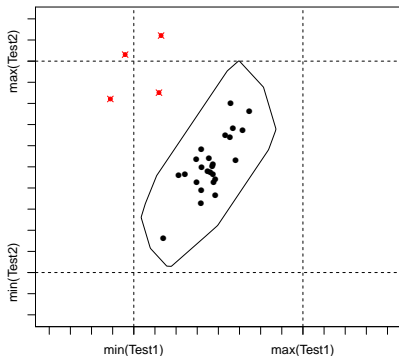
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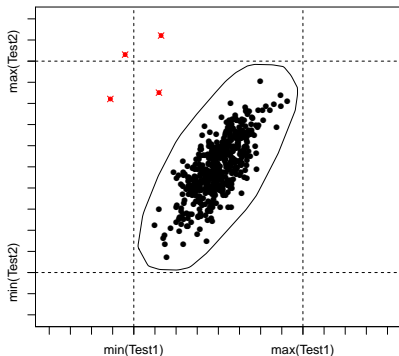


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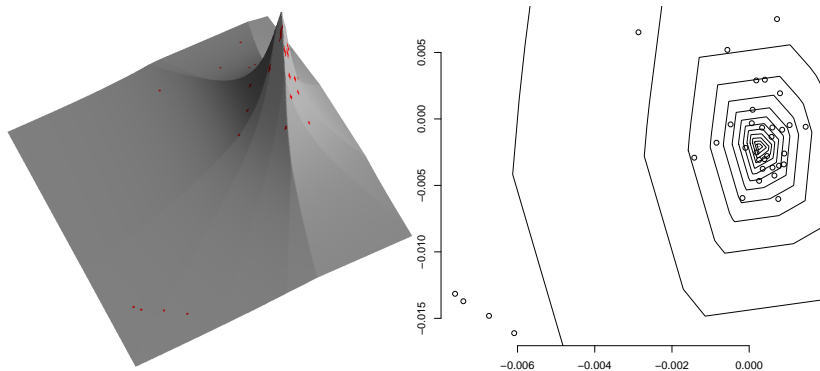
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# Projection depth (Zuo & Serfling, 2000)



## Spatial depth (Vardi & Zhang, 2000; Serfling 2002)

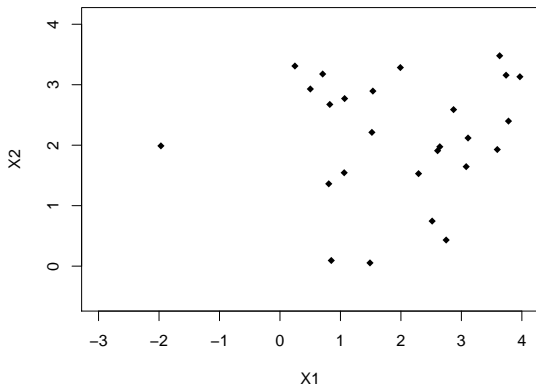
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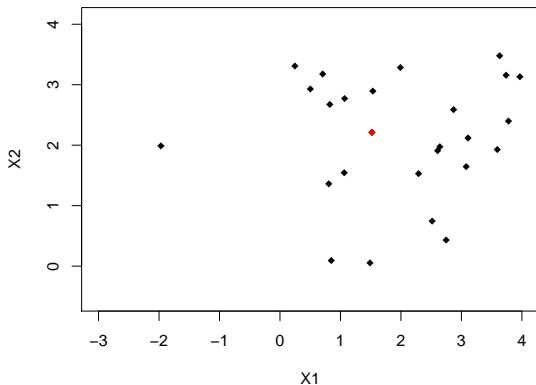
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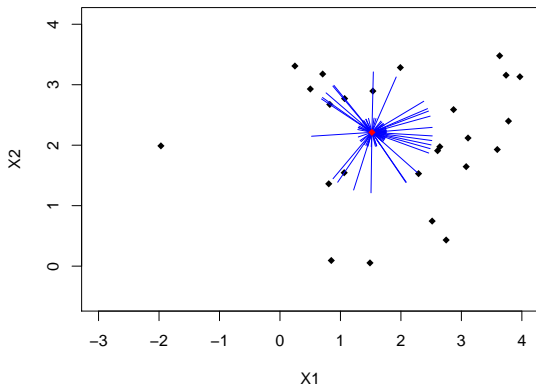
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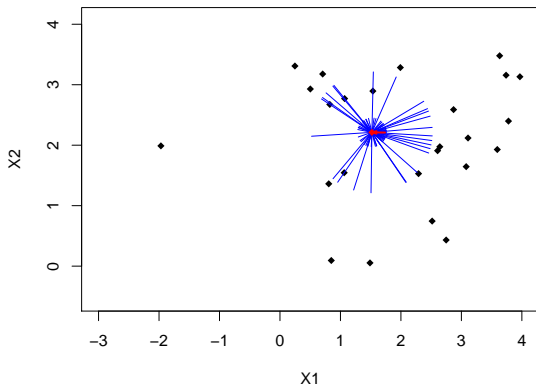
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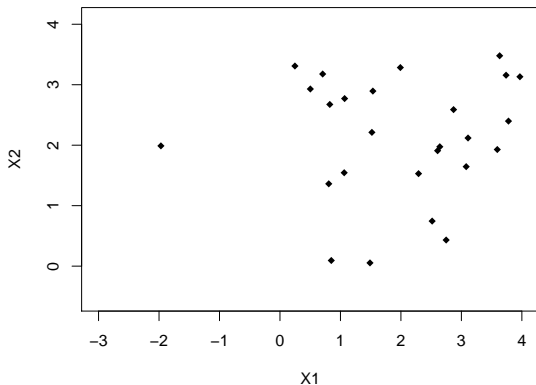




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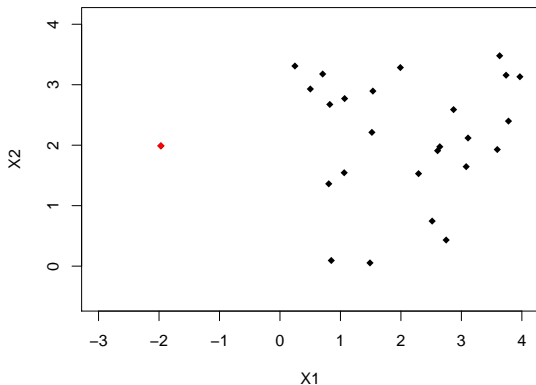
$$D^{spt}(\mathbf{x}|X) = 1 - \left\| \mathbb{E} \left[ \frac{\mathbf{x} - X}{\|\mathbf{x} - X\|} \right] \right\| \quad \text{with} \quad \frac{\mathbf{x} - X}{\|\mathbf{x} - X\|} = 0 \quad \text{if} \quad \mathbf{x} - X = \mathbf{0}.$$



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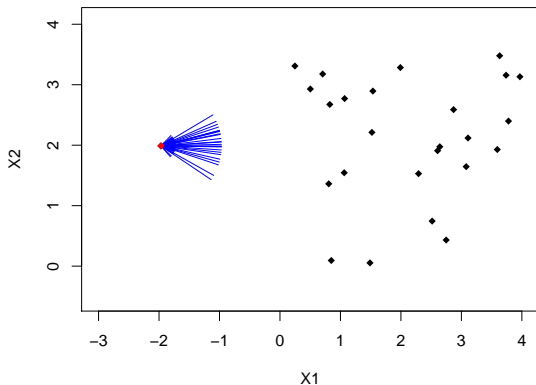
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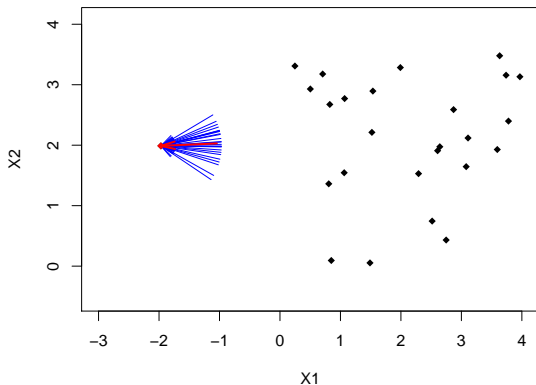
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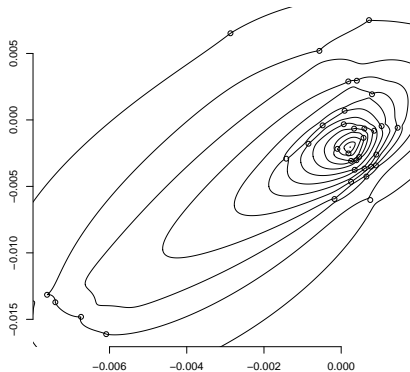
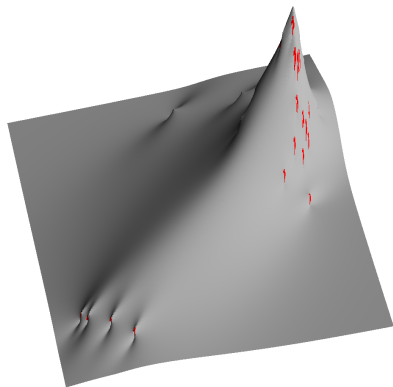
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- ▶ with **D2iso** its maximum (say  $\mathbf{x}^*$ ) is referred to as **spatial median**, a multivariate location estimator having asymptotic breakdown point of 0.5.



# Spatial depth (Vardi & Zhang, 2000; Serfling 2002)



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## Functional anomaly detection

- Integrated data depth

- Functional isolation forest

- Depth for curve data

## Practical session

# Functional data framework

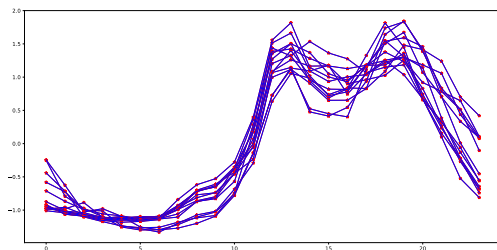
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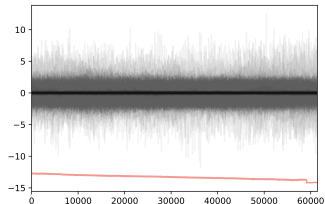
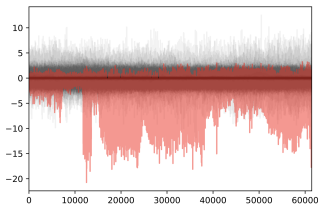
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- ▶ The first step: reconstruct **functional object** from partial observations (time-series) with interpolation or basis decomposition.



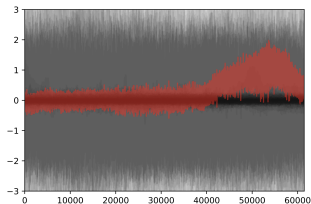
# Taxonomy of functional anomalies

A non-complete taxonomy of functional abnormalities:

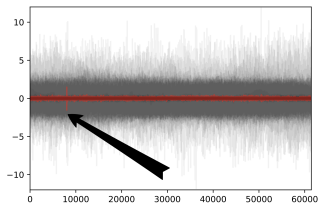
## Magnitude (=location, shift) anomalies



## Shape anomalies



## Isolated anomalies



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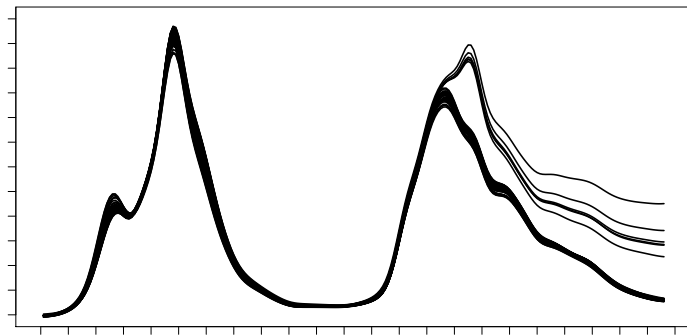
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Functional isolation forest

Depth for curve data

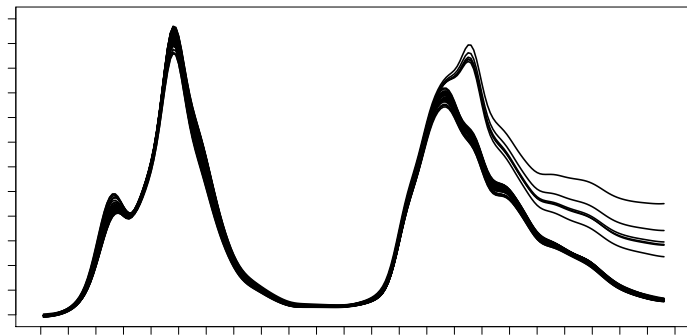
## Practical session

# Detection of (multivariate) functional anomalies





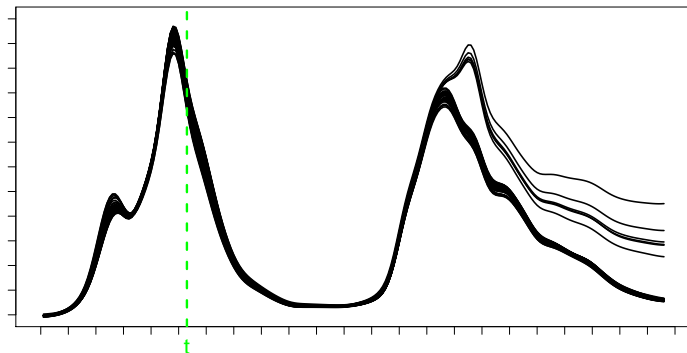
# Detection of (multivariate) functional anomalies



- **Functional depth** of  $\mathbf{f}$  w.r.t.  $\mathcal{F} = \{\mathbf{f}_i\}_{i=1}^n$ :

$$D(\mathbf{f}|\mathcal{F}) = \int_{t_{\min}}^{t_{\max}} D^1(\mathbf{f}(t)|\mathcal{F}(t)) dt ,$$

# Detection of (multivariate) functional anomalies

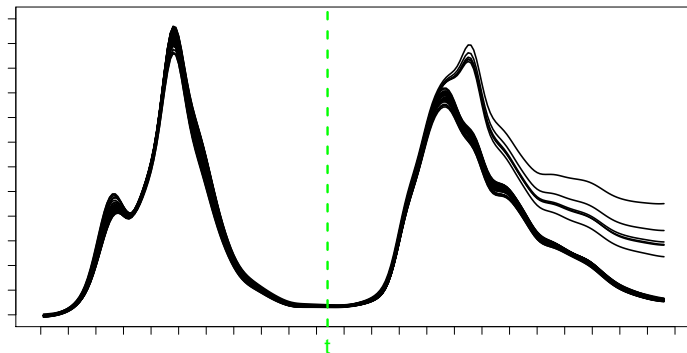


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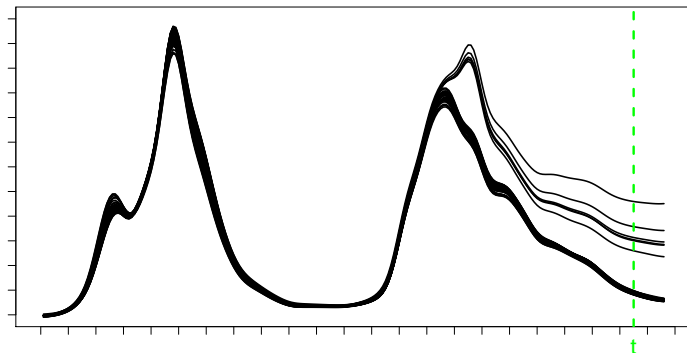


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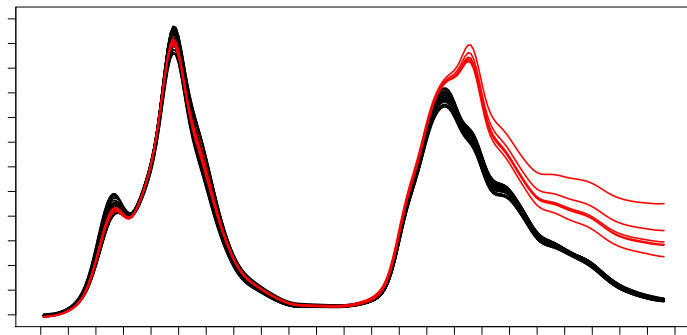


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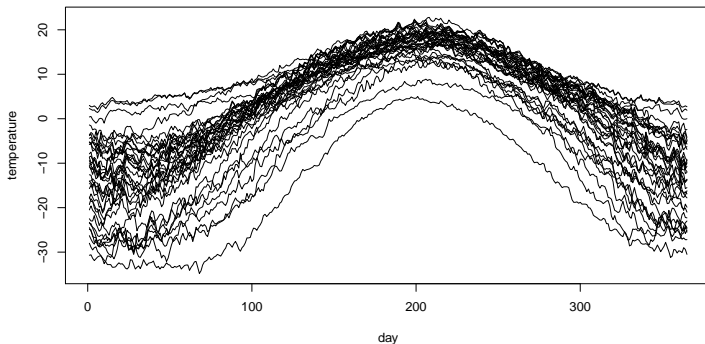
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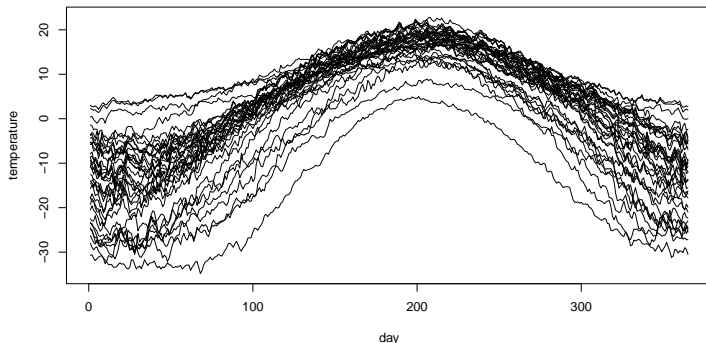
- Label  $\mathbf{f}$  as **anomaly** if  $D(\mathbf{f}|\mathcal{F}) < \min(D)$ .

# Integrated depth for functional data



Let  $\mathbf{F}$  be a stochastic process with continuous paths defined on  $[0, 1]$ , and  $\mathbf{f}$  its realization.

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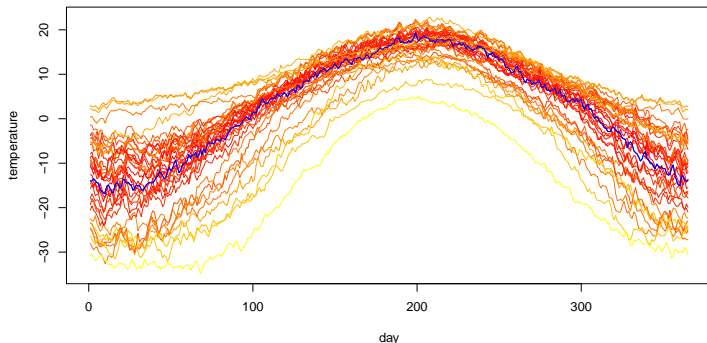


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see Fraiman, Muniz, 2001; also López-Pintado, Romo, 2011.

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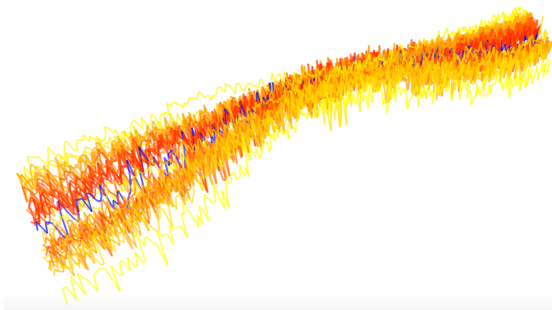
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$$D(\mathbf{f}|\mathbf{F}) = \int_0^1 \min\{F_{\mathbf{F}(t)}(\mathbf{f}(t)), 1 - F_{\mathbf{F}(t)}(\mathbf{f}(t)^-)\} dt.$$

see Fraiman, Muniz, 2001; also López-Pintado, Romo, 2011.



# Multivariate functional halfspace depth



Let  $\mathbf{F}$  be a  $d$ -real-valued stochastic process with continuous paths defined on  $[0, 1]$ , and  $\mathbf{f}$  its realization. Then:

$$MFD(\mathbf{f}|\mathbf{F}) = \int_0^1 D(\mathbf{f}(t)|\mathbf{F}(t)) \cdot w(t) dt,$$
$$w(t) = w_\alpha(t, \mathbf{F}(t)) = \frac{\text{vol}\{D_\alpha(\mathbf{F}(t))\}}{\int_0^1 \text{vol}\{D_\alpha(\mathbf{F}(u))\} du}.$$

see Claeskens, Hubert, Slaets, Vakili, 2014.

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(Staerman, M., Clémenton, d'Alché-Buc; 2019)

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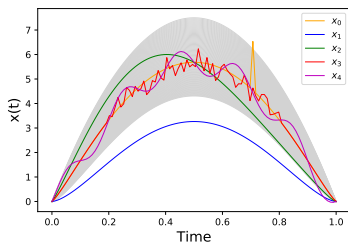
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- ▶ To account for both **location** and **shape** anomalies, we suggest the following **scalar product** that provides a compromise between the both (for  $\lambda = 0.5$ , Sobolev  $W_{1,2}$  scalar product):

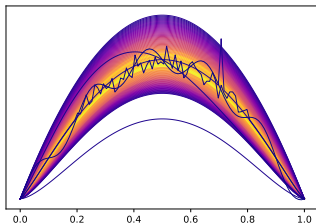
$$\langle \mathbf{f}, \mathbf{d} \rangle := \lambda \times \frac{\langle \mathbf{f}, \mathbf{d} \rangle_{L_2}}{\|\mathbf{f}\| \|\mathbf{d}\|} + (1 - \lambda) \times \frac{\langle \mathbf{f}', \mathbf{d}' \rangle_{L_2}}{\|\mathbf{f}'\| \|\mathbf{d}'\|}, \quad \lambda \in [0, 1].$$

# Functional isolation forest: an example

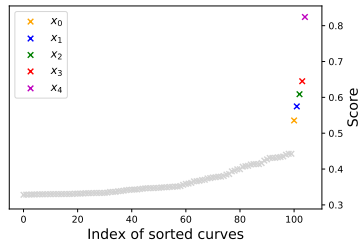
Functional **data set** with **anomalies**



Color-indicated anomaly score



Anomaly score





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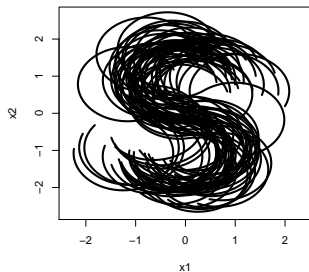
Integrated data depth

Functional isolation forest

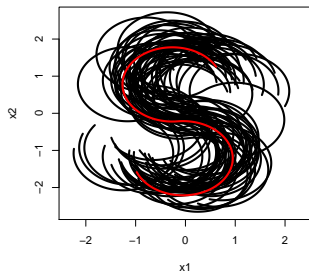
Depth for curve data

## Practical session

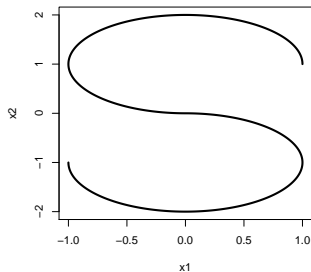
# Functional depth: Motivation 1



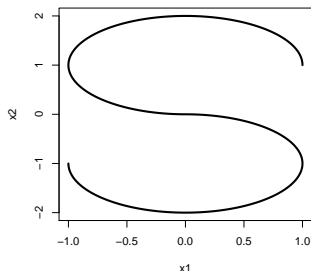
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Regard the following different parametrizations of a curve:

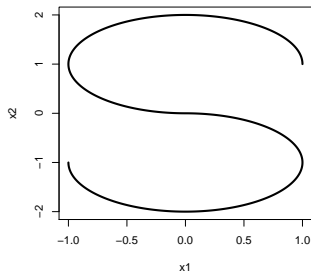
**Parametrization A:**

$$\begin{aligned}x_1(t) &= -(\cos(t)+1)\mathbb{1}\{t < \frac{3\pi}{2}\} - (\cos(3t-3\pi) + 1)\mathbb{1}\{t \geq \frac{3\pi}{2}\} + 1 \\x_2(t) &= (\sin(t) + 1)\mathbb{1}\{t < \frac{3\pi}{2}\} - (\sin(3t - 3\pi) + 1)\mathbb{1}\{t \geq \frac{3\pi}{2}\}\end{aligned}$$

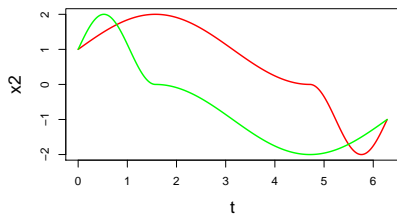
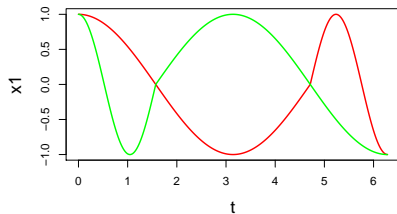
**Parametrization B:**

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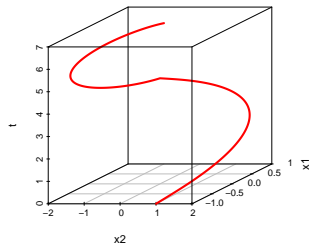


Regard the following different parametrizations of a curve:

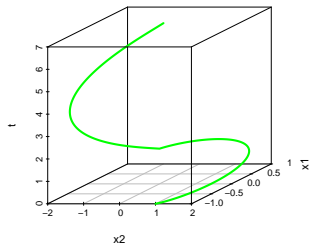


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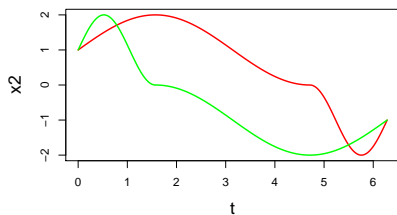
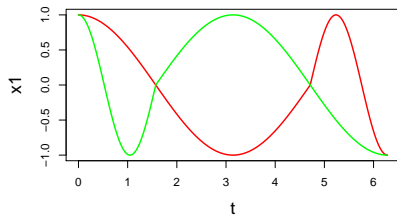
Parametrization A



Parametrization B

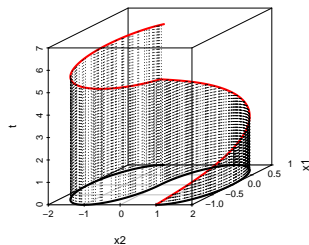


Parametrization:

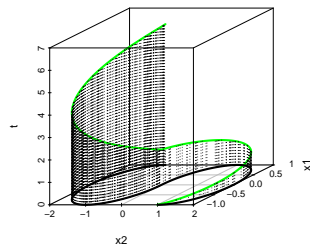


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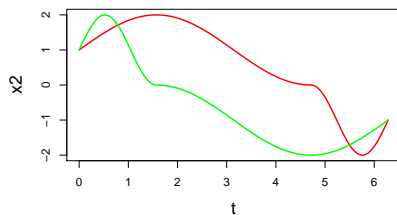
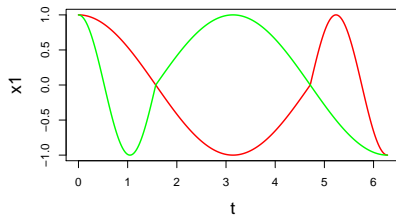
Parametrization A



Parametrization B



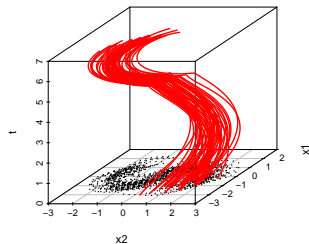
Parametrization:



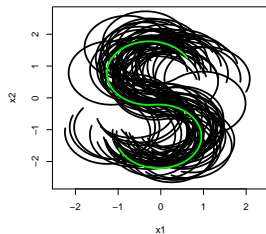
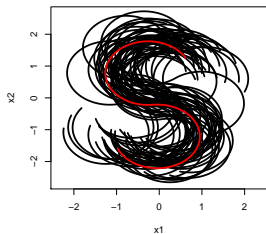
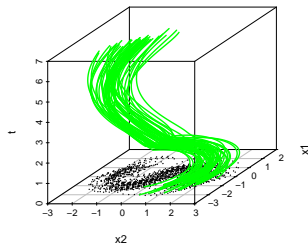


# Functional depth: Motivation 1

Parametrization A

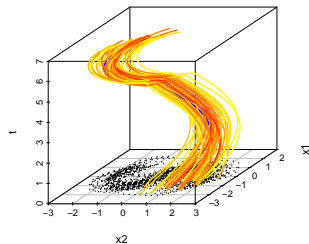


Parametrization B

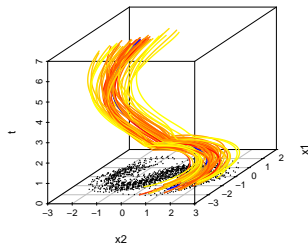


# Functional depth: Motivation 1

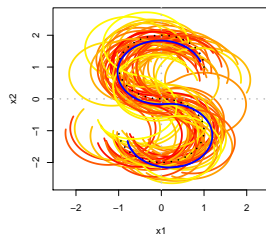
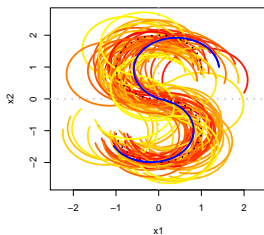
Parametrization A



Parametrization B



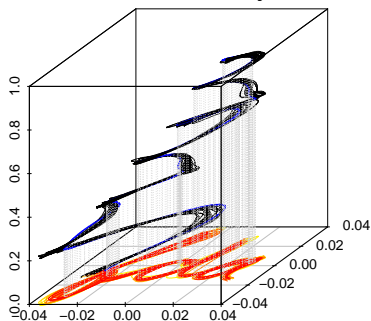
The depth-induced orders differ!



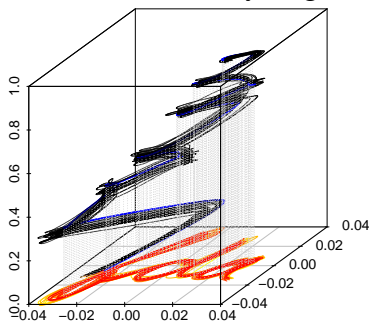
# Functional depth: Motivation 2

## Functional halfspace depth for the FDA-data

Parametrization by time



Parametrization by length



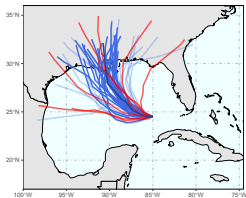
Depth-induced ranking for parametrizations by time and by length:

Time	2	3	13	12	4	8	1	17	11	9	7	19	15	20	18	16	14	5	6	10
Length	6	3	16	14	5	7	13	11	1	17	2	19	8	20	12	18	15	4	9	10

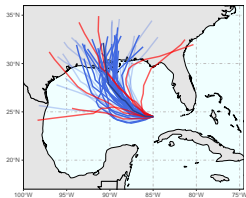
# Functional depth: Motivation 3

## Simulated hurricane tracks: **curve boxplot**

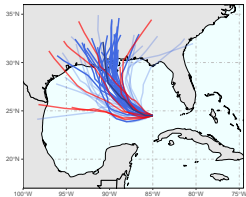
MFH depth – par. time



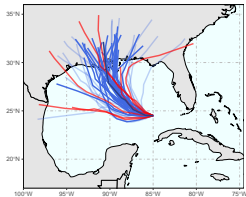
MFH depth - par. length



mSB depth – par. time



mSB depth – par. length



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- ▶ Let  $(\mathbb{R}^d, |\cdot|_2)$  be the Euclidean space.

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- ▶ A *parametrized curve*  $\beta : [0, 1] \rightarrow \mathbb{R}^d$  is a continuous map.  
A reparametrization  $\gamma : [0, 1] \rightarrow [0, 1]$  is increasing continuous function:  $\gamma(0) = 0$  and  $\gamma(1) = 1$ .

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$$\mathfrak{B} = \{\mathcal{C}_\beta : \beta \in \mathcal{C}([0, 1], \mathbb{R}^d)\}.$$



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- ▶ We endow  $\mathfrak{B}$  with the Fréchet *metric*:

$$d_{\mathfrak{B}}(\mathcal{C}_1, \mathcal{C}_2) = \inf \{\|\beta_1 - \beta_2\|_\infty, \beta_1 \in \mathcal{C}_1, \beta_2 \in \mathcal{C}_2\}, \quad \mathcal{C}_1, \mathcal{C}_2 \in \mathfrak{B}.$$

## Associated distribution and the sampling scheme

- Let  $\mathcal{C}$  be an unparameterized curve. The *length* of  $\mathcal{C}$ :

$$L(\mathcal{C}) = \sup_{\tau} \left\{ \sum_{i=1}^N |\beta(\tau_i) - \beta(\tau_{i-1})|_2 : \tau \text{ is a partition of } [0, 1] \right\},$$

for all  $\beta \in \mathcal{C}$ .

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- ▶ An unparametrized curve  $\mathcal{C}$  is called *rectifiable* if  $L(\mathcal{C})$  is finite. The length  $L : \mathfrak{B} \rightarrow \mathbb{R} + \cup\{\infty\}$  is measurable:

$$\mathcal{P} = \left\{ P \text{ prob. measure on } (\mathfrak{B}, d_{\mathfrak{B}}) : P(\{\mathcal{C} \in \mathfrak{B}; 0 < L(\mathcal{C}) < \infty\}) = 1 \right\}.$$

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- ▶ Let  $\mathcal{X}$  be a random element of  $\mathfrak{B}$  stemming from distribution  $P \in \mathcal{P}$ .
- ▶ We derive the probability distribution  $Q_P$  on  $\mathbb{R}^d$  as follows:  
if  $X \sim Q_P$ , then distribution of  $X \mid \mathcal{X} = \mathcal{C}$  is the (uniform on  $\mathcal{C}$ ) probability distribution  $\mu_{\mathcal{C}}$ :

$$\mu_{\mathcal{C}}(A) = \int_{\mathcal{C}} \mathbb{1}_A(x) dx.$$

# Associated distribution and the sampling scheme

The statistical model:

$$\mathcal{X}_1, \dots, \mathcal{X}_n \text{ i.i.d. from } P.$$

For Monte-Carlo estimation, we can consider the following **sampling scheme**:

$$\left\{ \begin{array}{l} \mathcal{X}_1, \dots, \mathcal{X}_n \text{ i.i.d. from } P, \\ \text{for all } i = 1, \dots, n \\ \quad X_{i,1}, \dots, X_{i,m} \text{ i.i.d. from } \mu_{\mathcal{X}_i}. \end{array} \right.$$

# Data depth for an unparametrized curve

## Definition

The **Tukey curve depth** of  $\mathcal{C} \in \mathfrak{B}$  w.r.t.  $Q_P$  is defined as:

$$D(\mathcal{C}|Q_P) = \int_{\mathcal{C}} D(\mathbf{x}|Q_P, \mu_{\mathcal{C}}) d\mu_{\mathcal{C}}(\mathbf{x}),$$

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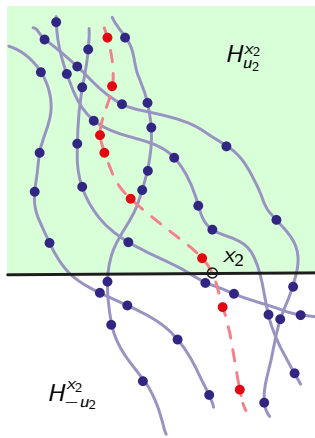
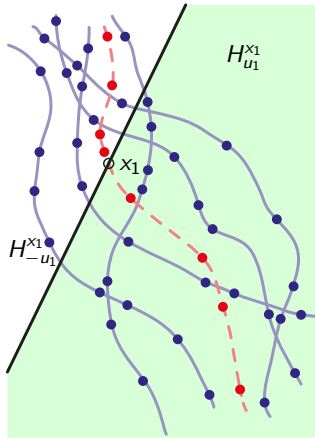
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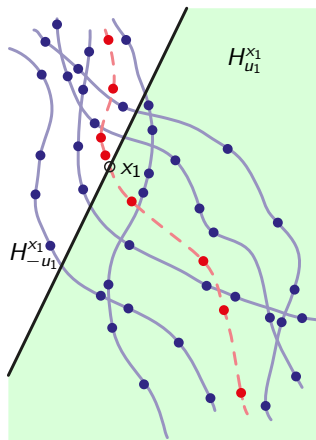
$$D(\mathcal{C}|\mathcal{X}_1, \dots, \mathcal{X}_n) = \int_{\mathcal{C}} D(\mathbf{x}|Q_n, \mu_{\mathcal{C}}) d\mu_{\mathcal{C}}(\mathbf{x}),$$

where  $Q_n = (\mu_{\mathcal{X}_1} + \dots + \mu_{\mathcal{X}_n})/n$ .

# Data depth for an unparametrized curve: intuition

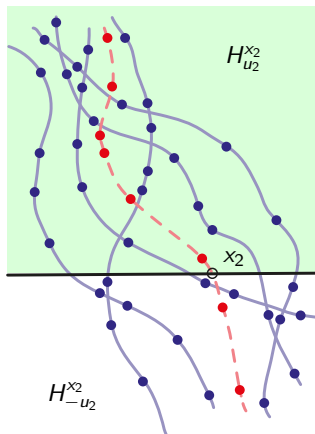


# Data depth for an unparametrized curve: intuition



**Traditional reasoning:**

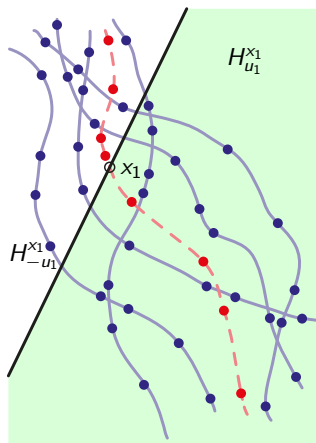
$$\begin{aligned}\hat{Q}_P(H_{u_1}^{x_1}) &= \frac{25}{40}, \quad \hat{\mu}_C(H_{u_1}^{x_1}) = \frac{4}{8} \\ \hat{Q}_P(H_{-u_1}^{x_1}) &= \frac{15}{40}, \quad \hat{\mu}_C(H_{-u_1}^{x_1}) = \frac{4}{8}\end{aligned}$$



**Curve-based reasoning:**

$$\begin{aligned}\hat{Q}_P(H_{u_2}^{x_2}) &= \frac{25}{40}, \quad \hat{\mu}_C(H_{u_2}^{x_2}) = \frac{6}{8} \\ \hat{Q}_P(H_{-u_2}^{x_2}) &= \frac{15}{40}, \quad \hat{\mu}_C(H_{-u_2}^{x_2}) = \frac{2}{8}\end{aligned}$$

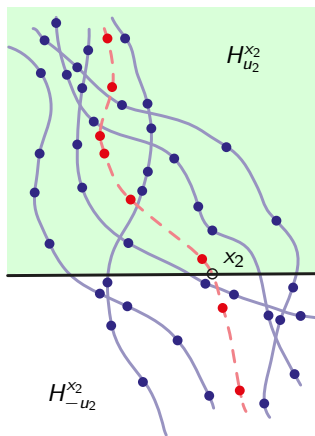
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- ▶ Let a chosen curve consist of two (independently drawn on  $\mathcal{C}$ ) parts  $\mathbb{Y}_{1,m} = (Y_{1,1}, \dots, Y_{1,m})$  and  $\mathbb{Y}_{2,m} = (Y_{2,1}, \dots, Y_{2,m})$  with empirical distribution

$$\hat{\mu}_m = \frac{1}{m} \sum_{i=1}^m \delta_{Y_{1,i}},$$

where  $\delta_{\mathbf{x}}$  is the Dirac measure in  $\mathbf{x} \in \mathbb{R}^d$ .

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- ▶ Let  $\hat{Q}_{n,m}$  be the empirical distribution (observed sample)  
 $\mathbb{X}_{n,m} = \{X_{i,j}, i = 1, \dots, n, j = 1, \dots, m\}$

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- ▶ To compute the sample Tukey curve depth, a Monte Carlo approximation is used.



## Data depth for an unparametrized curve: empirical version

- ▶ Let  $H$  be a closed halfspace in  $\mathbb{R}^d$  and  $\mathcal{H}_\Delta^{n,m}$  denote a collection of such halfspaces such that for all  $H \in \mathcal{H}_\Delta^{n,m}$  either  $\hat{Q}_{n,m}(H) = 0$  or  $\hat{\mu}_m(H) > \Delta$ , almost surely, for  $\Delta \in (0, \frac{1}{2})$ .

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## Definition

The **Monte Carlo approximation** of the **Tukey curve depth** of  $\mathcal{C}$  w.r.t.  $\mathcal{X}_1, \dots, \mathcal{X}_n$  is defined as:

$$\hat{D}_{n,m,\Delta}(\mathcal{C}|\mathcal{X}_1, \dots, \mathcal{X}_n) = \frac{1}{m} \sum_{i=1}^m \hat{D}(Y_{2,i} | \hat{Q}_{n,m}, \hat{\mu}_m, \mathcal{H}_{\Delta}^{n,m}),$$

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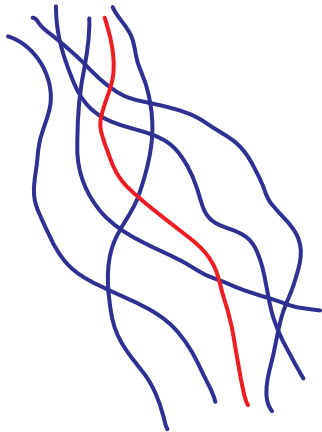
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with the depth of an arbitrary point  $\mathbf{x} \in \mathbb{R}^d$  w.r.t.  $\hat{Q}_{n,m}$  being:

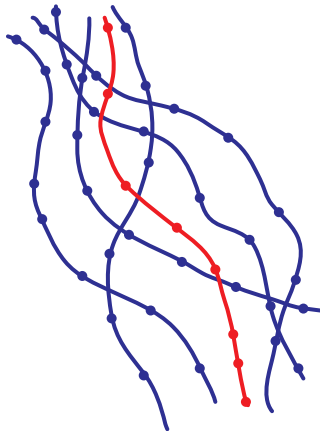
$$\hat{D}(\mathbf{x}|\hat{Q}_{n,m}, \hat{\mu}_m, \mathcal{H}_\Delta^{n,m}) = \inf \left\{ \frac{\hat{Q}_{n,m}(H)}{\hat{\mu}_m(H)} : H \in \mathcal{H}_\Delta^{n,m}, \mathbf{x} \in \partial H \right\}$$

and  $\frac{0}{0} = 0$  as before.

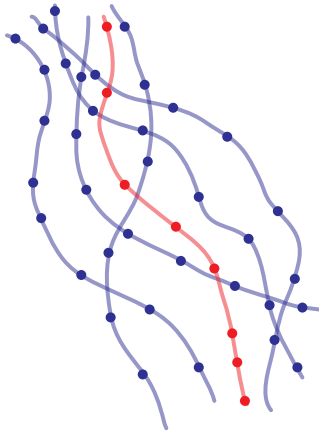
# Calculation of the Tukey curve depth



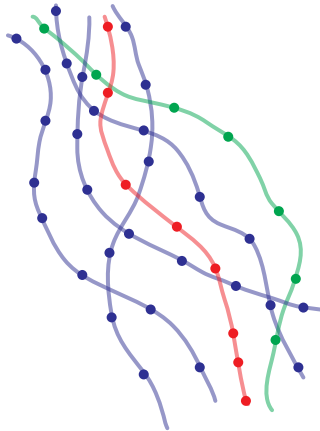
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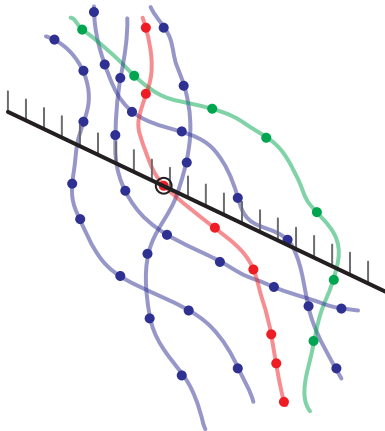
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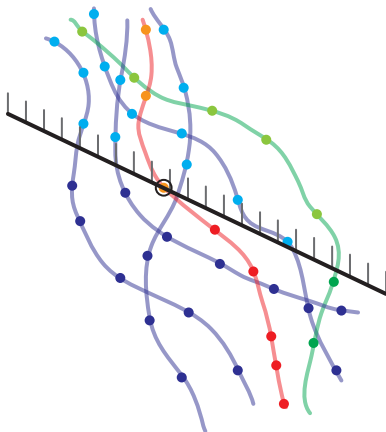


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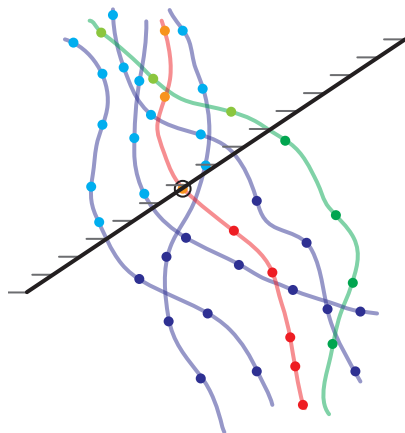


# Calculation of the Tukey curve depth



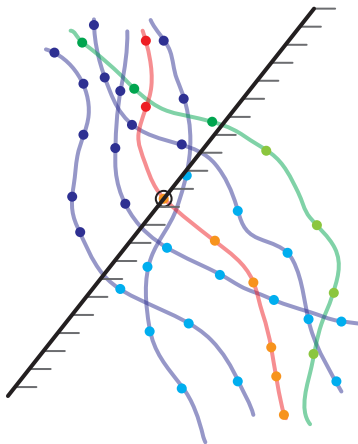
$$D(Y_{2,c}|Q_m, \mathcal{H}_{m,b}) = \frac{\frac{1}{5} \left( \frac{5}{7} + \frac{3}{8} + \frac{6}{8} + \frac{2}{7} + \frac{3}{6} \right)}{2.1} = 2.1$$

# Calculation of the Tukey curve depth



$$D(Y_{2,c}|Q_m, \mathcal{H}_{m,b}) = \frac{\frac{1}{5} \left( \frac{3}{7} + \frac{5}{8} + \frac{4}{8} + \frac{3}{7} + \frac{3}{6} \right)}{2.08} = 1.9857$$

# Calculation of the Tukey curve depth



$$D(Y_{2,c}|Q_m, \mathcal{H}_{m,b}) = \frac{\frac{1}{5} \left( \frac{4}{7} + \frac{3}{8} + \frac{4}{8} + \frac{4}{7} + \frac{4}{6} \right)}{5} = 0.7159$$

## Data depth for an unparametrized curve: properties

Restrict to  $\mathfrak{B}_\ell$ , the subset of unparametrized curves of positive length bounded by  $\ell > 0$ . Then the Tukey curve depth satisfies the following properties:

- ▶ **Nonnegativity and boundedness by one:**

$$D(\mathcal{C}|Q_P) \in [0, 1].$$

## Data depth for an unparametrized curve: properties

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- ▶ **Similarity invariance:** Let  $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$  be a similarity, i.e. there exists an orthogonal matrix  $A$ , a factor  $r > 0$  and a vector  $\mathbf{b} \in \mathbb{R}^d$  such that for all  $\mathbf{x} \in \mathbb{R}^d$ ,  $f(\mathbf{x}) = rA\mathbf{x} + \mathbf{b}$ . In particular for all  $\mathbf{x}$  and  $\mathbf{y}$  in  $\mathbb{R}^d$ ,  $|f(\mathbf{x}) - f(\mathbf{y})|_2 = r|\mathbf{x} - \mathbf{y}|_2$ . Denote by  $P_f$  the distribution of the image through  $f$  of a stochastic process having a distribution  $P$ . Then

$$D(f \circ \mathcal{C}|Q_{P_f}) = D(\mathcal{C}|Q_P).$$

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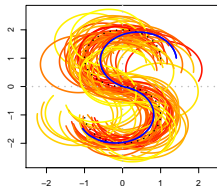
- ▶ **Vanishing at infinity:**

$$\lim_{d_G(\mathcal{C}, \mathbf{0}) \rightarrow \infty, \mathcal{C} \in \mathfrak{B}_\ell} D(\mathcal{C}, Q_P) = \inf_{\mathcal{C} \in \mathfrak{B}_\ell} D(\mathcal{C}, Q_P) = 0.$$

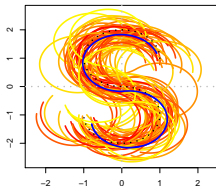
# Comparison with functional depth: Example 1

Simulated S letters: **depth-induced ranking**

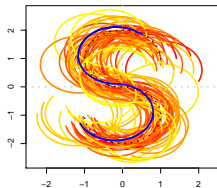
MFHD – time



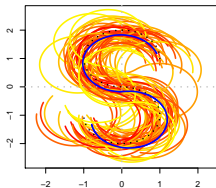
MFHD - length



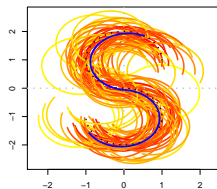
mSBD – time



mSBD – length



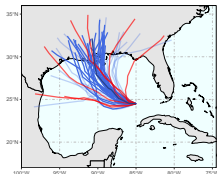
Curve depth



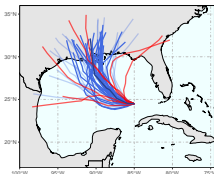
# Comparison with functional depth: Example 2

Simulated hurricane tracks: **curve boxplot**

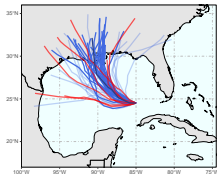
MFHD – time



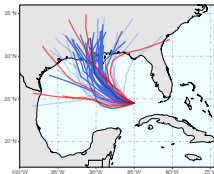
MFHD - length



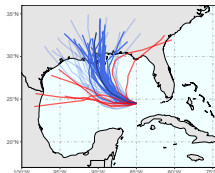
mSBD – time



mSBD – length



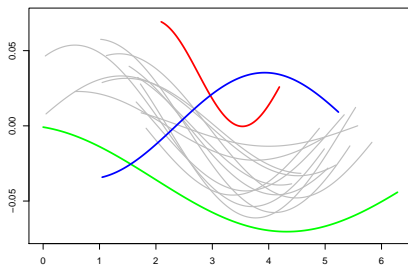
Curve depth





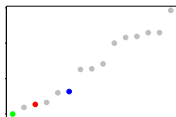
# Comparison with functional depth: Anomaly detection 1

Data set 1 with introduced anomalies:

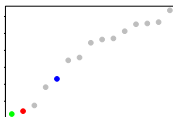


Ordered depth values:

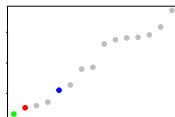
mSBD



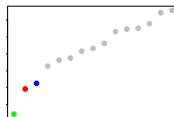
saPRJ



MFHD

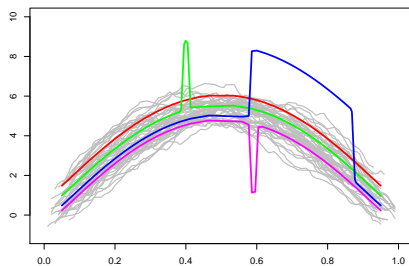


Curve depth



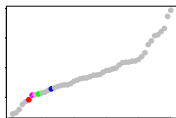
# Comparison with functional depth: Anomaly detection 2

Data set 2 with introduced anomalies:

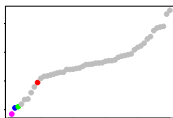


Ordered depth values:

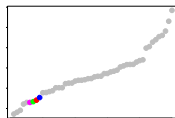
mSBD



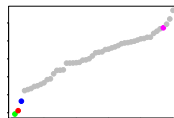
saPRJ



MFHD



Curve depth



# Contents

## Introduction

## Non-parametric approaches

- One-class support vector machines

- Local outlier factor

- Isolation forest

## Systematic orderings: data depth

- The notion of depth and the Tukey depth

- Central regions

- Further depth notions

## Functional anomaly detection

- Integrated data depth

- Functional isolation forest

- Depth for curve data

## Practical session

# Thank you for attention! (and a short list of literature)

- ▶ Chandola, V., Banerjee, A., and Kumar, V. (2009). Anomaly detection: A survey. *ACM Computing Surveys (CSUR)*, 41(3):15, 1–58.
- ▶ Breunig, M.M., Kriegel, H.-P., Ng, R.T., and Sander, J. (2000). LOF: Identifying density-based local outliers. In: *Proceedings of the 2000 ACM SIGMOD International Conference on Management of Data*, 29, 93–104.
- ▶ Schölkopf, B., Platt, J.C., Shawe-Taylor, J., Smola, A., and Williamson, R. (2001). Estimating the support of a high-dimensional distribution. *Neural Computation*, 13(7), 1443–1471.
- ▶ Liu, F.T., Ting, K.M., and Zhou, Z. (2008). Isolation forest. In: *Proceedings of the 2008 Eighth IEEE International Conference on Data Mining*, 413–422.
- ▶ Mosler, K. (2013). Depth statistics. In: *Robustness and Complex Data Structures: Festschrift in Honour of Ursula Gather*, 17–34.
- ▶ Hubert, M., Rousseeuw, P.J., and Segaert, P. (2015). Multivariate functional outlier detection. *Statistical Methods & Applications*, 24(2), 177–202.

# Practical session

## Notebooks:

- ▶ `anomdet_simulation1.Rmd`,
- ▶ `anomdet_hurricanes.Rmd`,
- ▶ `anomdet_brainimaging.Rmd`,
- ▶ `anomdet_cars.ipynb`,
- ▶ `anomdet_airbus.ipynb`.

## Data sets:

- ▶ `carsanom.csv`: Data set on anomaly detection for cars.
- ▶ `airbus_data.csv`: Data set from Airbus.
- ▶ `hurdat2-1851-2019-052520.txt`: Historical hurricane data.
- ▶ `101_1_dwi_fa.nii`: Anatomical brain volume data.
- ▶ `101_1_dwi.voxelcoordsL.txt`: Left brain fiber's bundle.
- ▶ `101_1_dwi.voxelcoordsR.txt`: Right brain fiber's bundle.

## Supplementary scripts:

- ▶ `depth_routines.py`: Routines for data depth calculation.
- ▶ `FIF.py`: Implementation of the functional isolation forest.
- ▶ `depth_routines.R`: Routines for curves' parametrization.
- ▶ `DTI.R`: Routines for input of brain imaging data.

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- ▶ Chandola, V., Banerjee, A., and Kumar, V. (2009). Anomaly detection: A survey. *ACM Computing Surveys (CSUR)*, 41(3):15, 1–58.
- ▶ Chaudhuri P. (1996). On a geometric notion of quantiles for multivariate data. *Journal of the American Statistical Association*, 91, 862–872.
- ▶ Claeskens, G., Hubert, M., Slaets, L., and Vakili, K. (2014). Multivariate functional halfspace depth. *Journal of the American Statistical Association*, 109(505), 411–423.
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- ▶ Donoho D. (1982). *Breakdown Properties of Multivariate Location Estimators*. Ph.D. thesis, Harvard University.
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- ▶ Hariri, S., Carrasco Kind, M., and Brunner, R.J. (2018). Extended isolation forest. *arXiv:1811.02141*.
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## Literature (mentioned in the tutorial) (3)

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## Literature (mentioned in the tutorial) (4)

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