

Anomaly detection

Part I: Multivariate data

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Tutorial for the chair DSAIDIS

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Non-parametric approaches

- One-class support vector machines

- Local outlier factor

- Isolation forest

Systematic orderings: data depth

- The notion of data depth

- The Tukey depth function

- Central regions

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Practical session

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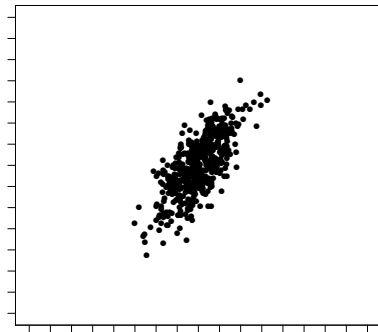
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Practical session

A real task

Regard two measurements during a test in a production process:

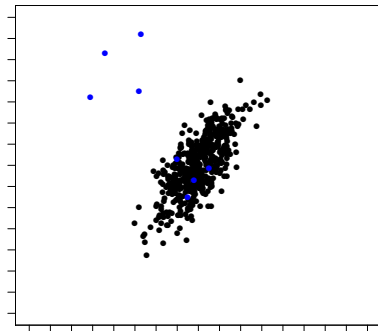


Given **training data**, polluted or not with anomalies:

- ▶ detect **anomalies** in the given data.

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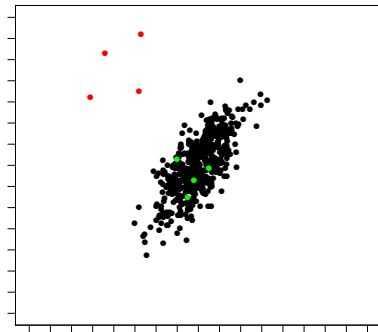
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For **new data**, determine:

- ▶ Whether new observations are **normal** data or **anomalies**?

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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 (parts I and II)

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

(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).
- ▶ Generalized portrait is the vector:

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

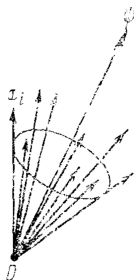


Рис. 24.

One-class support vector machines

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

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

- ▶ Let Φ be a feature map: $\mathbb{R}^d \mapsto \mathcal{H}$.

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- ▶ Let Φ be a feature map: $\mathbb{R}^d \mapsto \mathcal{H}$.
- ▶ Due to the **kernel trick**, the dot product in the image of φ can be computed by evaluation of a kernel K :

$$K(\mathbf{x}_i, \mathbf{x}_j) = \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle .$$

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$$K(\mathbf{x}_i, \mathbf{x}_j) = e^{-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2}$$

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Soft margin (Cortes, Vapnik; 1995):

- ▶ 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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Idea 1: Separate points from the origin.

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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 (ψ^*, ξ^*, ρ^*) 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:

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

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

with $\alpha = (\alpha_1, \dots, \alpha_n)^\top$.

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

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with $\alpha = (\alpha_1, \dots, \alpha_n)^\top$.

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 ρ 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**:

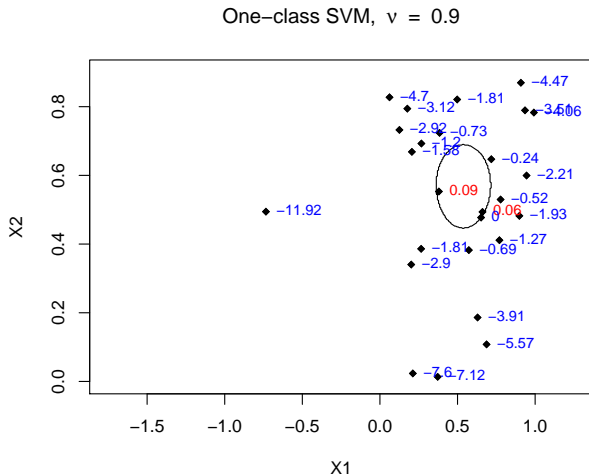
$$g_{\text{OCSVM}}(\mathbf{x}) = \left(R^2 - \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) + 2 \sum_{i=1}^n \alpha_i K(\mathbf{x}_i, \mathbf{x}) - K(\mathbf{x}, \mathbf{x}) \right),$$

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)

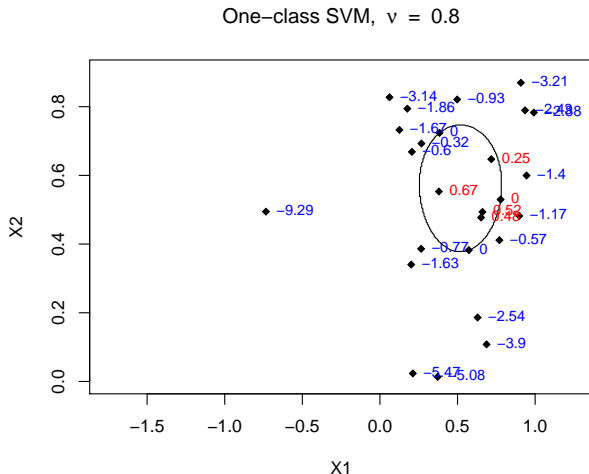
Illustration: Case 1



One-class support vector machines

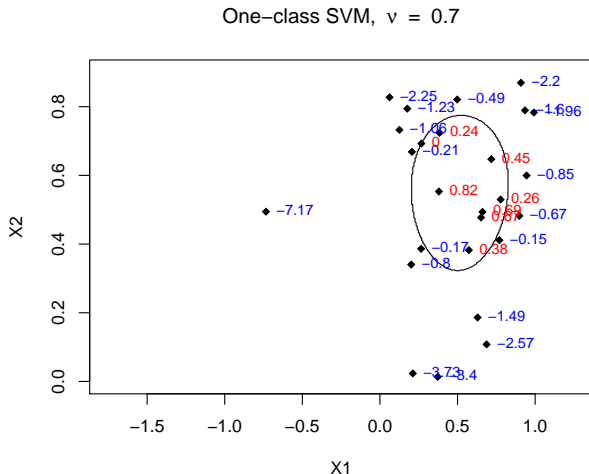
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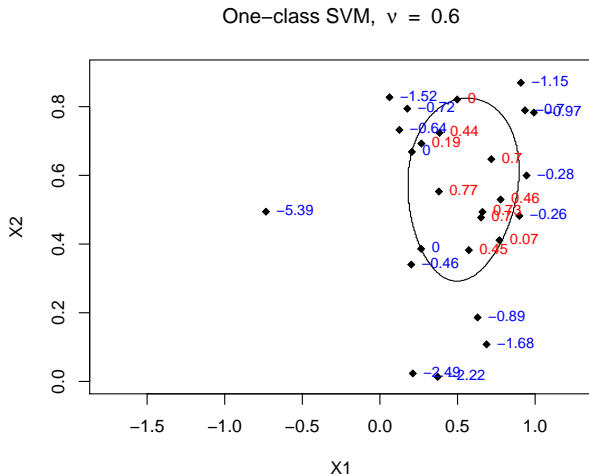
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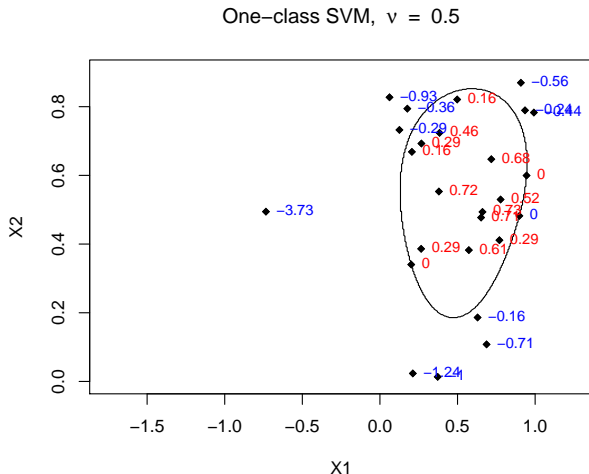
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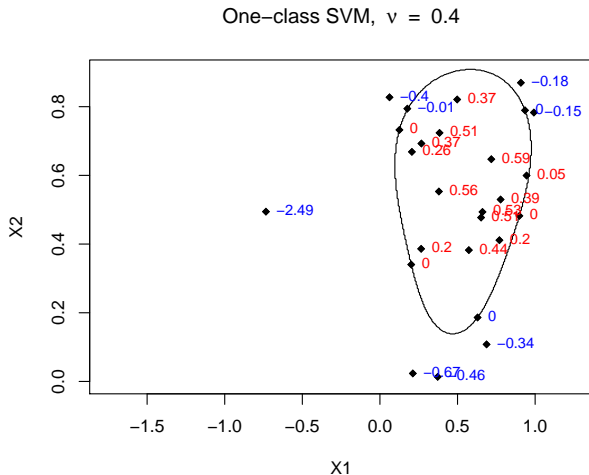
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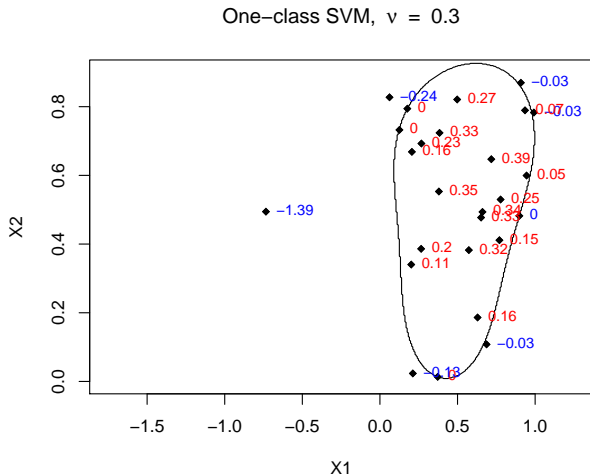
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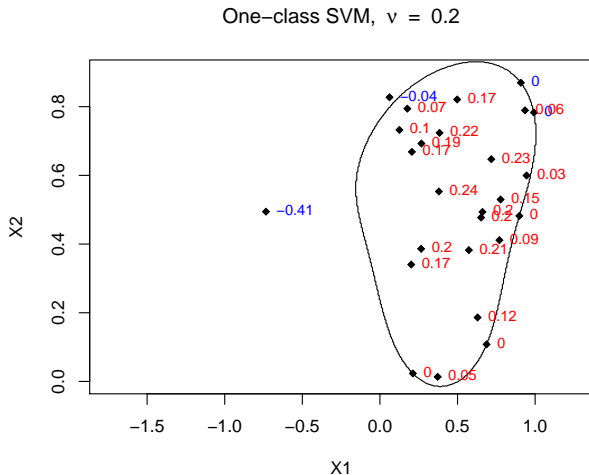
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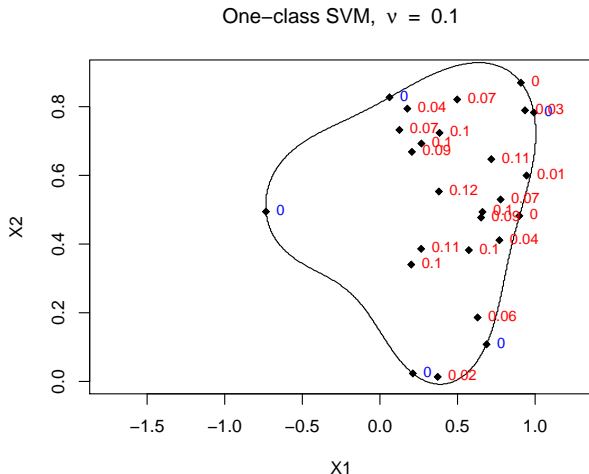
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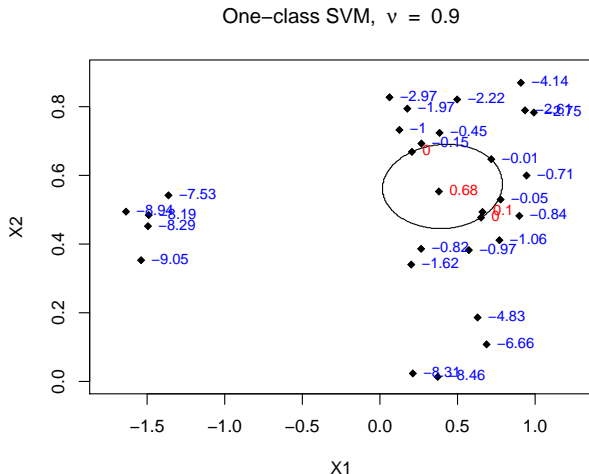
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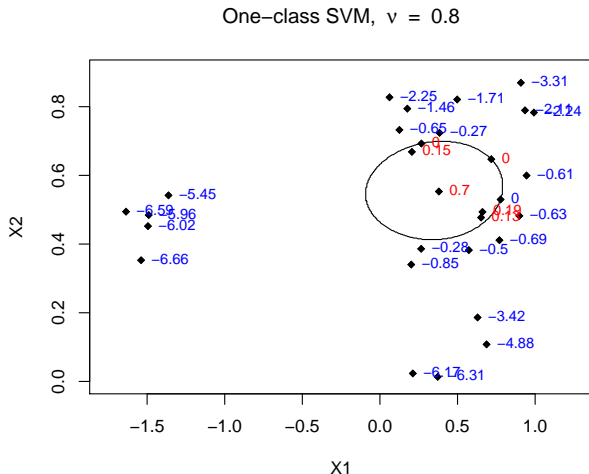
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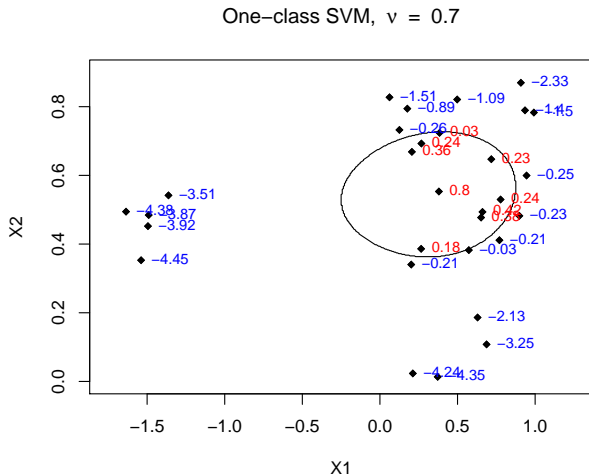
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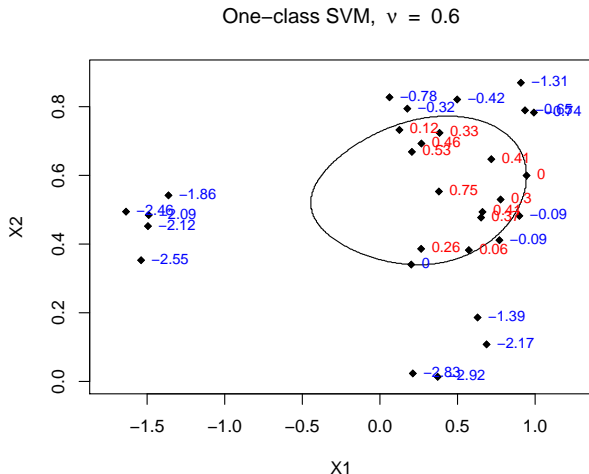
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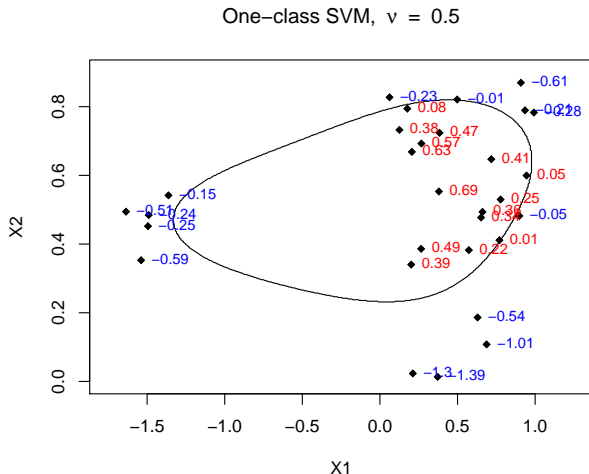
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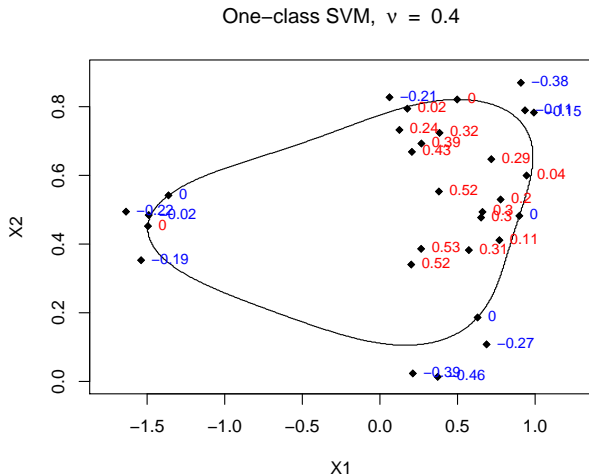
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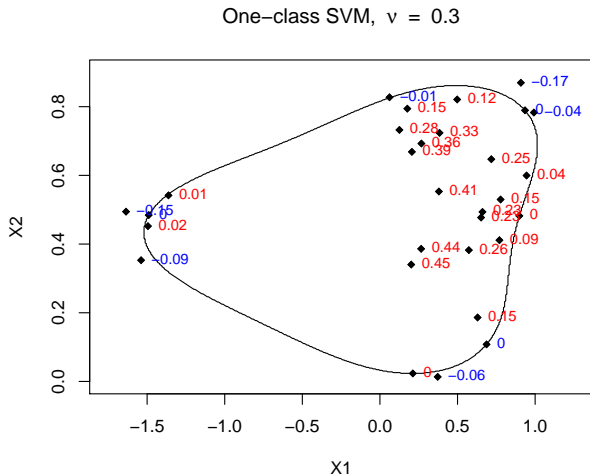
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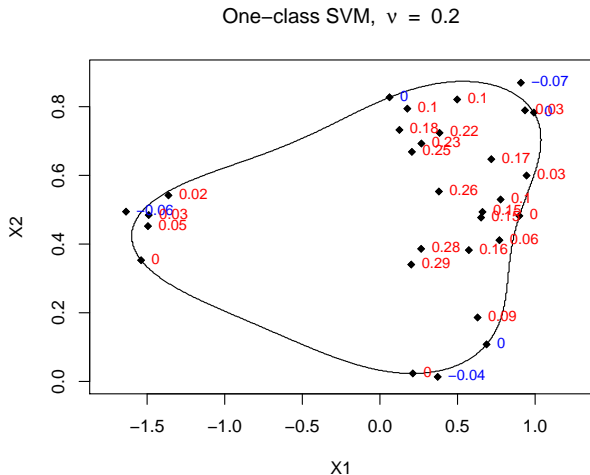
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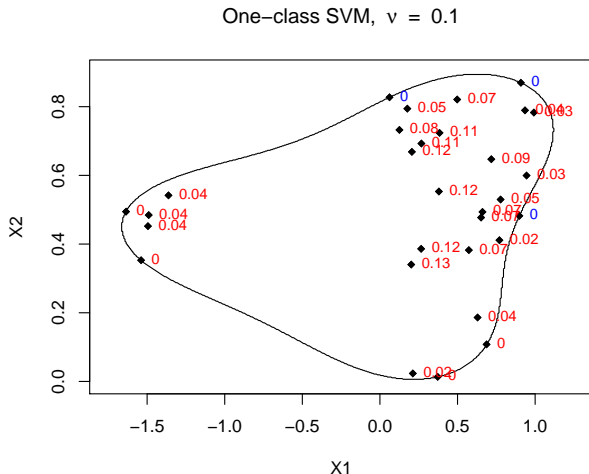
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Local outlier factor (Breunig, Kriegel, Ng, Sander; 2000)

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 $d(\mathbf{x}, \mathbf{o}') < d(\mathbf{x}, \mathbf{o})$.

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

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- ▶ 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.)

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.:

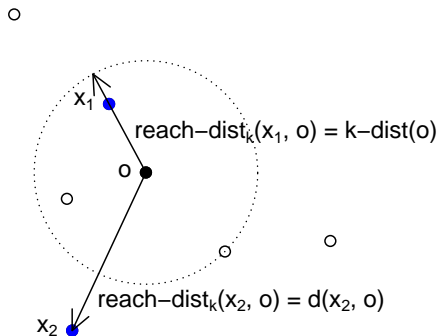
$$N_k(\mathbf{x}) = \{ \mathbf{q} \in \mathbf{X} \setminus \{\mathbf{x}\} \mid d(\mathbf{x}, \mathbf{q}) \leq k\text{-dist}(\mathbf{x}) \}.$$

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

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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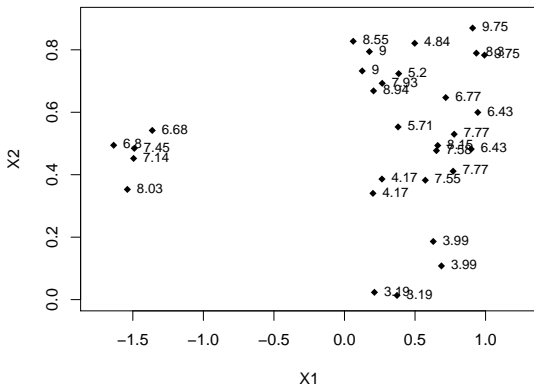
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Local reachability density, $k = 2$



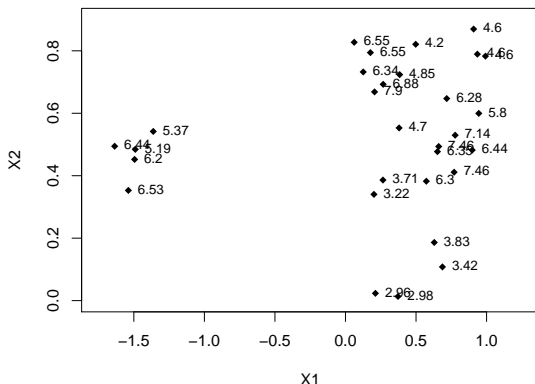
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Local reachability density, $k = 3$



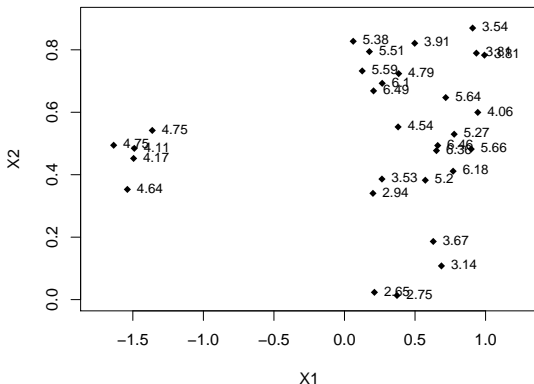
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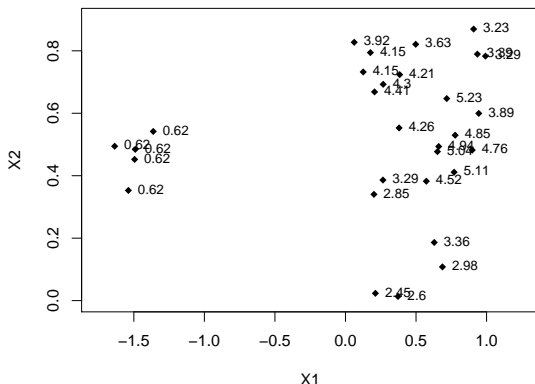
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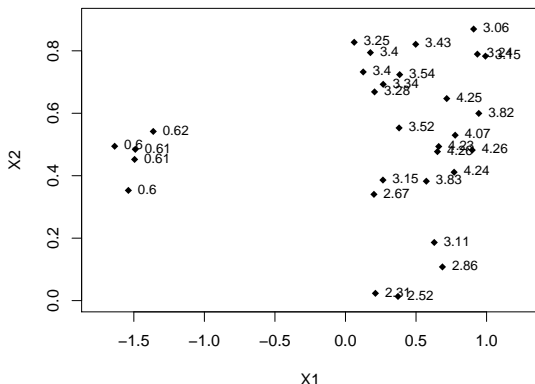
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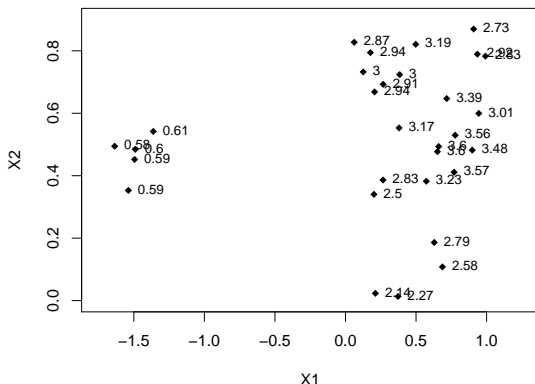
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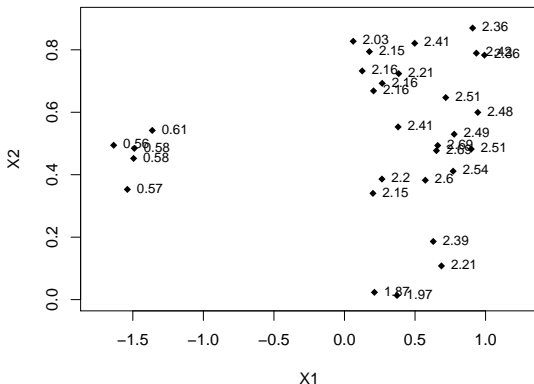
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Local reachability density, $k = 10$



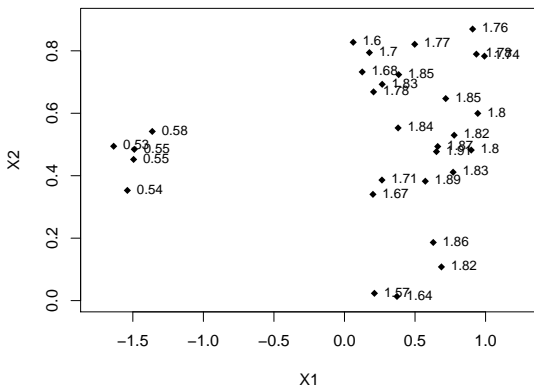
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Local reachability density, k = 15



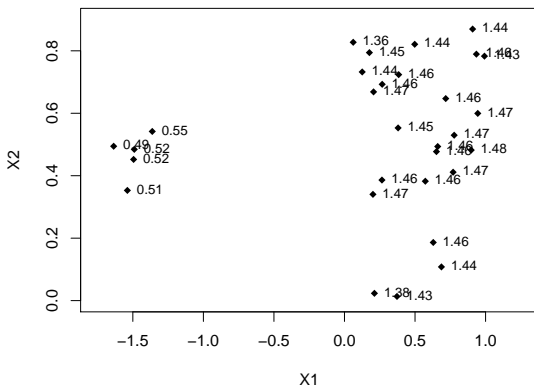
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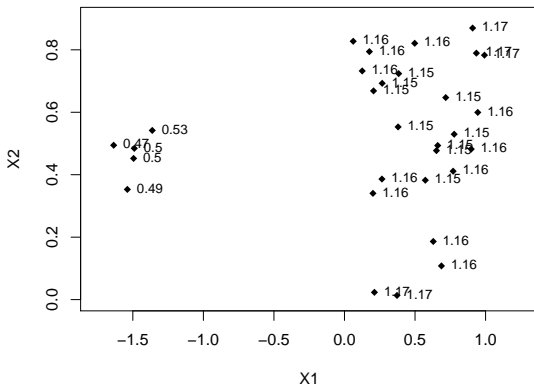
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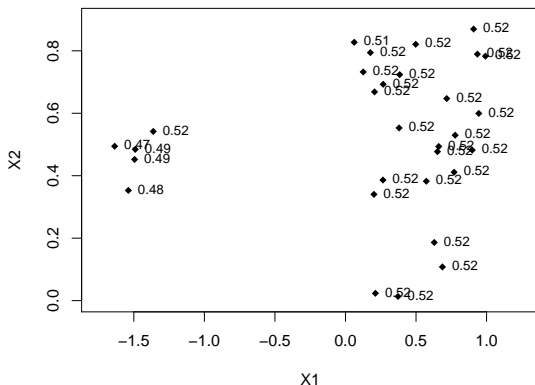
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Local reachability density, k = 25



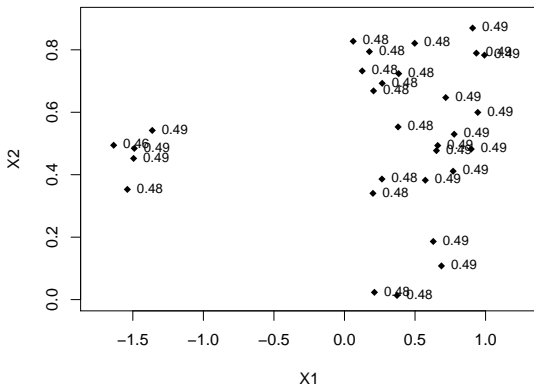
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Local reachability density, $k = 26$



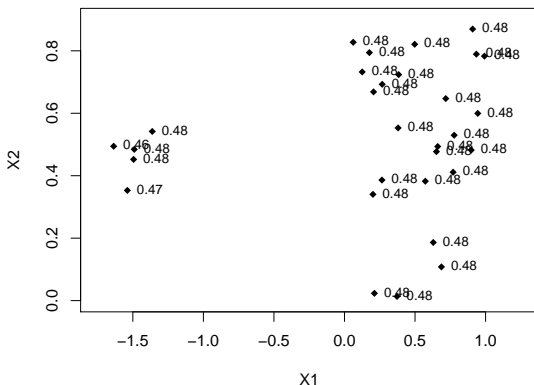
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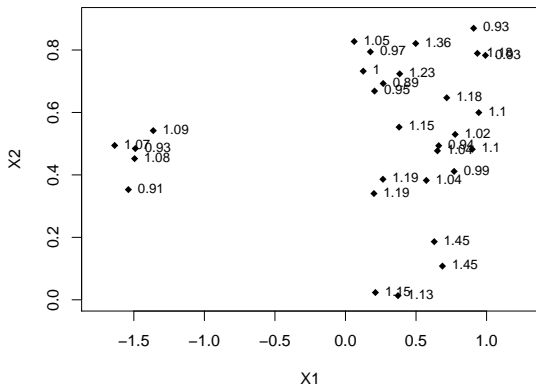
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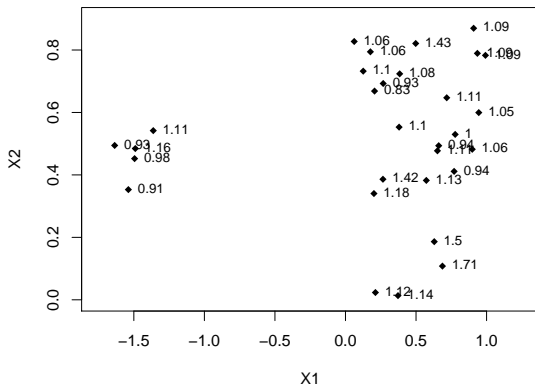
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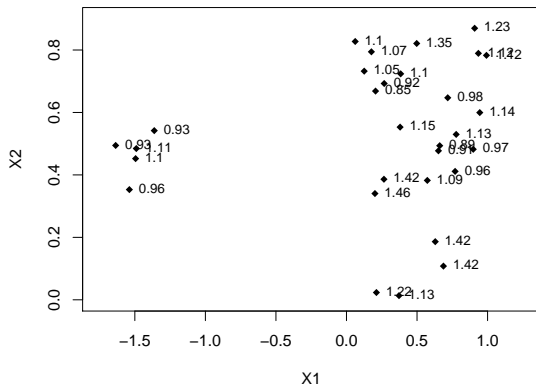
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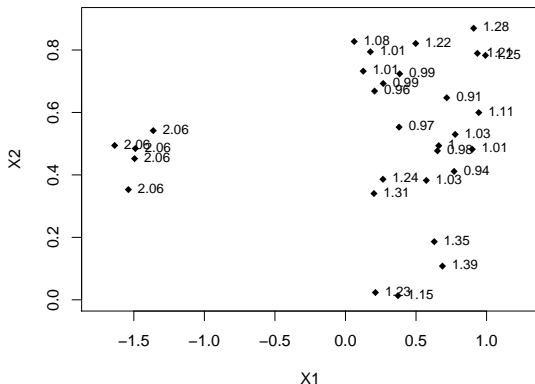
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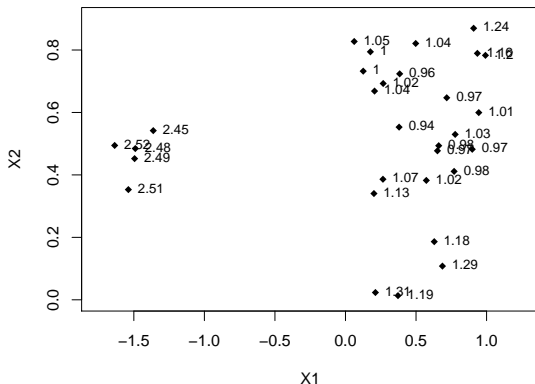
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Local outlier factor, $k = 6$



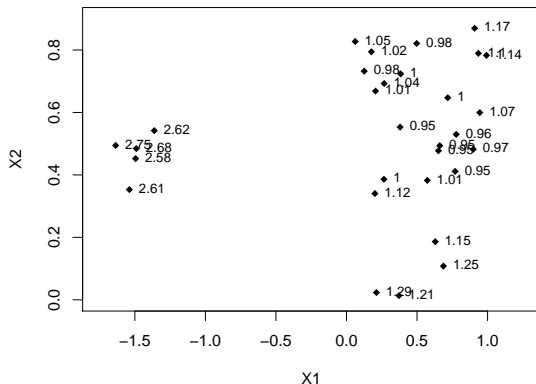
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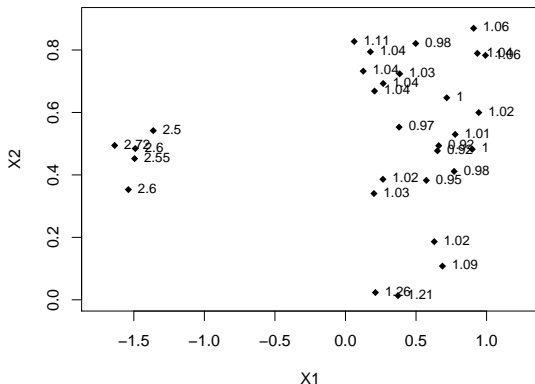
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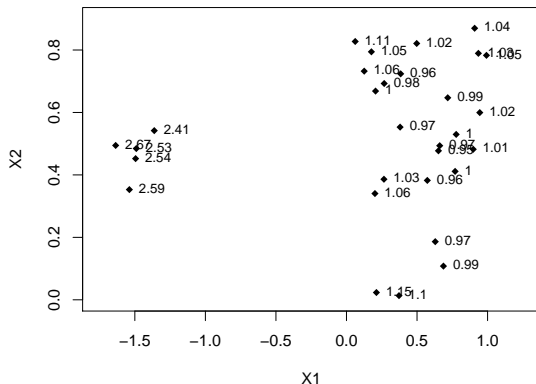
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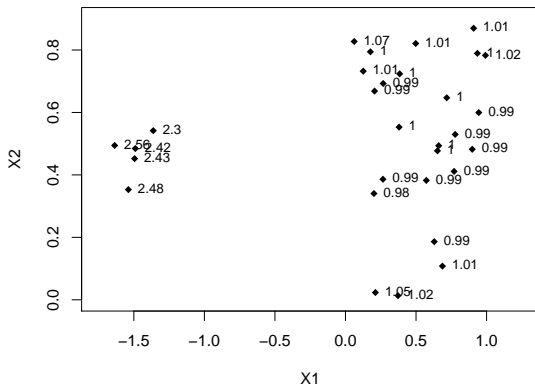
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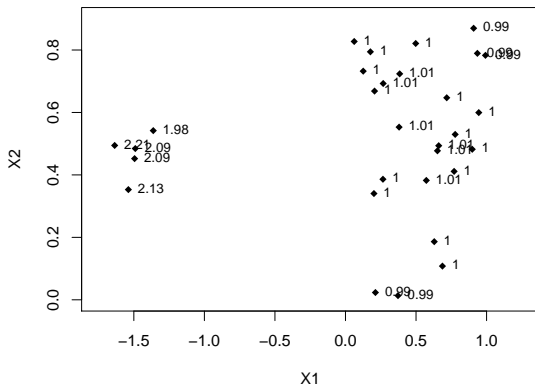
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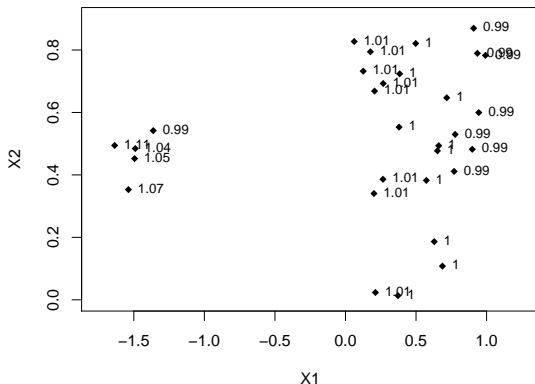
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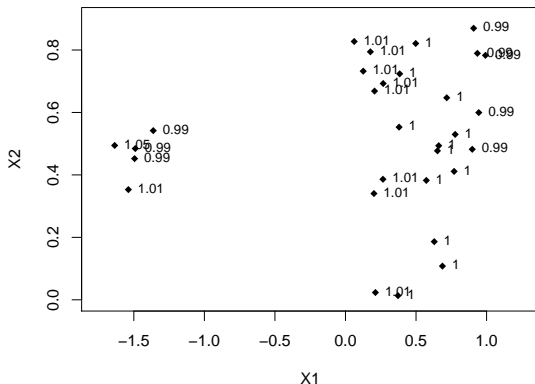
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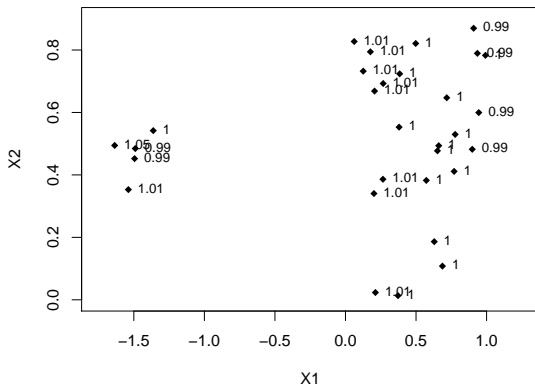
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Isolation forest (Liu, Ting, Zhou; 2008)

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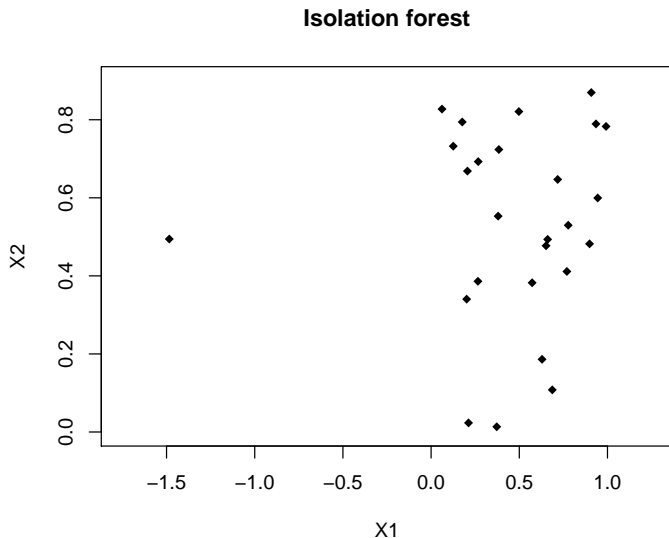
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Stop when only one observation is in each node: **isolation**. 

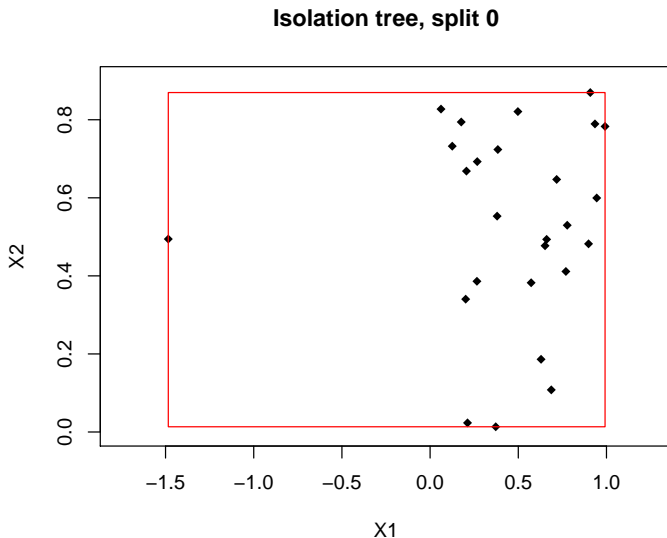
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Illustration: Isolation tree



Isolation forest (Liu, Ting, Zhou; 2008)

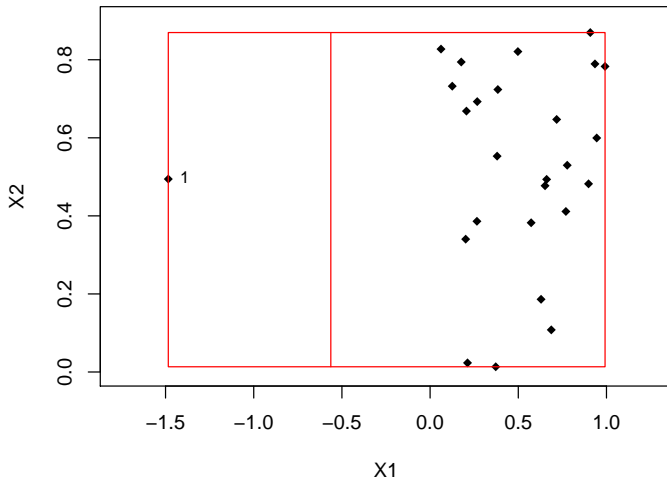
Illustration: Isolation tree



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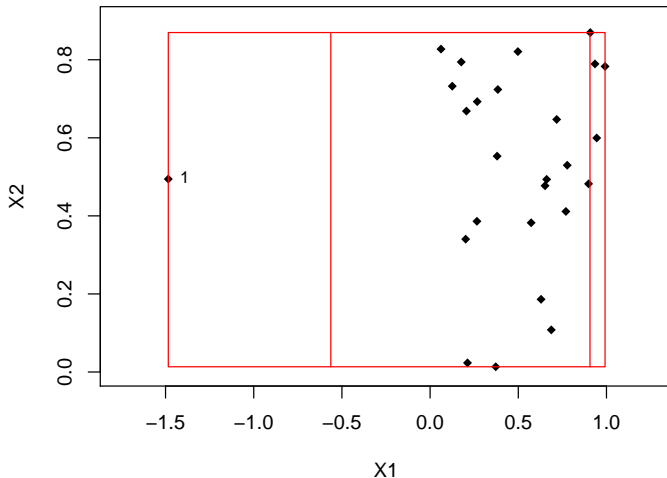
Isolation tree, split 1



Isolation forest (Liu, Ting, Zhou; 2008)

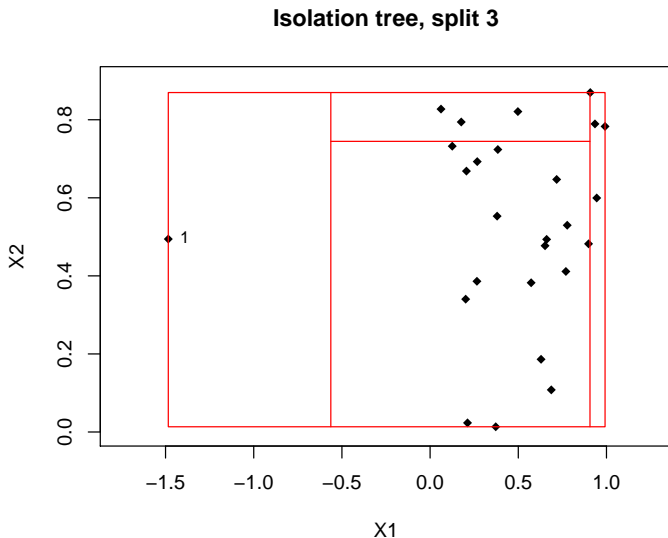
Illustration: Isolation tree

Isolation tree, split 2



Isolation forest (Liu, Ting, Zhou; 2008)

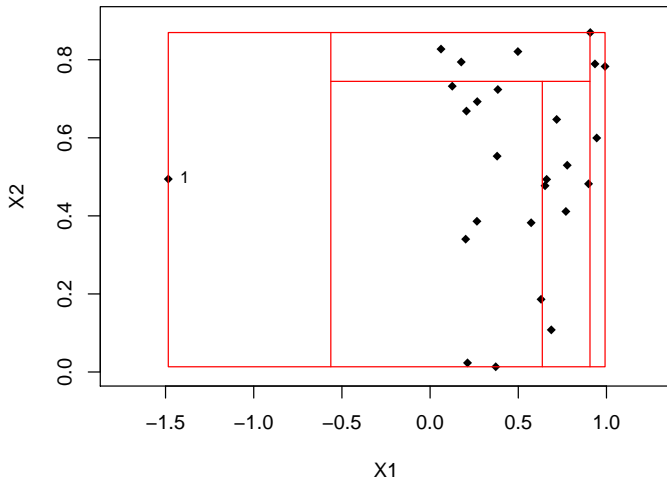
Illustration: Isolation tree



Isolation forest (Liu, Ting, Zhou; 2008)

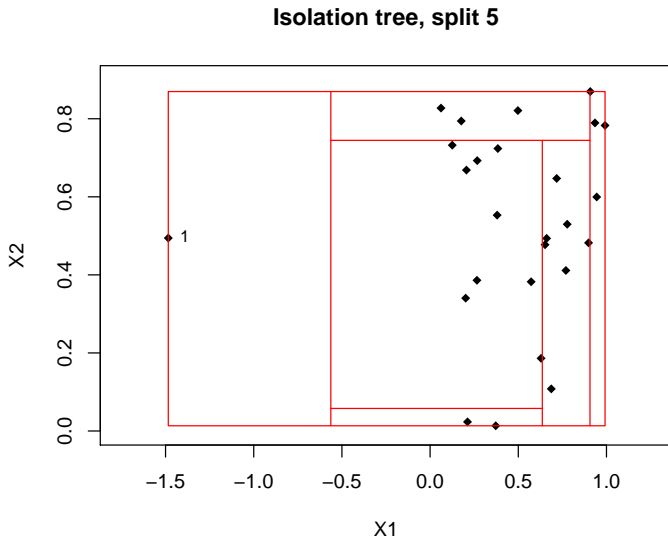
Illustration: Isolation tree

Isolation tree, split 4



Isolation forest (Liu, Ting, Zhou; 2008)

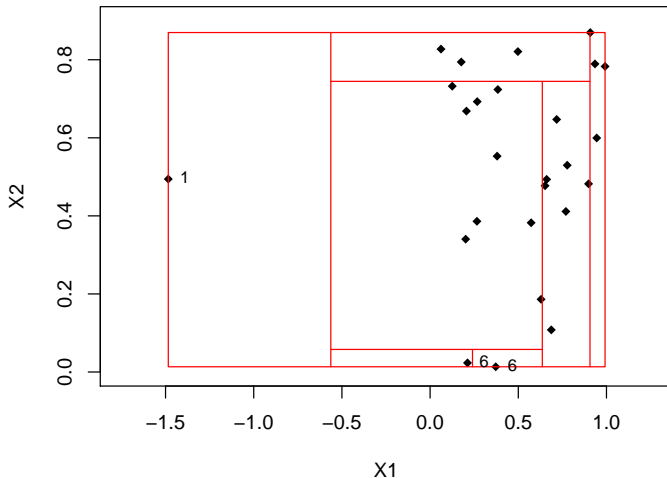
Illustration: Isolation tree



Isolation forest (Liu, Ting, Zhou; 2008)

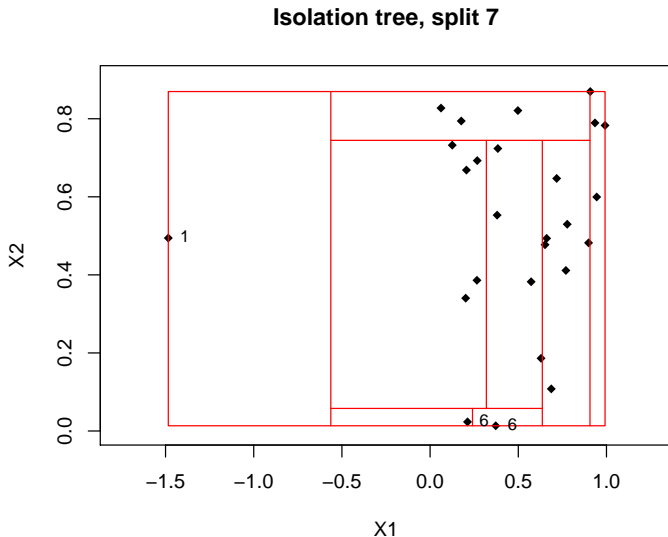
Illustration: Isolation tree

Isolation tree, split 6



Isolation forest (Liu, Ting, Zhou; 2008)

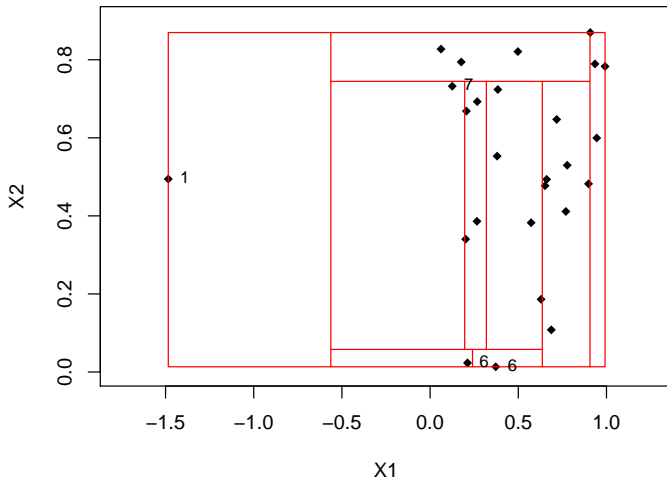
Illustration: Isolation tree



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

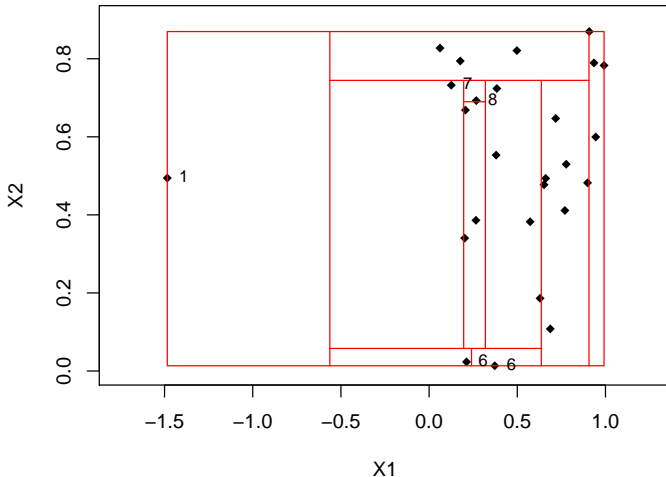
Isolation tree, split 8



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

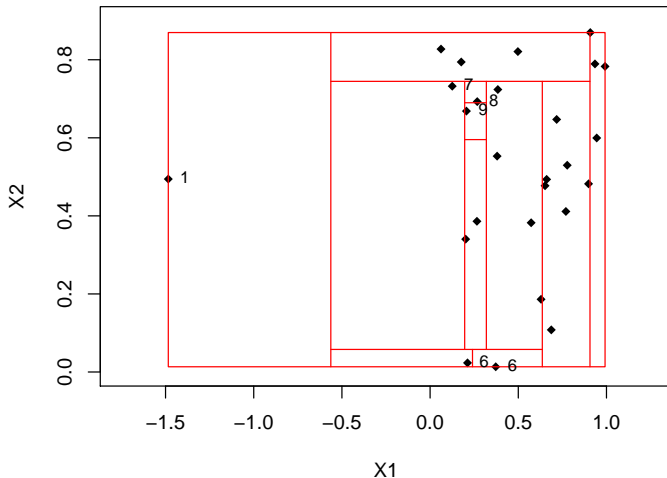
Isolation tree, split 9



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

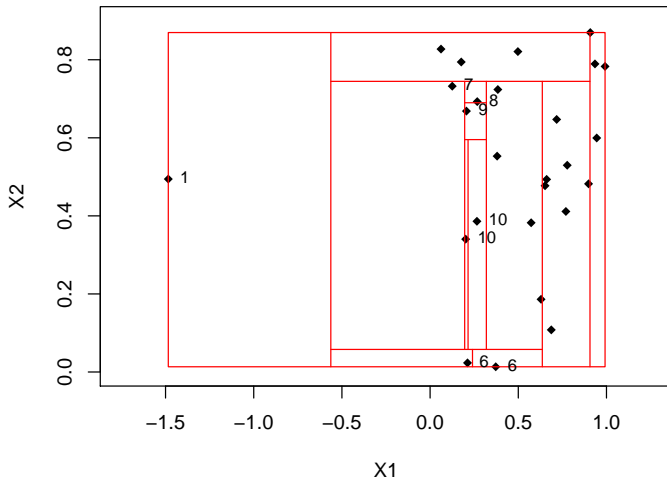
Isolation tree, split 10



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

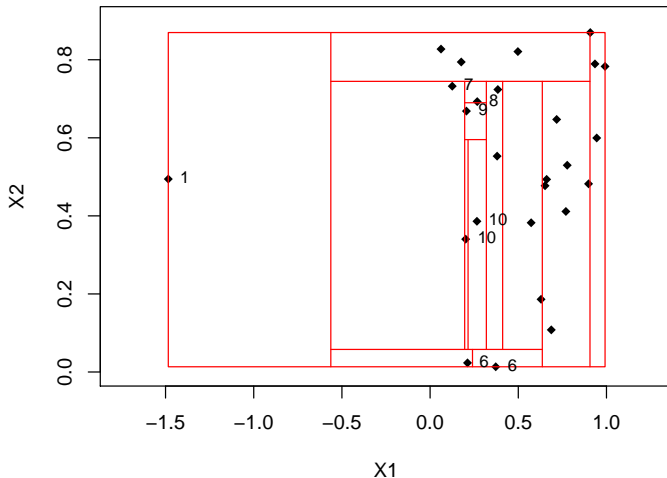
Isolation tree, split 11



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

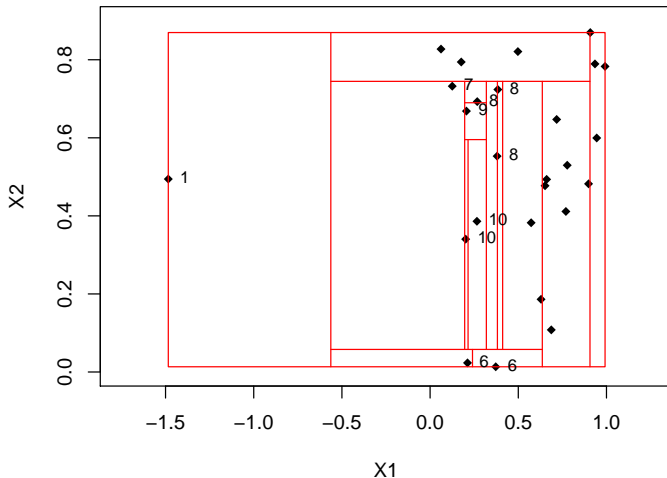
Isolation tree, split 12



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

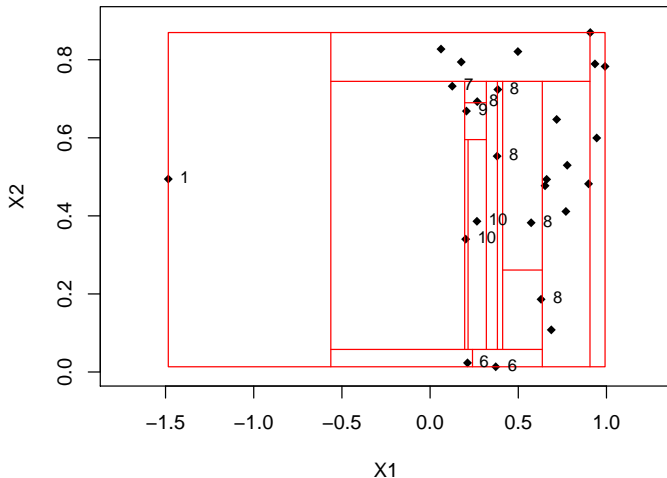
Isolation tree, split 13



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

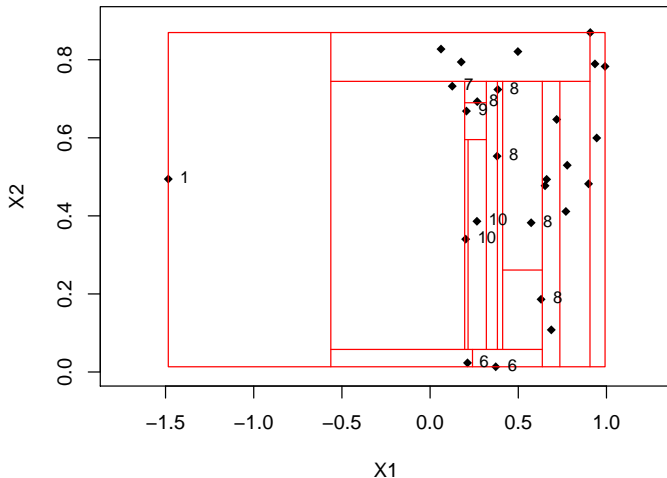
Isolation tree, split 14



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

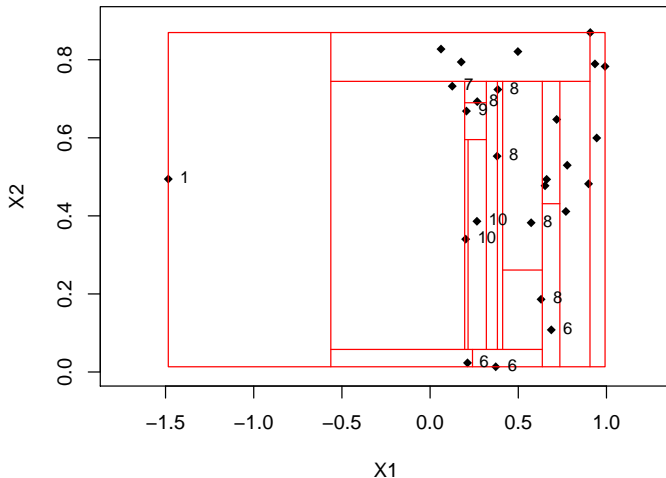
Isolation tree, split 15



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

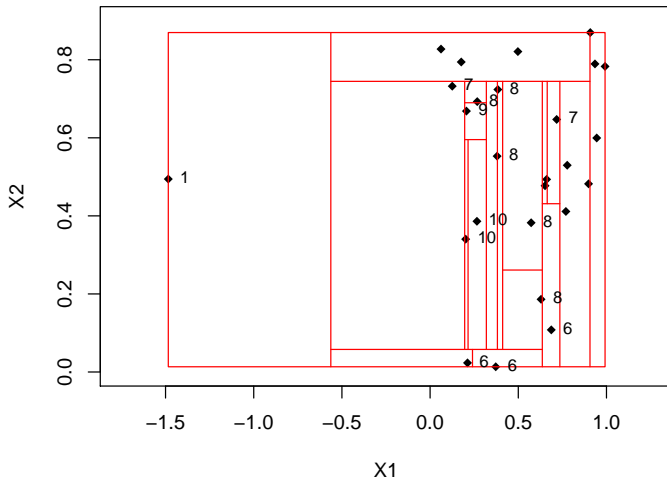
Isolation tree, split 16



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

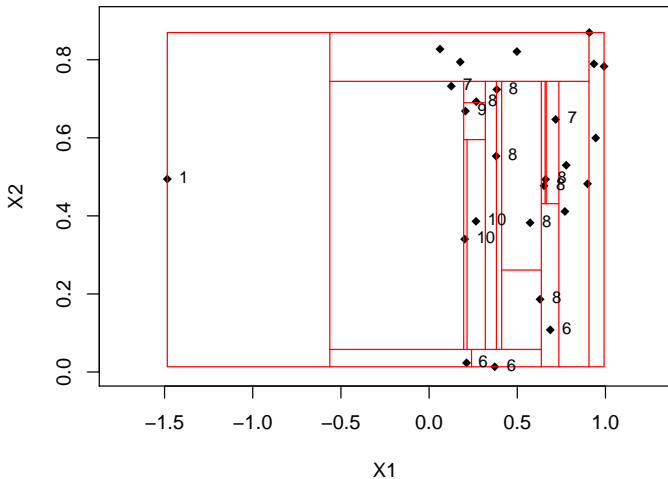
Isolation tree, split 17



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

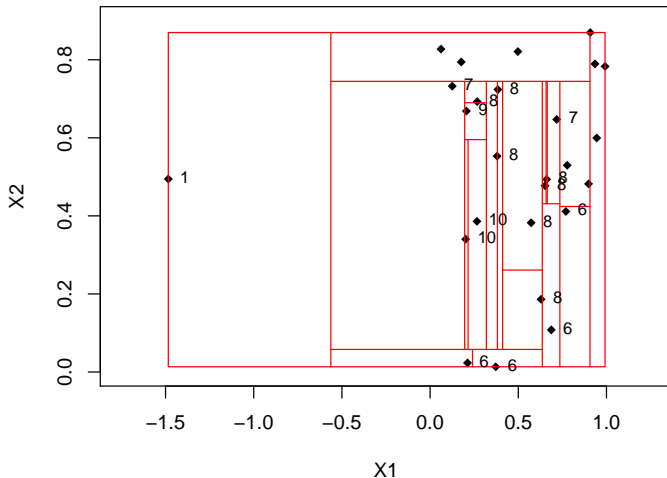
Isolation tree, split 18



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

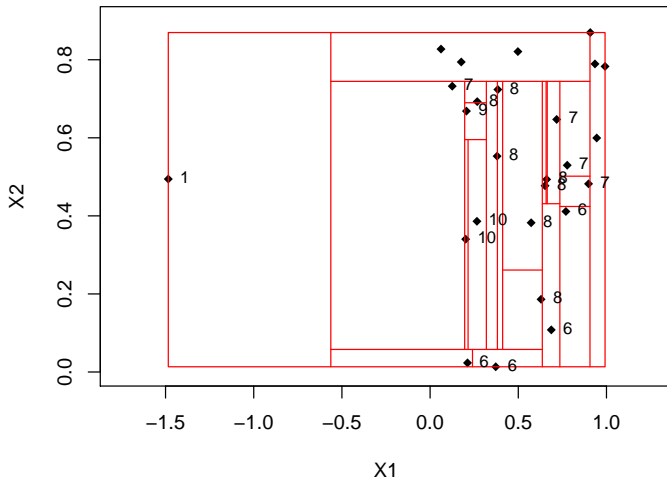
Isolation tree, split 19



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

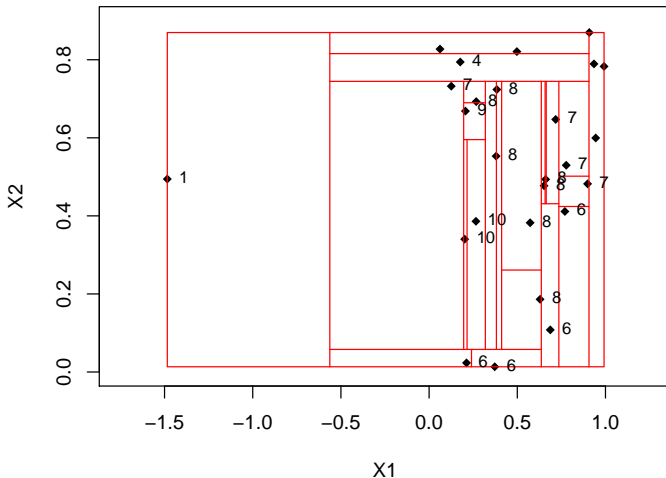
Isolation tree, split 20



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

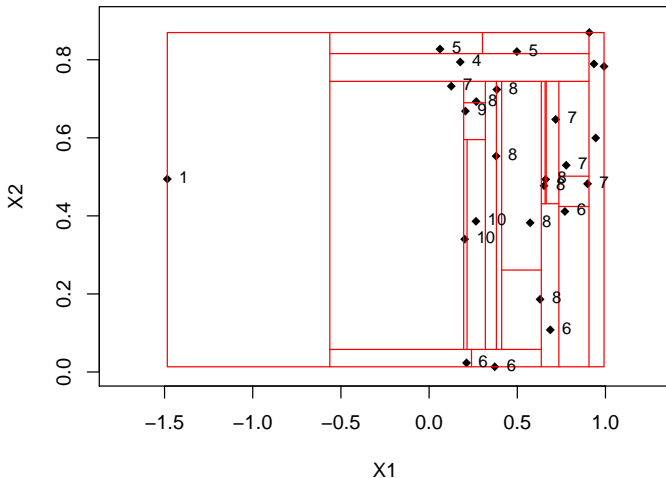
Isolation tree, split 21



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

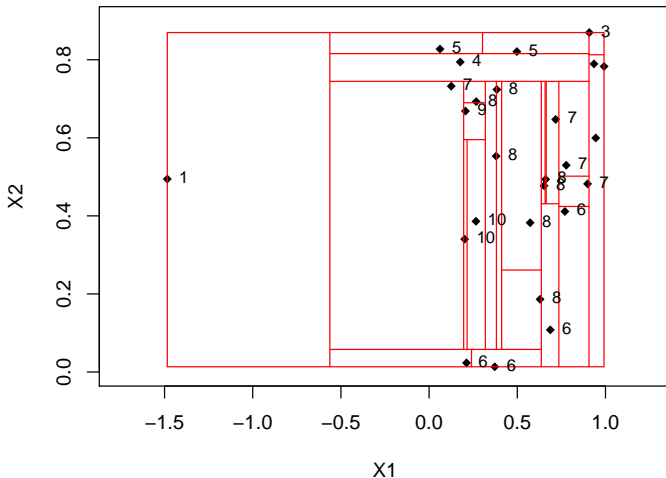
Isolation tree, split 22



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

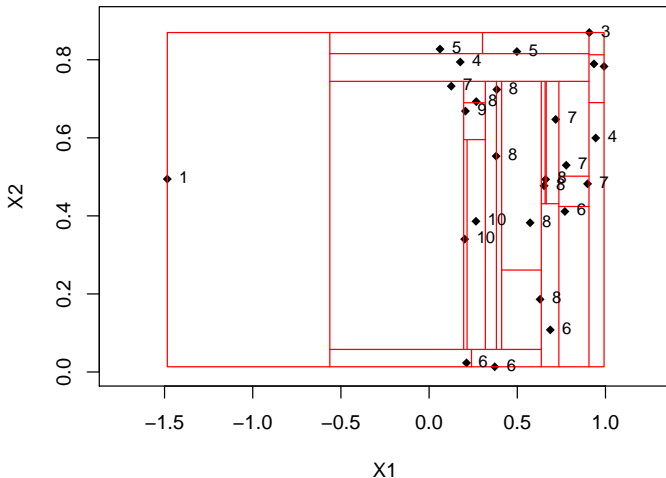
Isolation tree, split 23



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

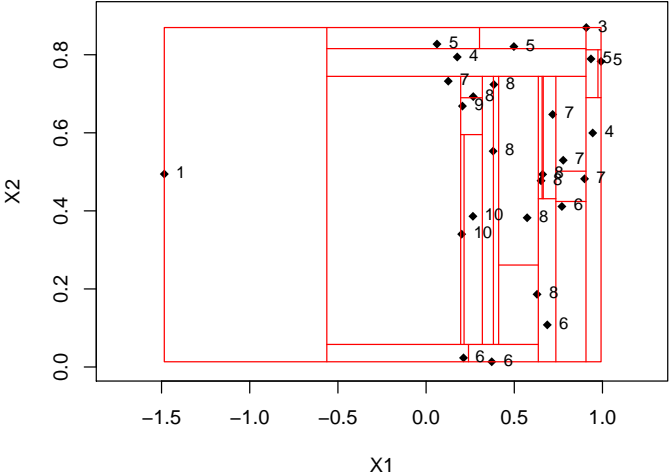
Isolation tree, split 24



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**:

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

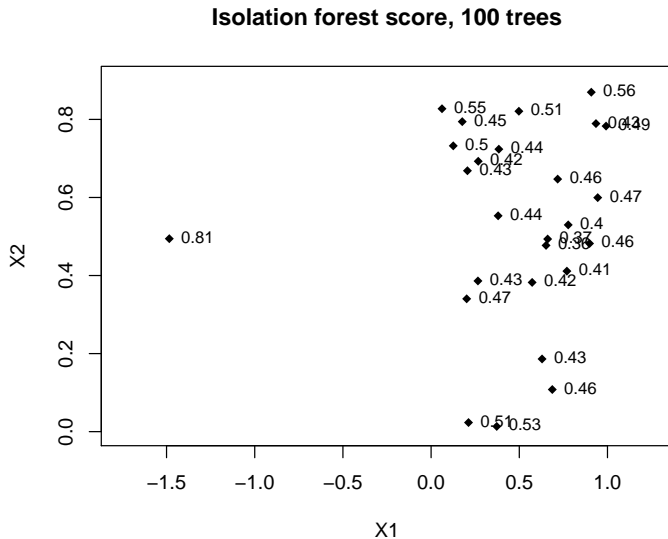
with $c(n) = 2H(n-1) - \frac{2(n-1)}{n}$ where $H(k)$ is the harmonic number and can be estimated by $\ln(k) + 0.5772156649$.

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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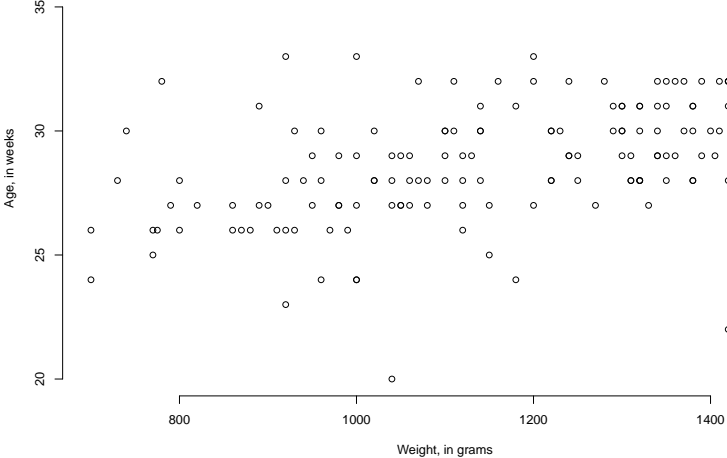
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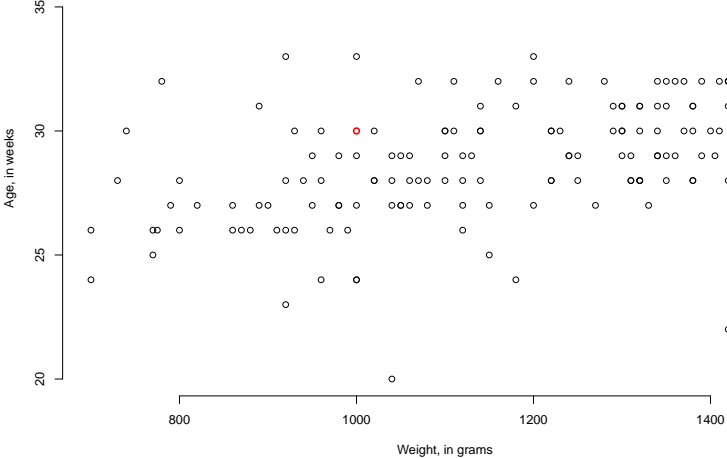
Data depth

Babies with low birth weight



Data depth

Babies with low birth weight



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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- D4 monotone on rays:** for any $\mathbf{x}^* \in \operatorname{argmax}_{\mathbf{x} \in \mathbb{R}^p} D(\mathbf{x}|X)$, any $\mathbf{x} \in \mathbb{R}^p$, and any $0 \leq \alpha \leq 1$ it holds:
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 $D(\mathbf{x}|X) \leq D(\mathbf{x}^* + \alpha(\mathbf{x} - \mathbf{x}^*)|X)$;
- 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 α .

Statistical data depth

Some remarks:

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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.

Python library **data-depth**: to be released soon.

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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} :

$$D^T(\mathbf{x}|X) = \inf\{P(H) : H \text{ is a closed halfspace, } \mathbf{x} \in H\},$$

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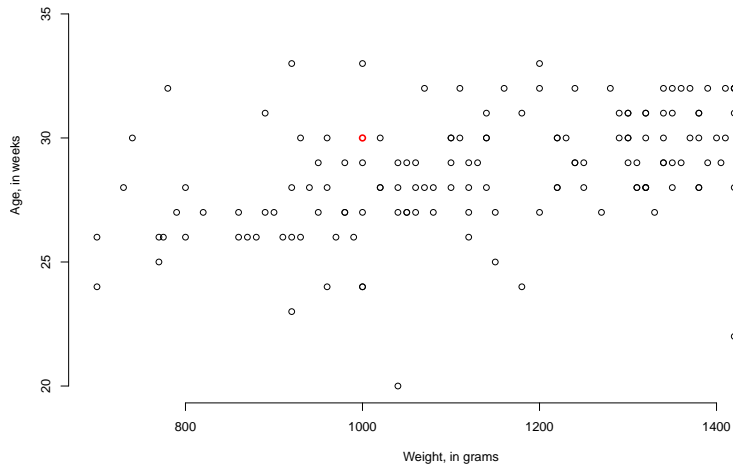
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Tukey depth

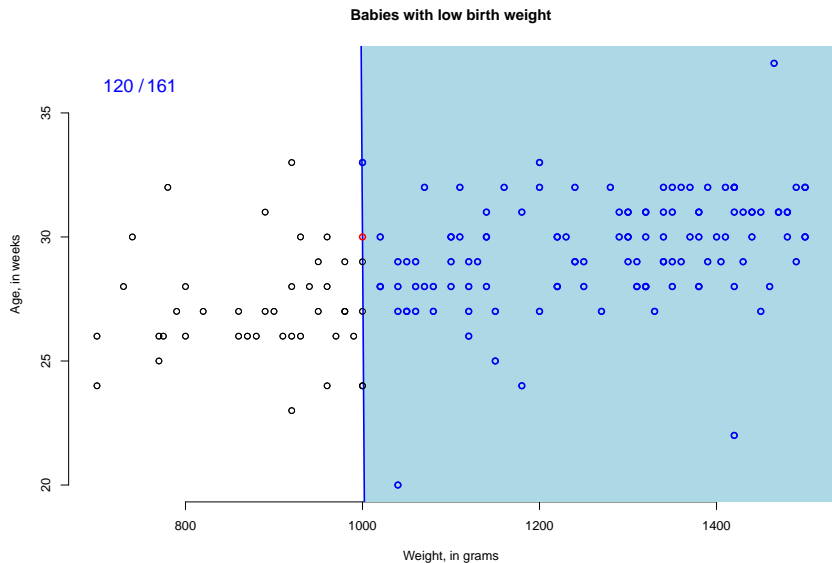
- ▶ satisfies all the above postulates,
- ▶ is purely non-parametric and robust,
- ▶ has direct connection to quantiles and many applications.

Tukey (=halfspace, location) data depth

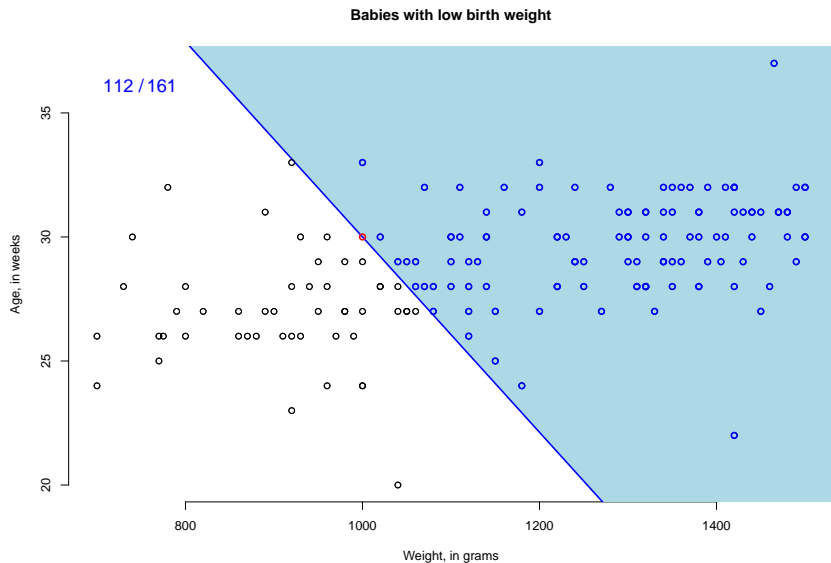
Babies with low birth weight



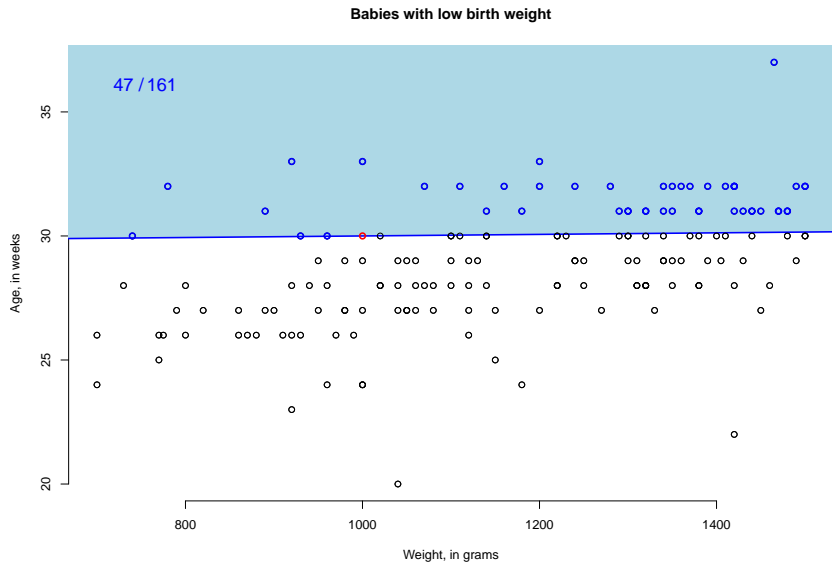
Tukey (=halfspace, location) data depth



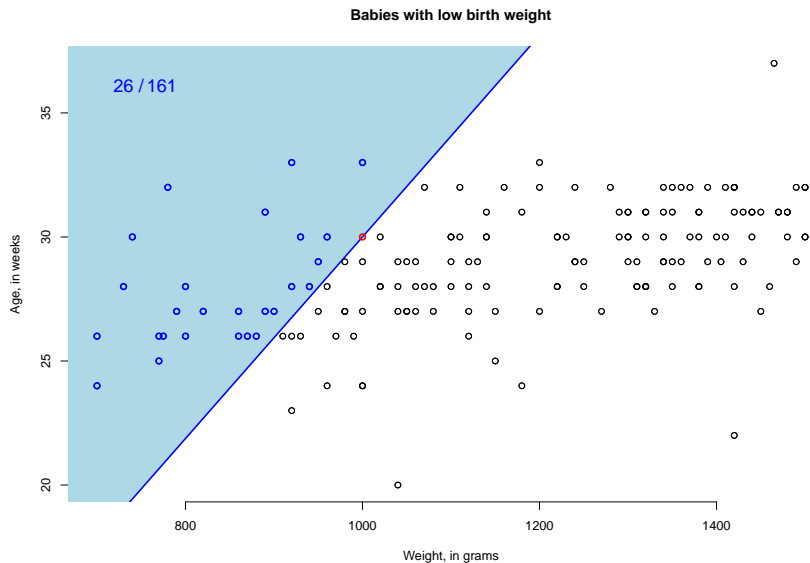
Tukey (=halfspace, location) data depth



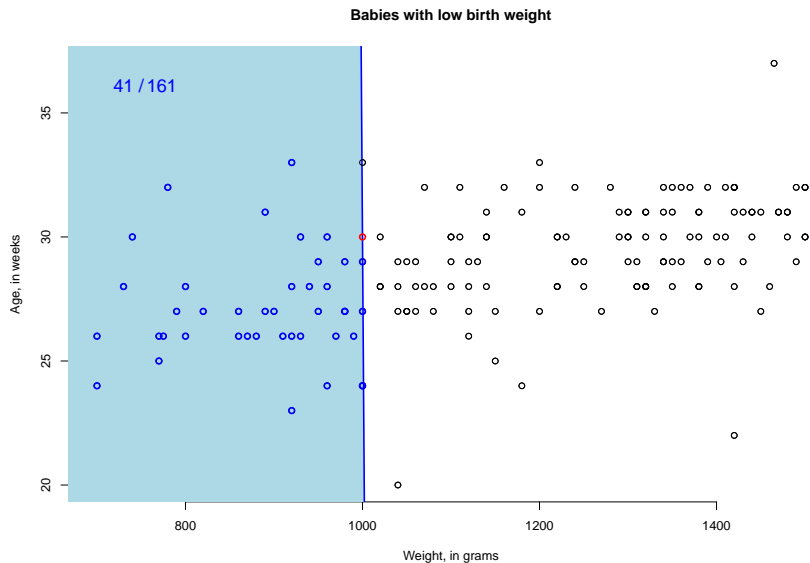
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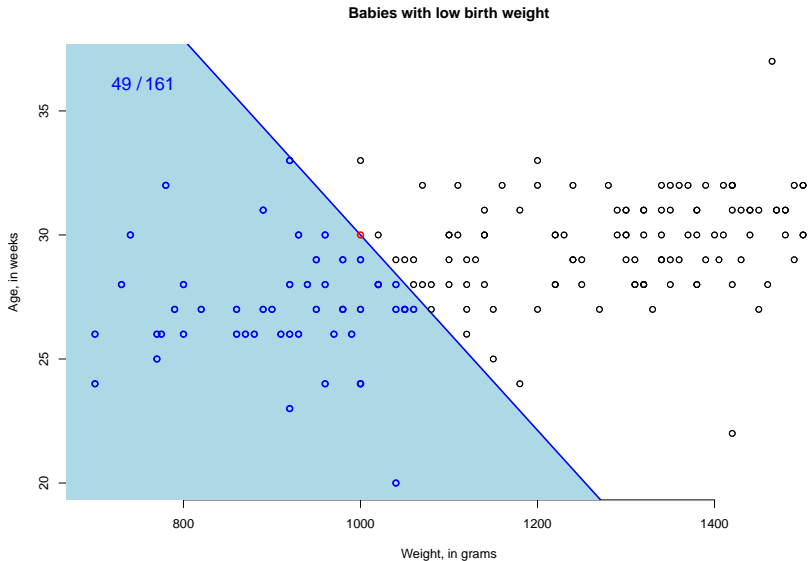
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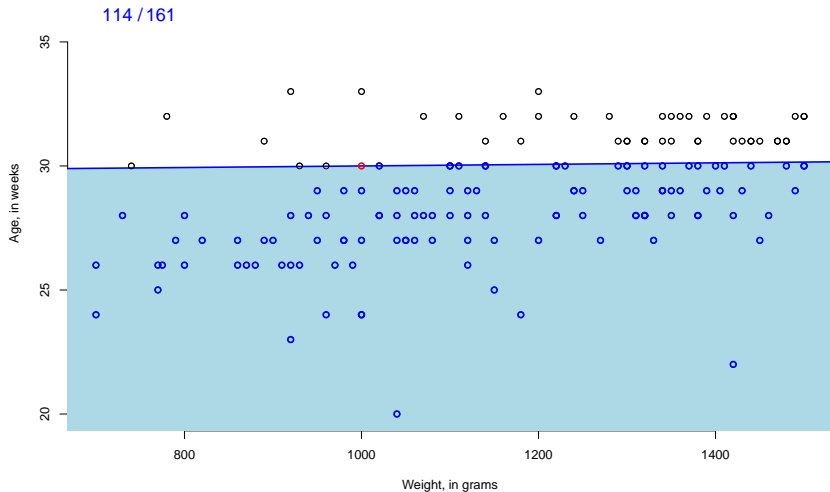


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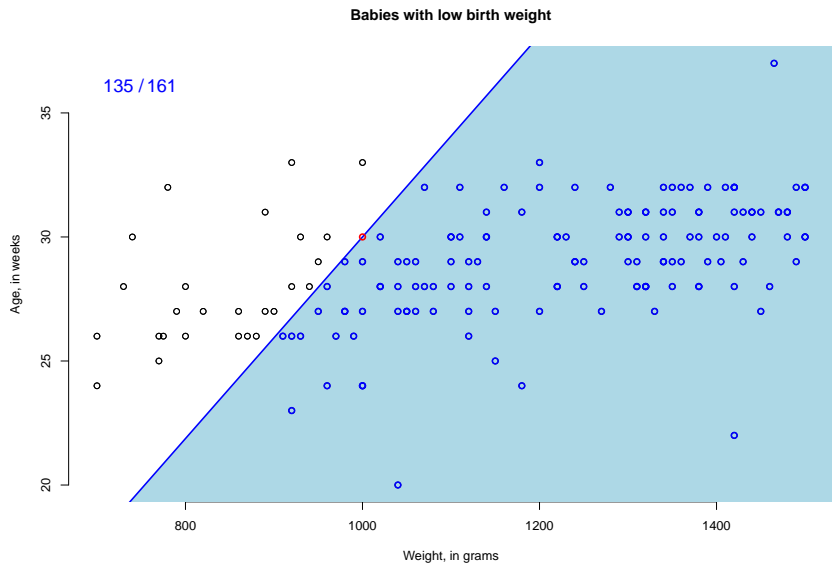


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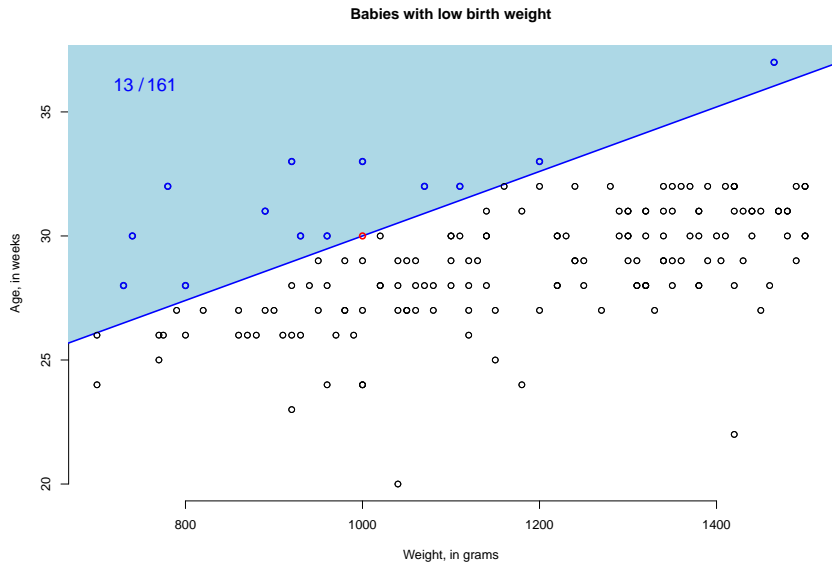
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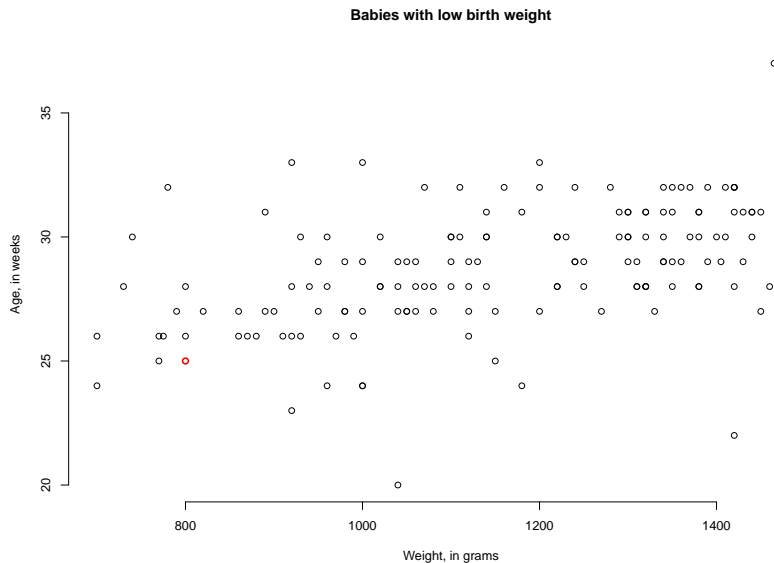
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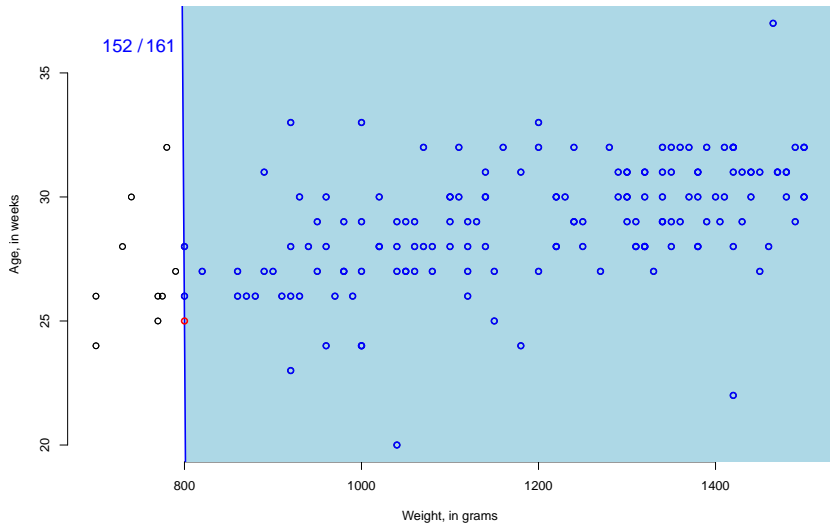


Tukey (=halfspace, location) data depth



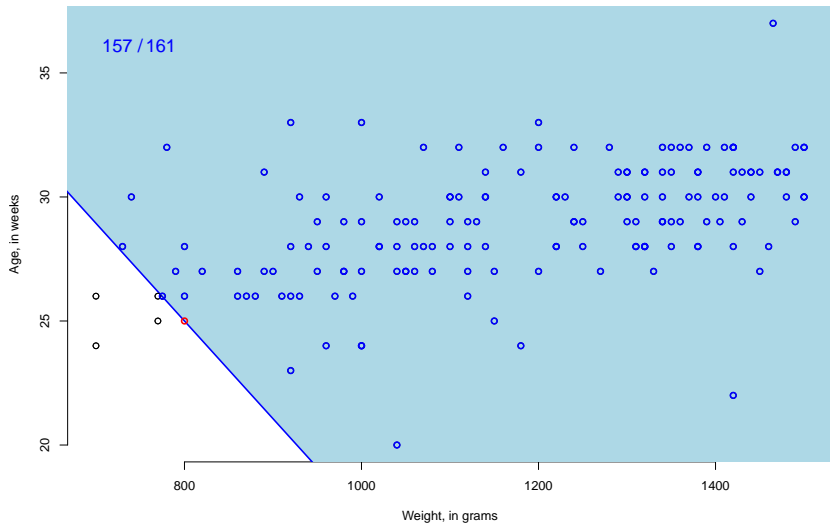
Tukey (=halfspace, location) data depth

Babies with low birth weight

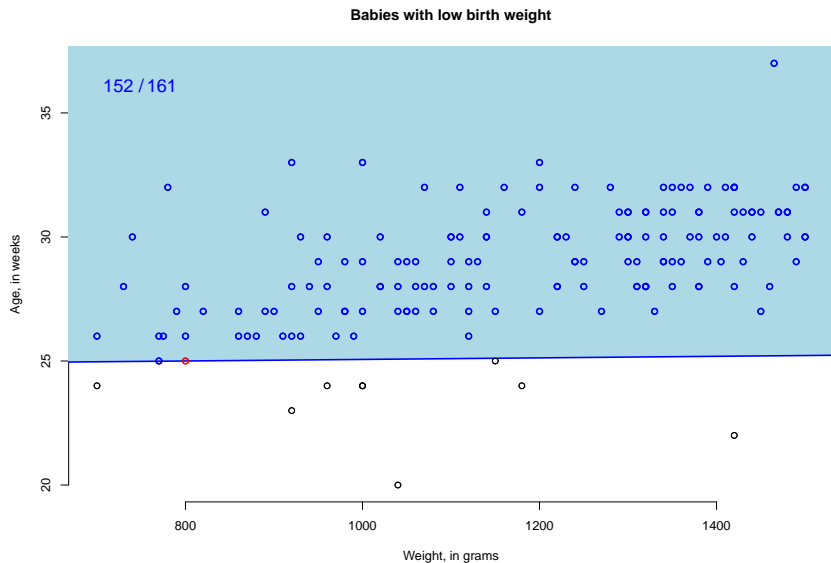


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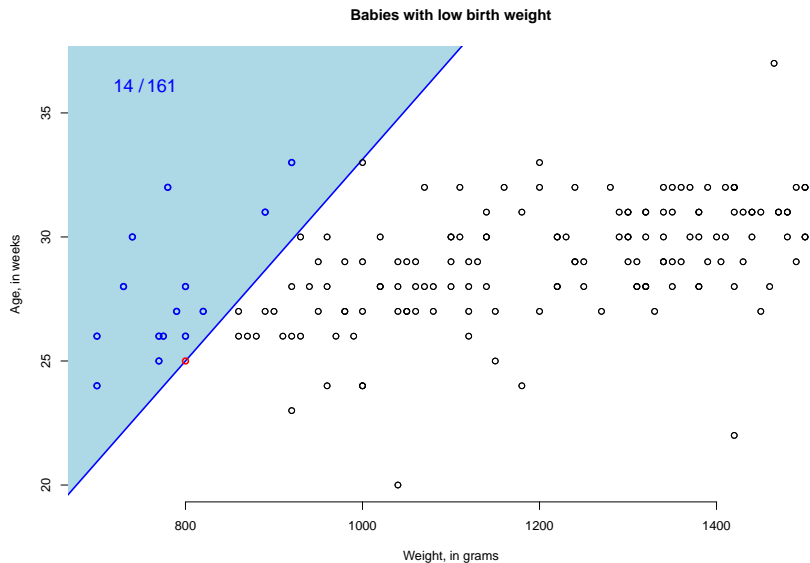
Babies with low birth weight



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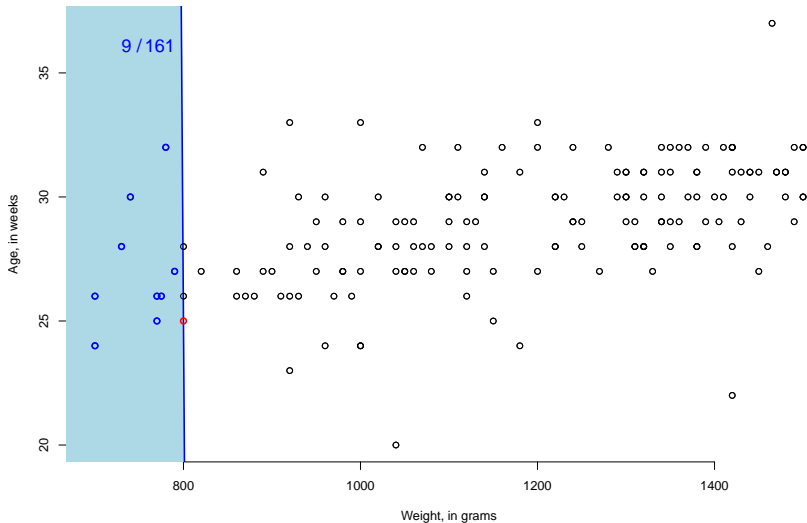


Tukey (=halfspace, location) data depth



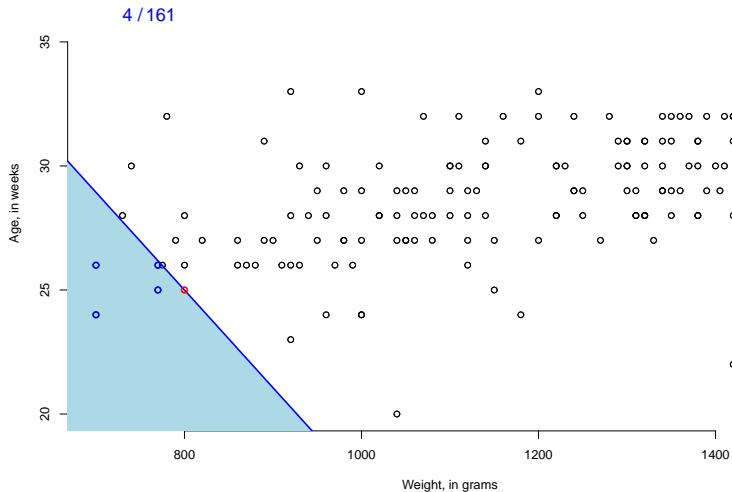
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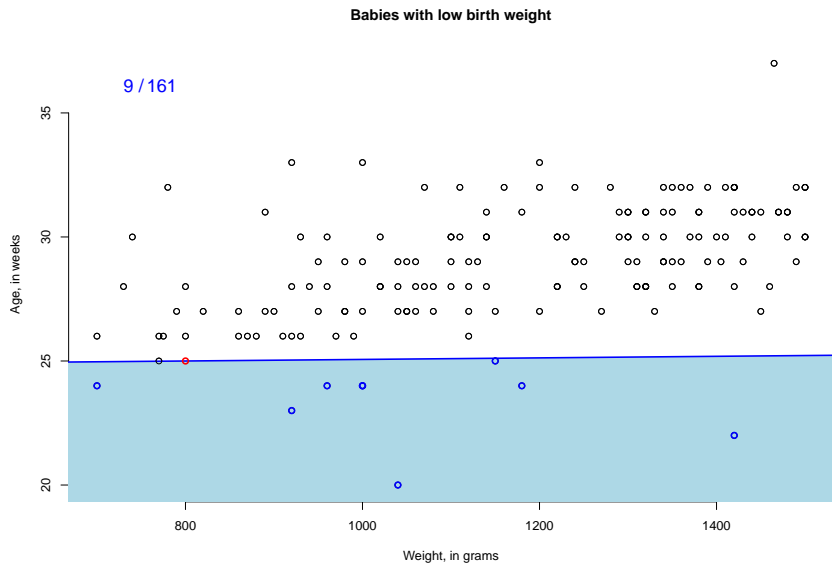


Tukey (=halfspace, location) data depth

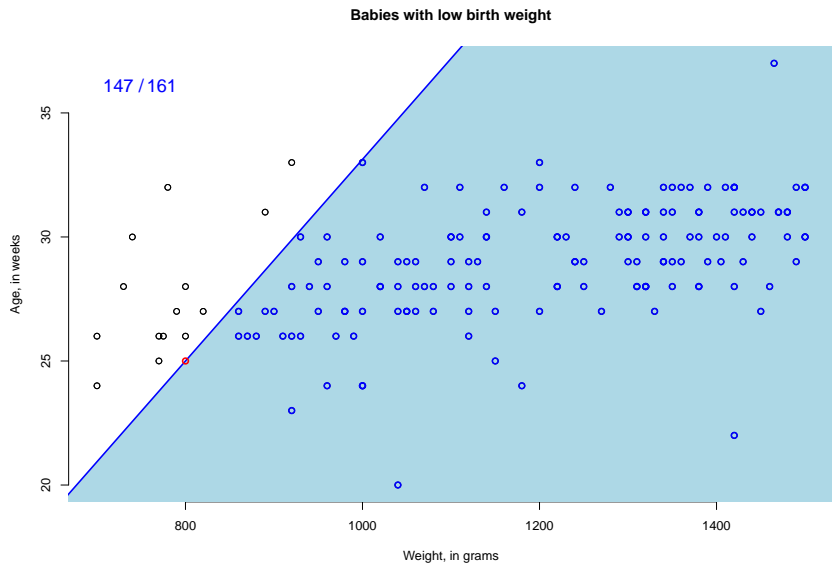
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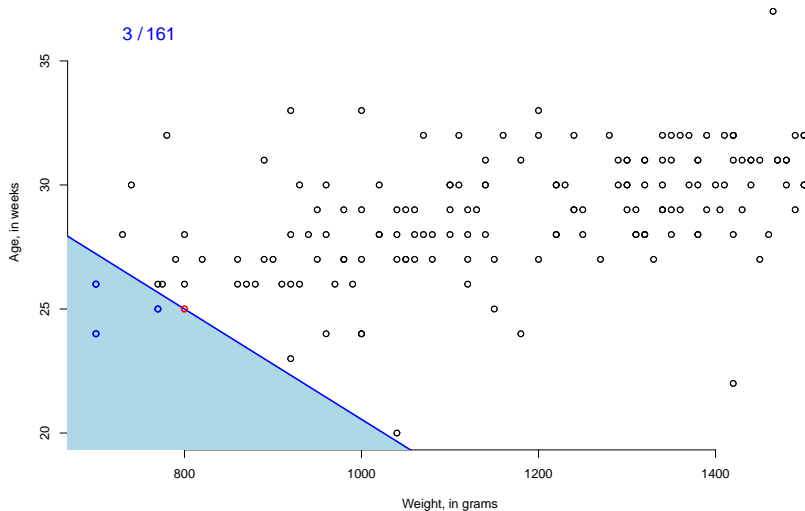


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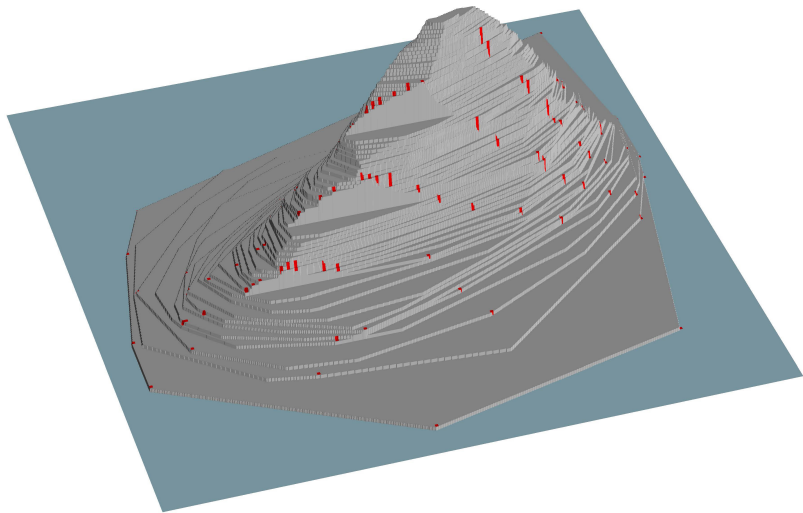


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Tukey (=halfspace, location) data depth



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Central regions

- ▶ For given distribution P and $\alpha \in [0, 1]$, the level sets $D_\alpha(P)$ form a family of **depth-trimmed** of **central regions**.

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Tukey-trimmed regions

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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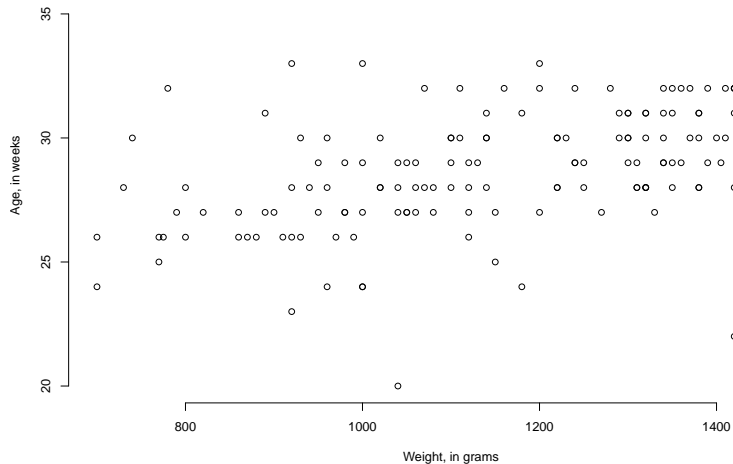
- ▶ Affine invariant;
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- ▶ Quasiconcave.

Regions:

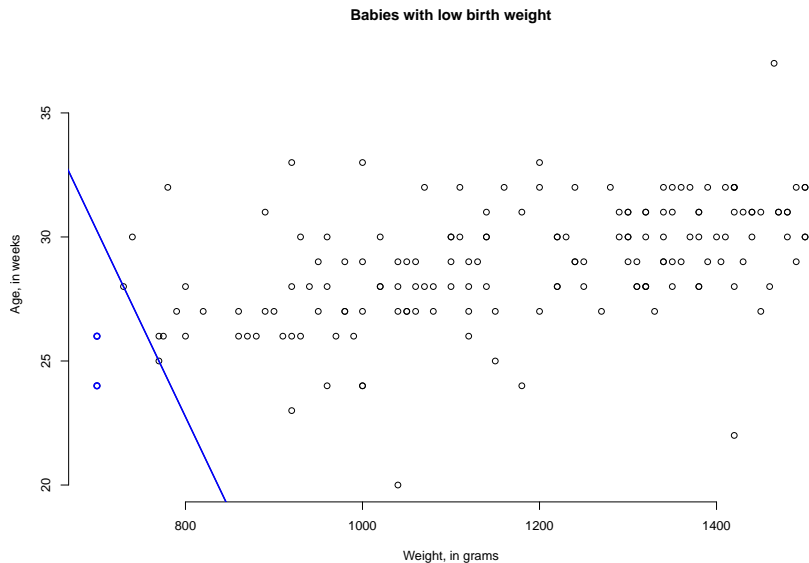
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Tukey (=halfspace, location) depth-trimmed regions

Babies with low birth weight

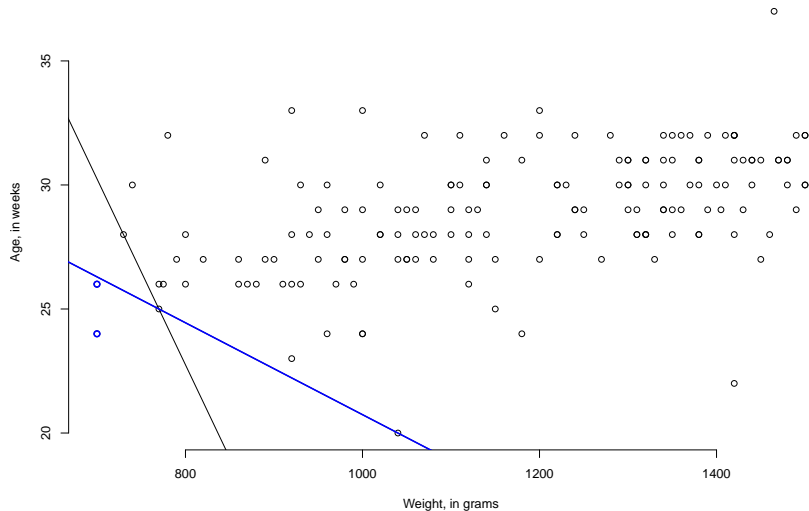


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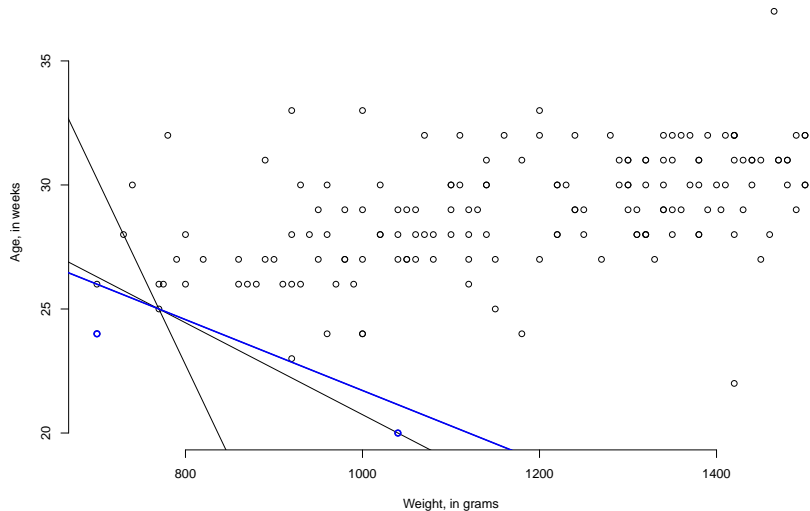
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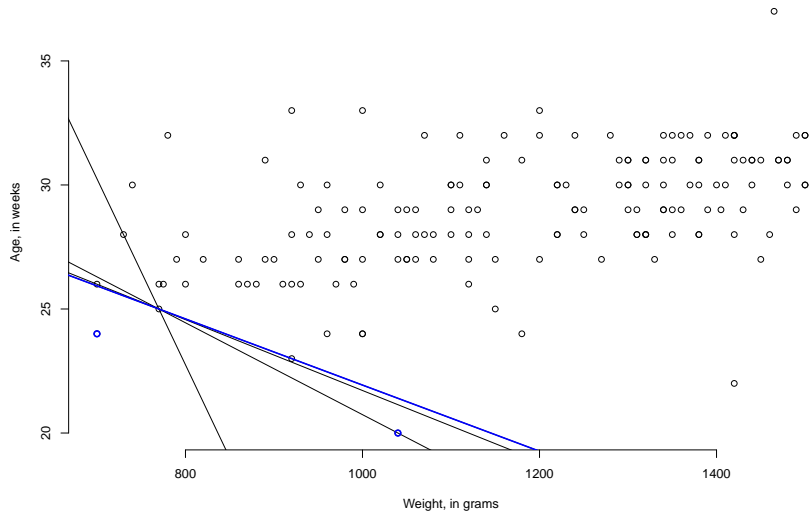
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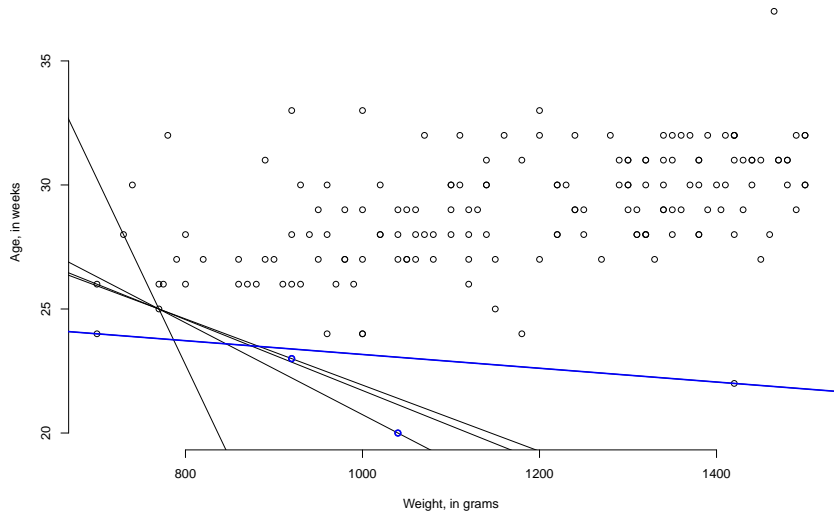
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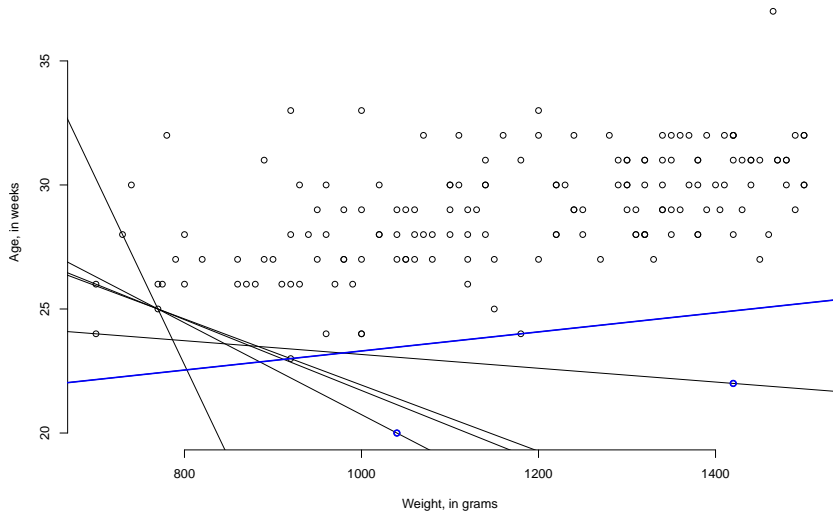
Tukey (=halfspace, location) depth-trimmed regions

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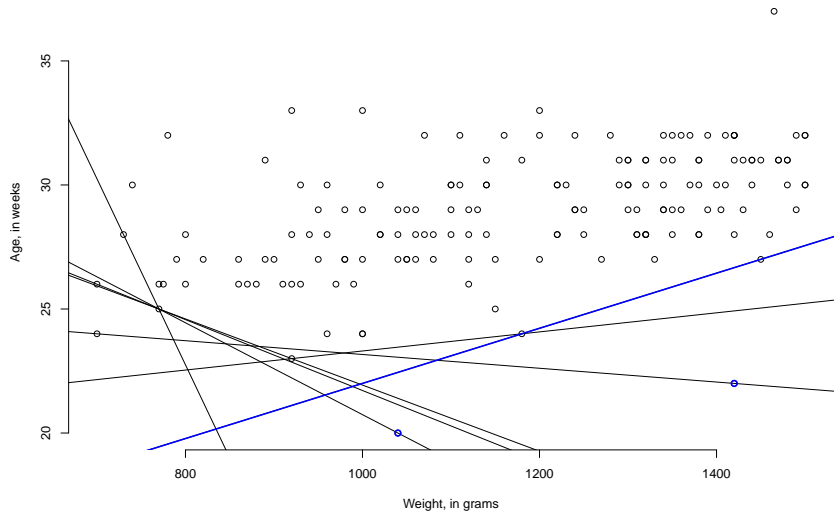
Tukey (=halfspace, location) depth-trimmed regions

Babies with low birth weight



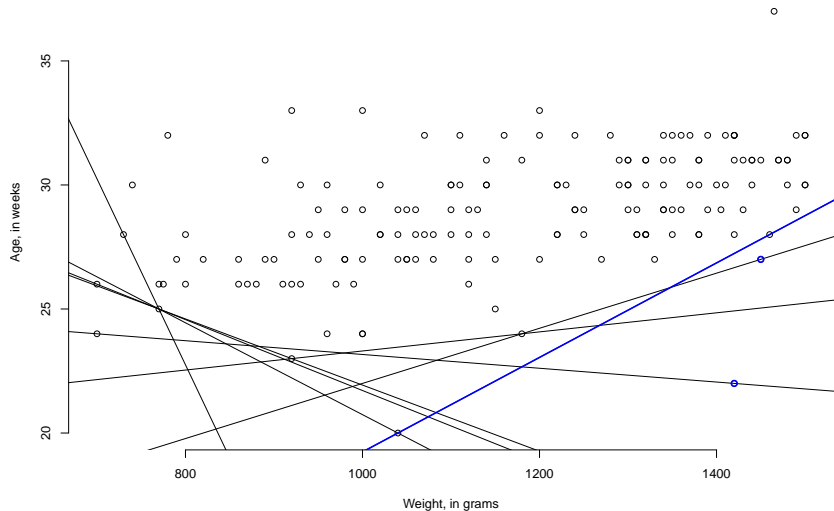
Tukey (=halfspace, location) depth-trimmed regions

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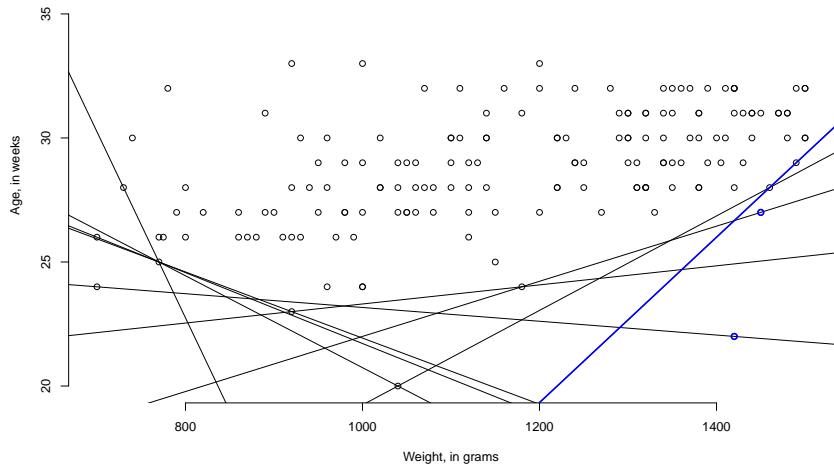
Tukey (=halfspace, location) depth-trimmed regions

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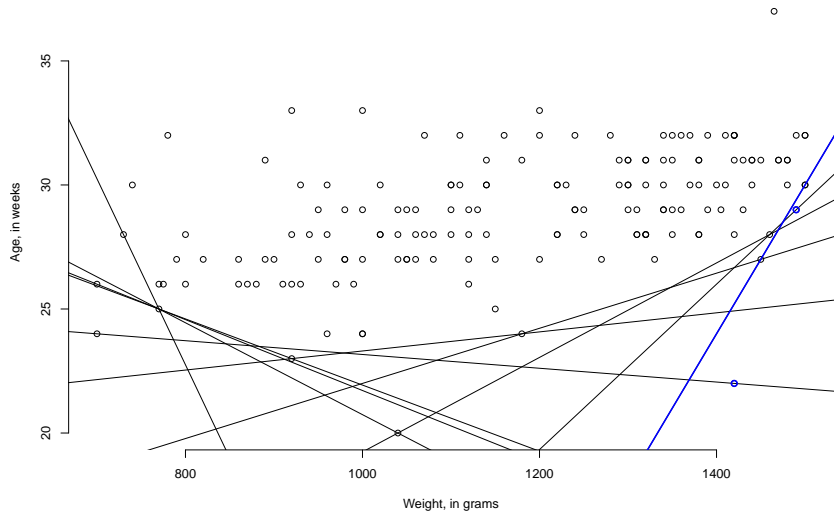
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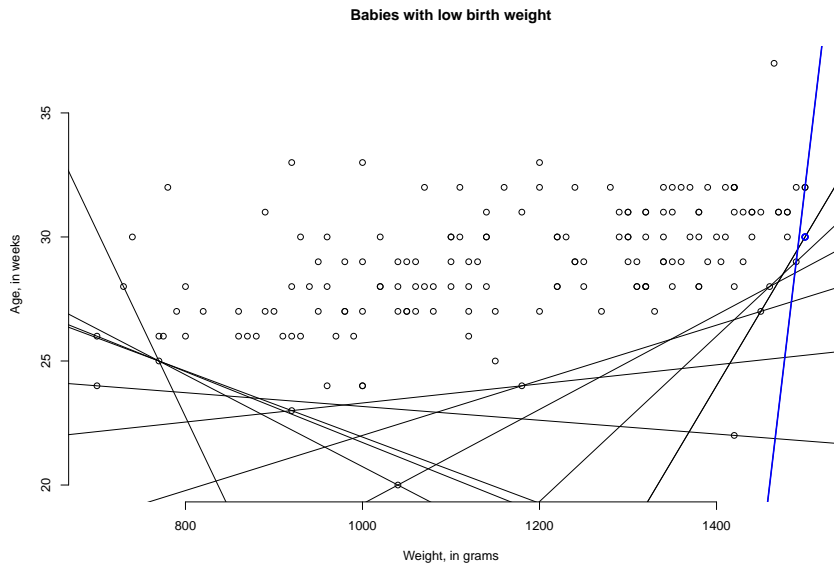


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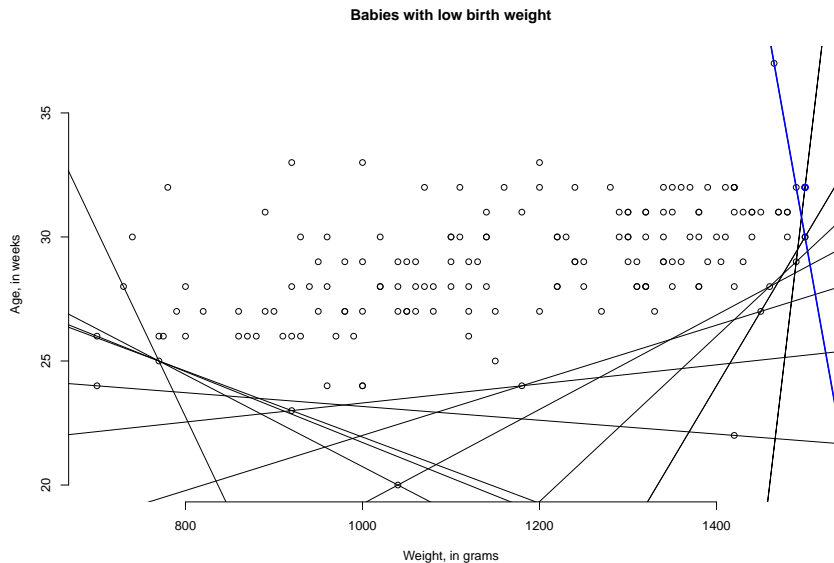
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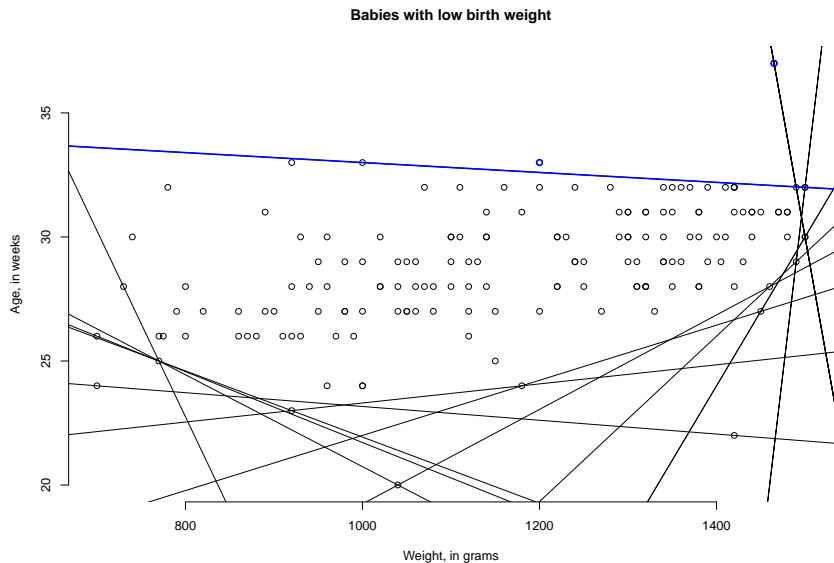
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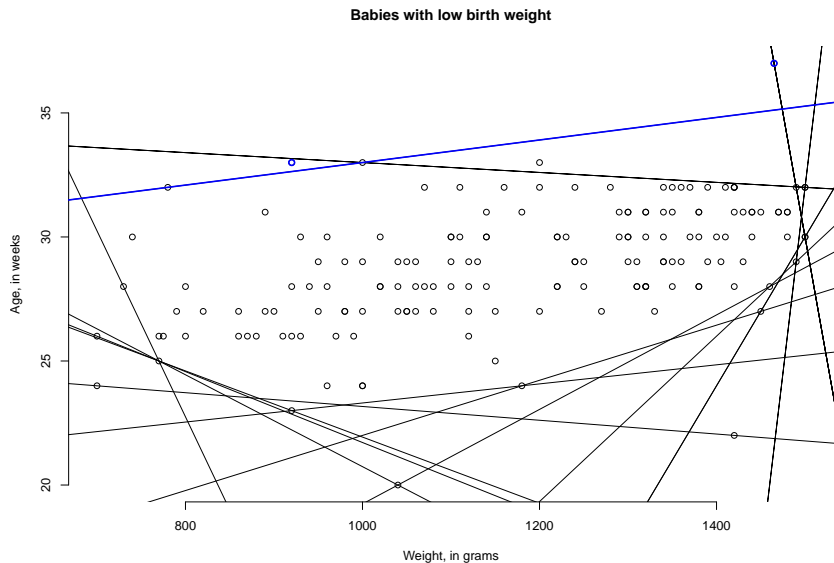
Tukey (=halfspace, location) depth-trimmed regions



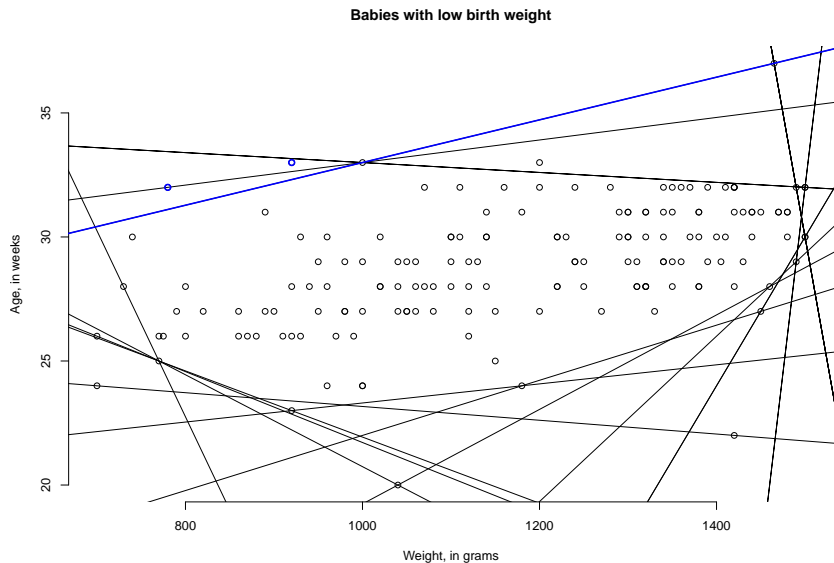
Tukey (=halfspace, location) depth-trimmed regions



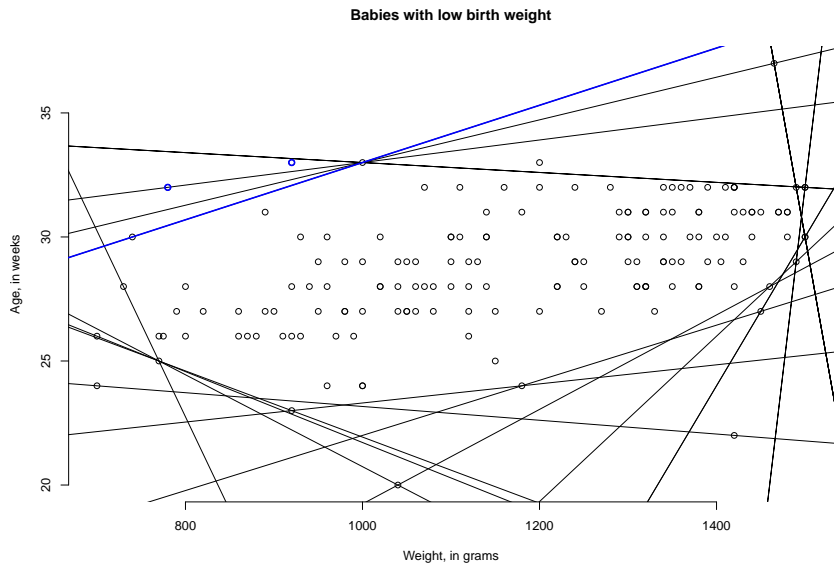
Tukey (=halfspace, location) depth-trimmed regions



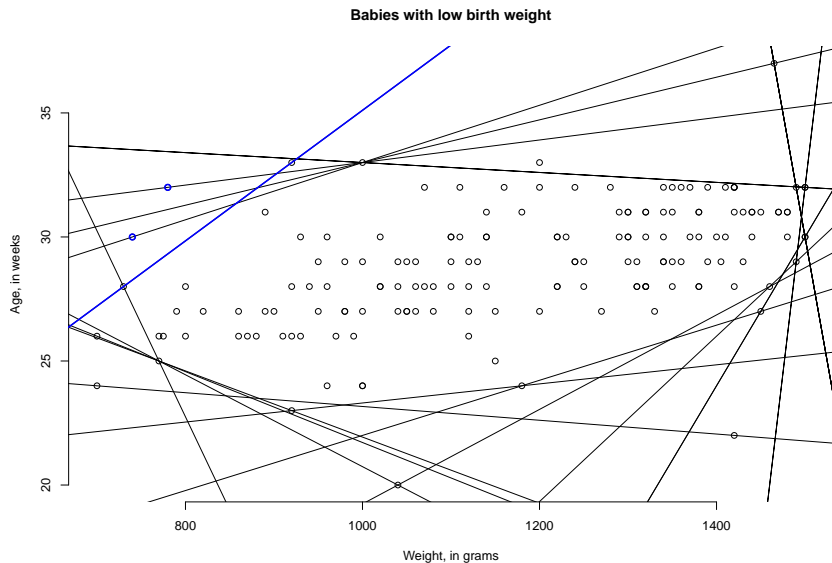
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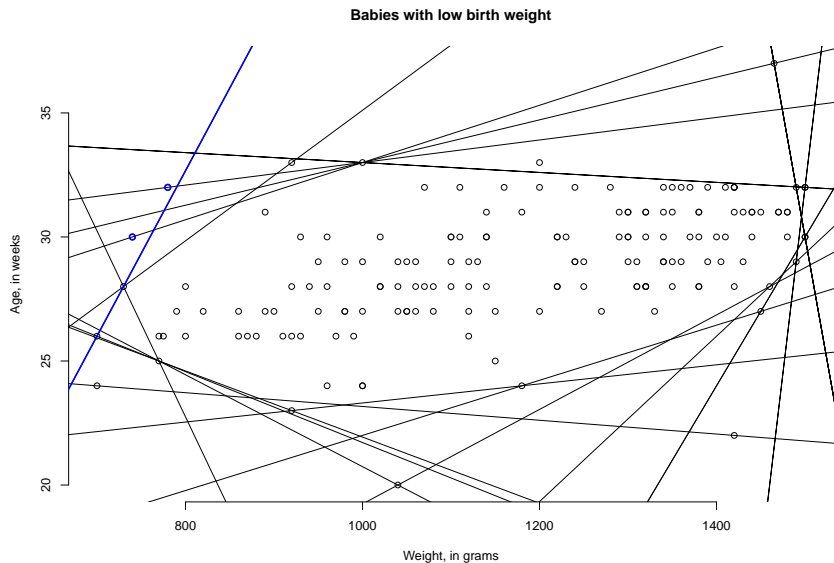
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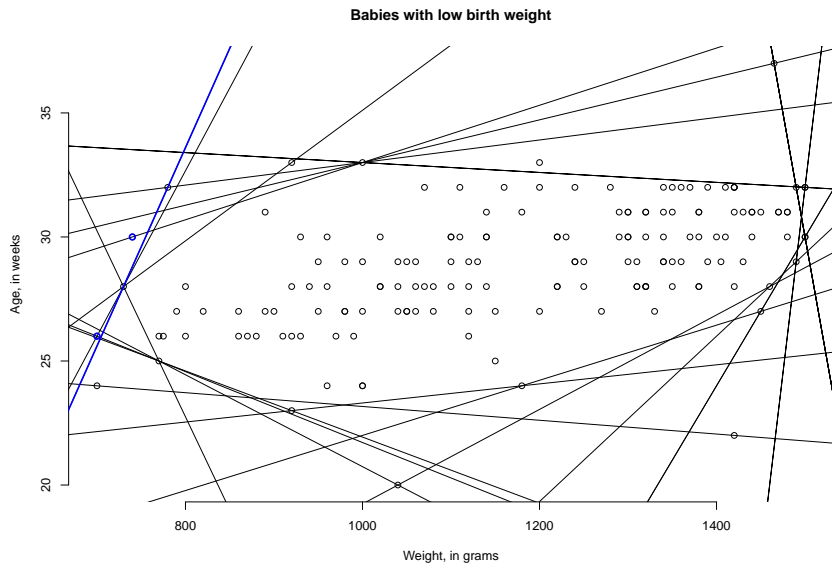
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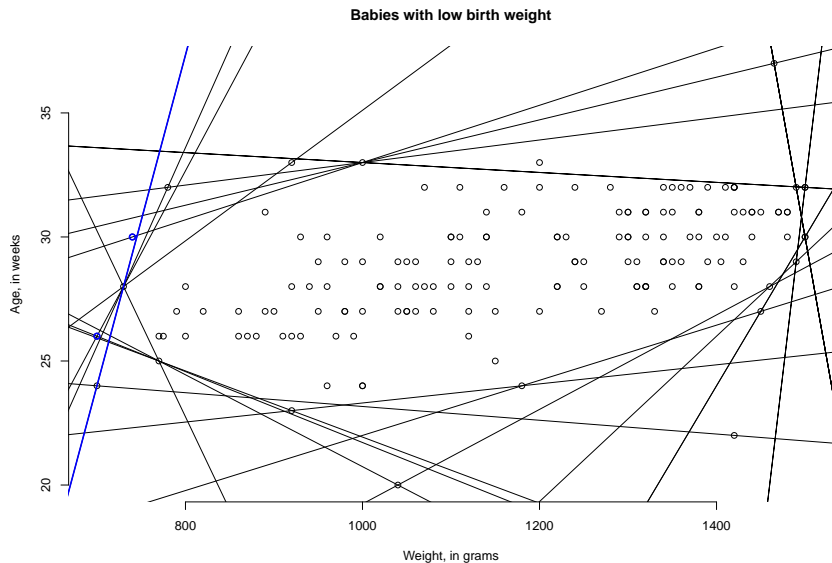
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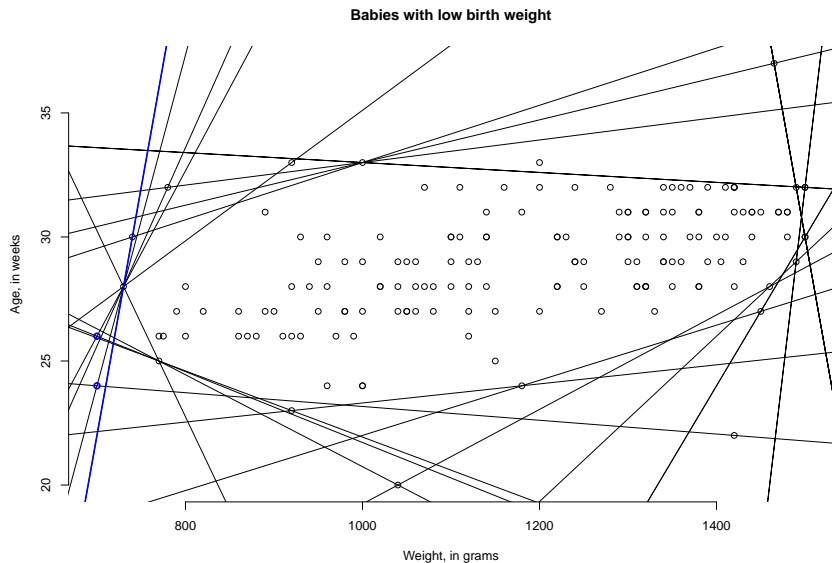
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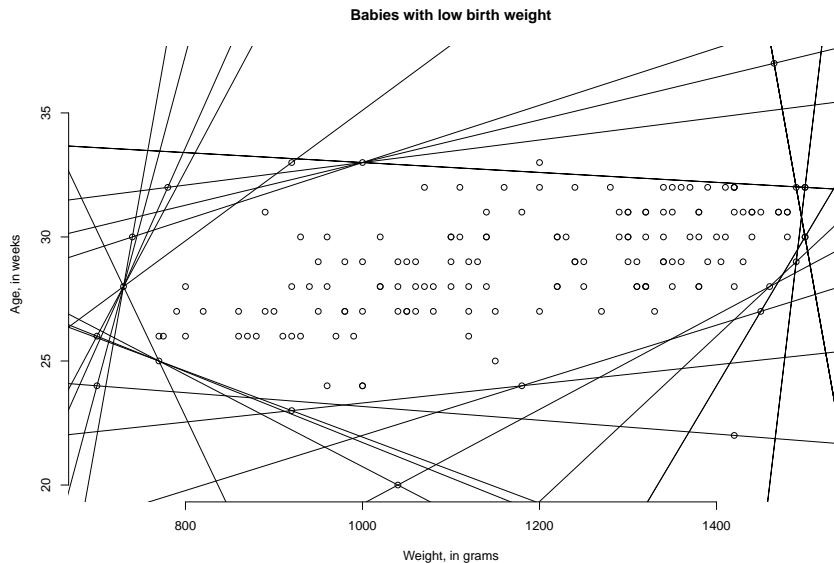
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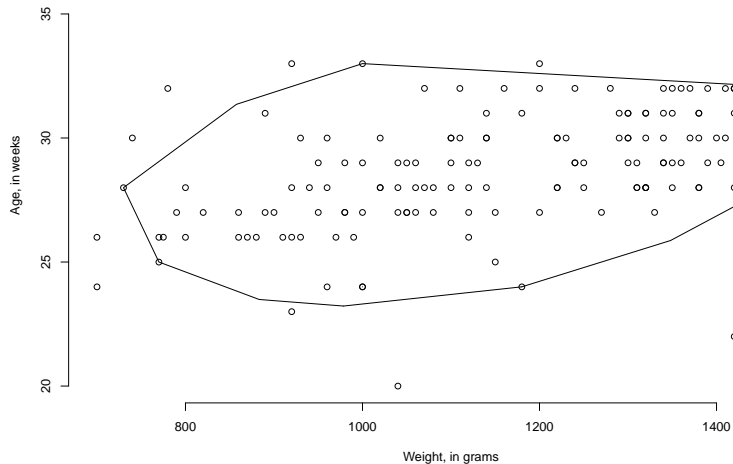


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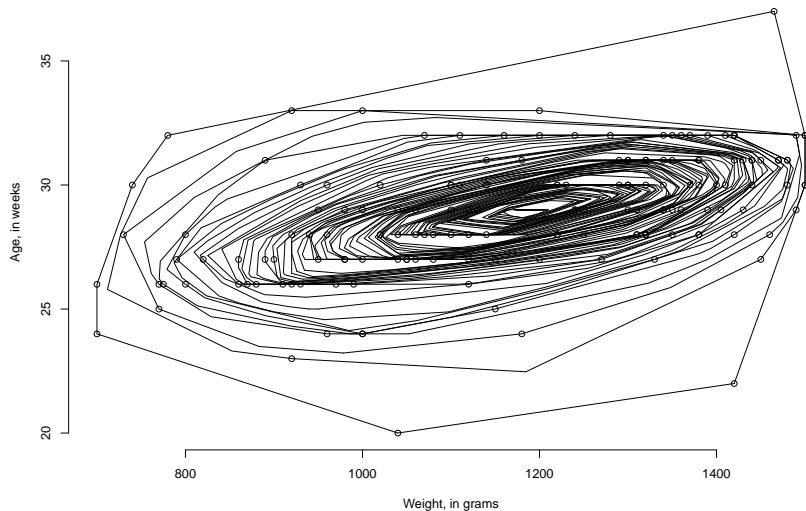
Tukey (=halfspace, location) depth-trimmed regions

Babies with low birth weight

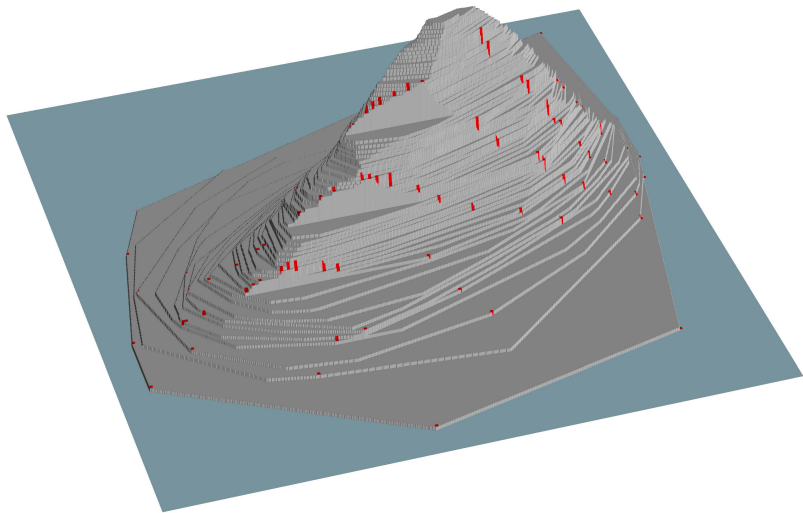


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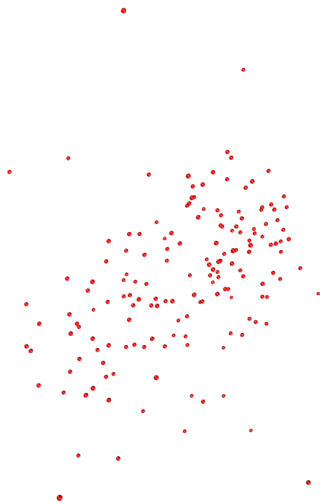
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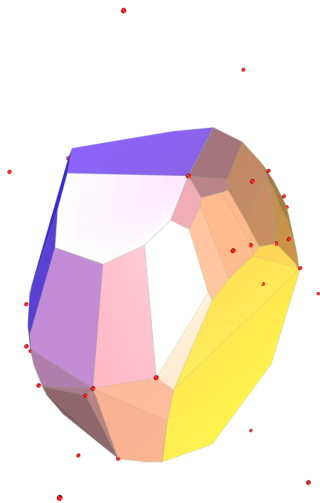
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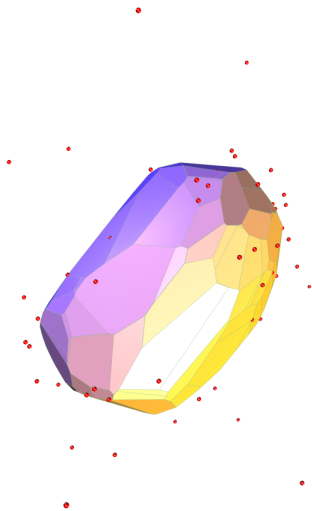
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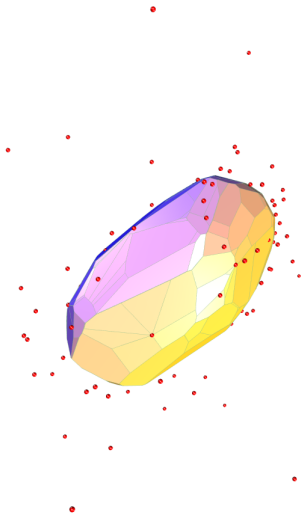
Tukey (=halfspace, location) depth region: $\tau = 2/161$



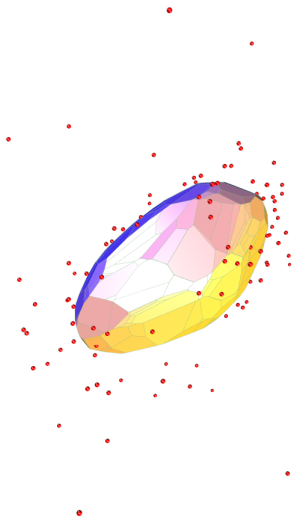
Tukey (=halfspace, location) depth region: $\tau = 5/161$



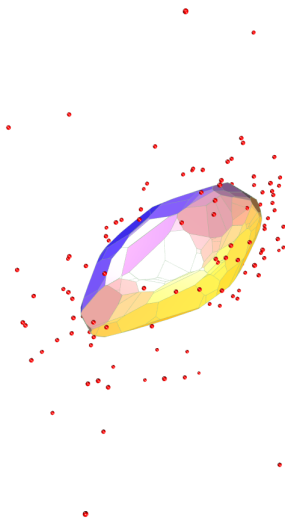
Tukey (=halfspace, location) depth region: $\tau = 9/161$



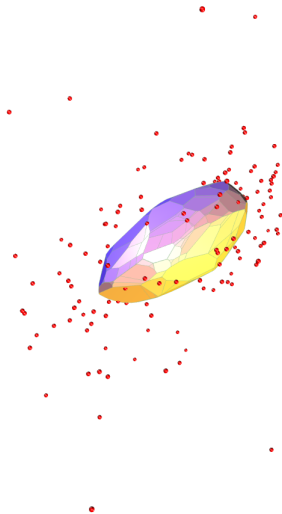
Tukey (=halfspace, location) depth region: $\tau = 13/161$



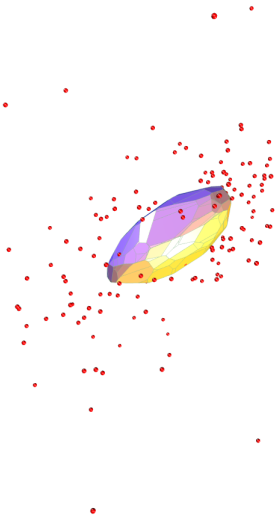
Tukey (=halfspace, location) depth region: $\tau = 17/161$



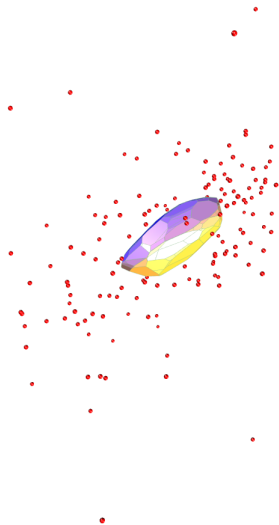
Tukey (=halfspace, location) depth region: $\tau = 25/161$



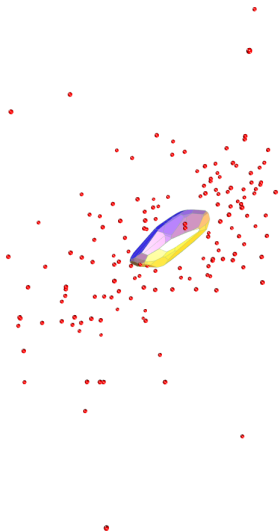
Tukey (=halfspace, location) depth region: $\tau = 33/161$



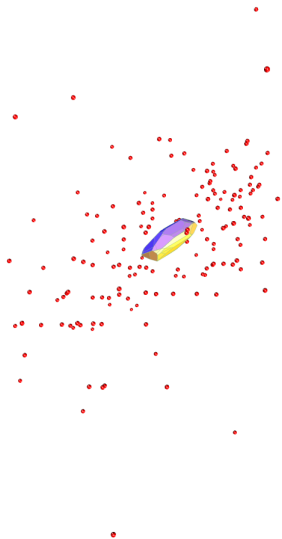
Tukey (=halfspace, location) depth region: $\tau = 41/161$



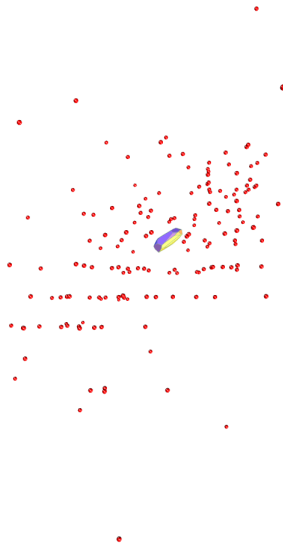
Tukey (=halfspace, location) depth region: $\tau = 49/161$



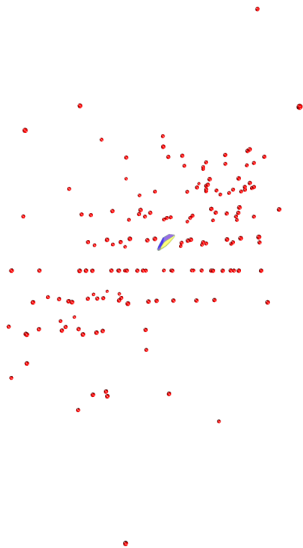
Tukey (=halfspace, location) depth region: $\tau = 57/161$



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



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



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Mahalanobis depth (Mahalanobis, 1936)

- ▶ **Mahalanobis depth** is defined as:

$$D^{Mah}(\mathbf{x}|X) = \frac{1}{1 + (\delta^{Mah})^2(\mathbf{x}|X)},$$

based on Mahalanobis distance:

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- ▶ In the empirical version, $\boldsymbol{\mu}_X$ and $\boldsymbol{\Sigma}_X$ are substituted by suitable estimates:
 - ▶ moment estimates;
 - ▶ robust estimates such as **minimum volume ellipsoid** or **minimum covariance determinant (MCD)**.
- ▶ Properties:
 - ▶ satisfies **D1 – D5** and **D4con**, is continuous;
 - ▶ being defined by $d(d + 1)$ parameters, can be seen as a **parametric depth**;

Mahalanobis depth (Mahalanobis, 1936)

- ▶ **Mahalanobis depth** is defined as:

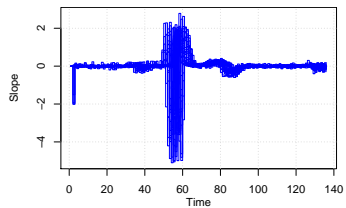
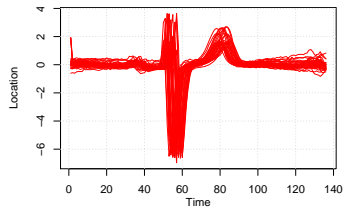
$$D^{Mah}(\mathbf{x}|X) = \frac{1}{1 + (\delta^{Mah})^2(\mathbf{x}|X)},$$

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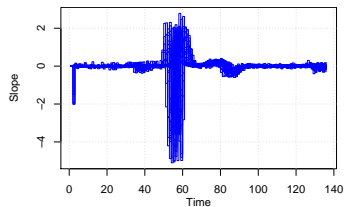
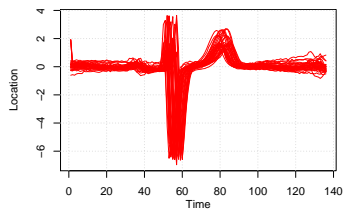
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 - ▶ by a single elliptical contour characterizes a multivariate **normal distribution** or one within an affine **family of non-degenerate elliptical distributions**.

ECG five days data



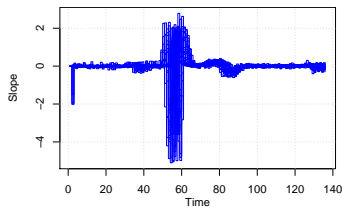
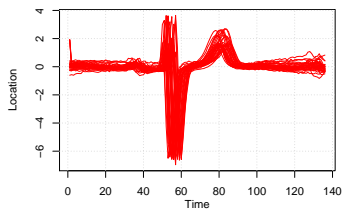
ECG five days data



$$\hat{f}_i \mapsto \mathbf{x}_i = \left[\int_0^T \hat{f}_i(t) dt, \int_0^T \hat{f}'_i(t) dt \right],$$

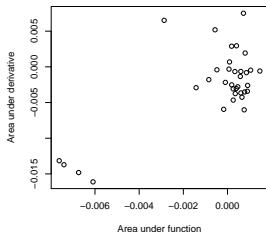
with $\hat{f}_i(t)$ being the function obtained by connecting the points $(t_{ij}, f_i(t_{ij}))$, $j = 1, \dots, N_i$ with line segments, $\hat{f}'_i(t)$ its derivative.

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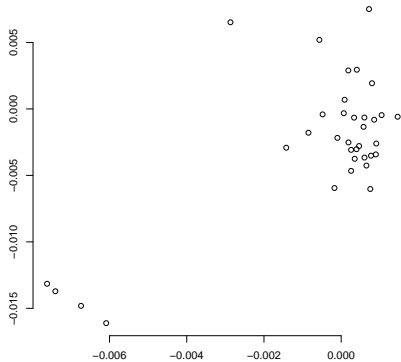


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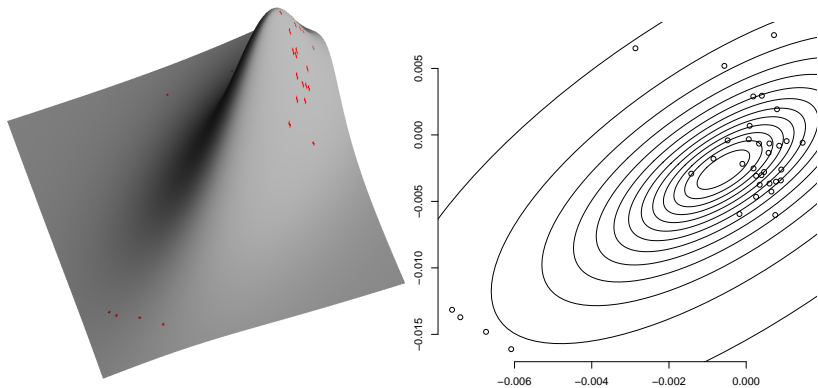
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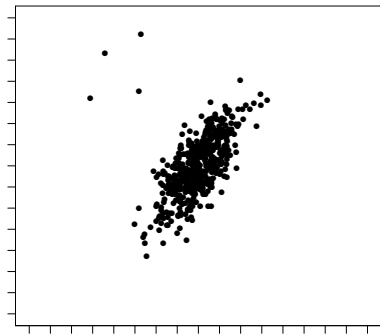
Mahalanobis depth (Mahalanobis, 1936)



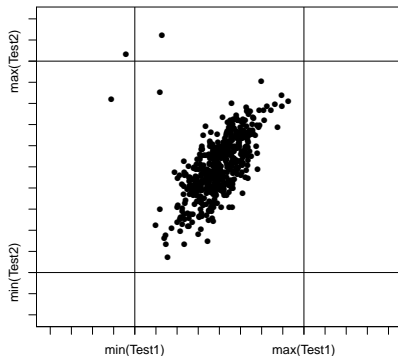
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Multivariate anomaly detection: an example

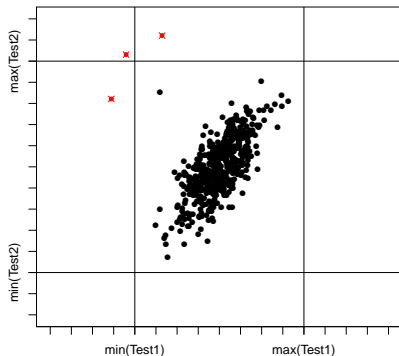


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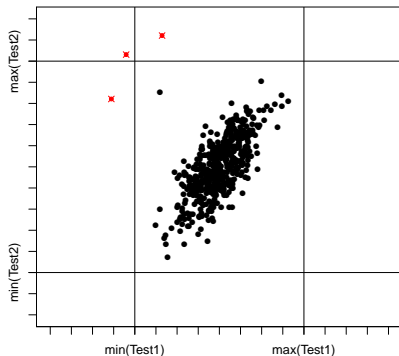
- ▶ Checking for **minimum** and **maximum** in each test result.

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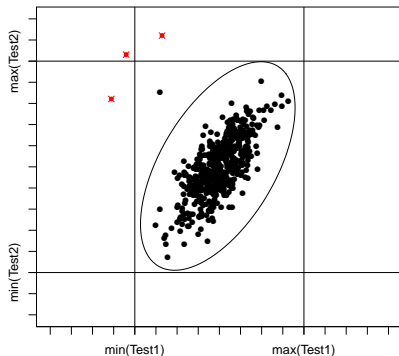
- ▶ Checking for **minimum** and **maximum** in each test result.
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- ▶ **Not all** anomalies can be detected.

Multivariate anomaly detection: an example

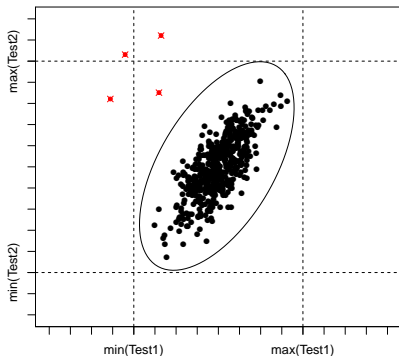


- **Mahalanobis distance** of an observation $\mathbf{x} \in \mathbb{R}^2$ (from the mean) is defined as follows:

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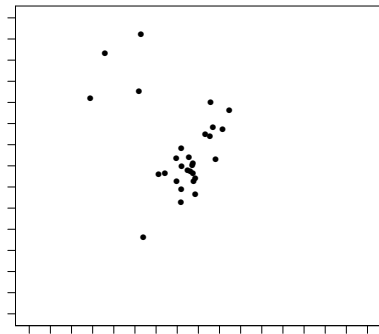
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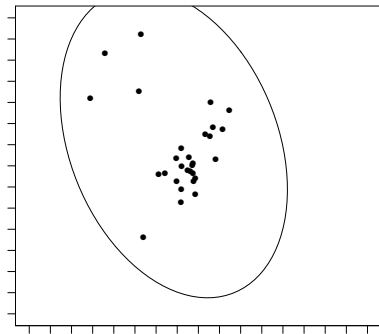
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Multivariate anomaly detection: robustness

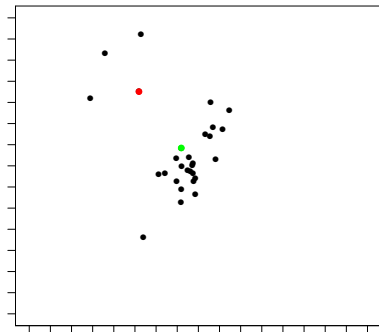


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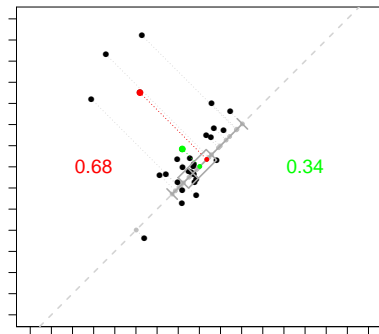
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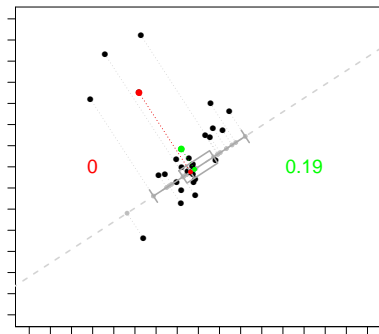
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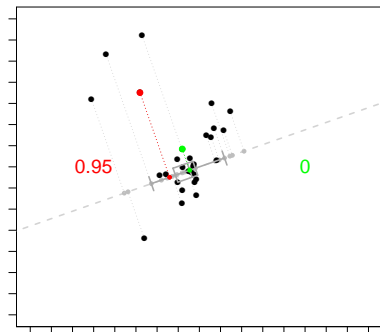
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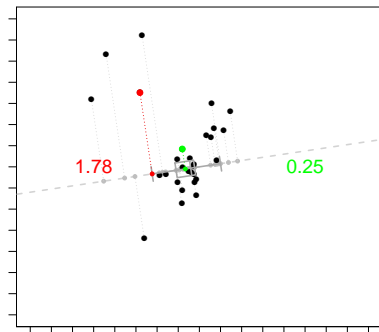
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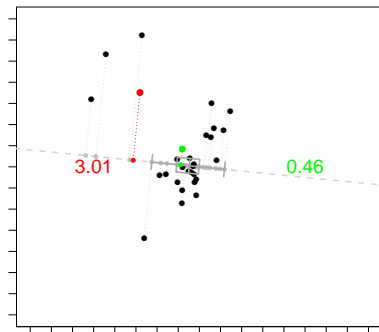
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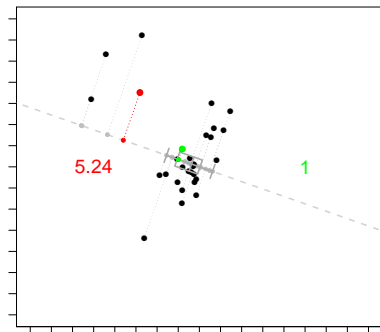
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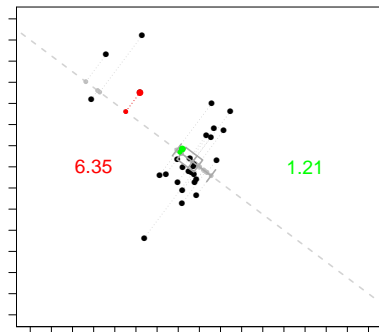
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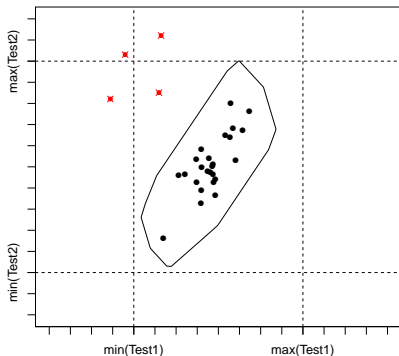
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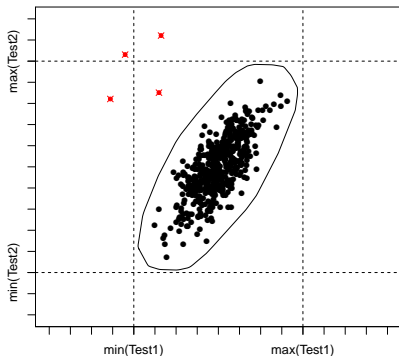


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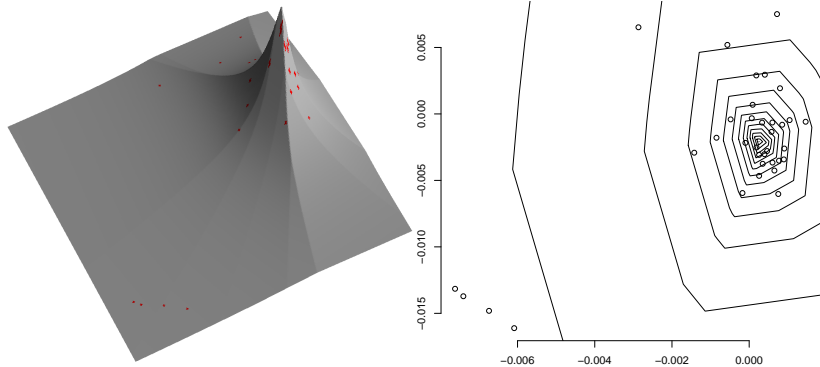
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Projection depth (Zuo & Serfling, 2000)



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

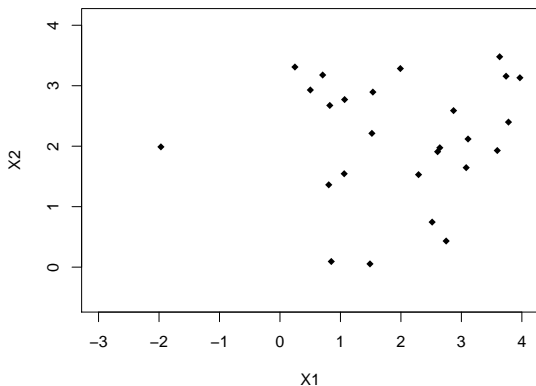
Exploiting the idea of spatial quantiles of Chaudhuri (1996) and Koltchinskii (1997), Vardi & Zhang (2000) and Serfling (2002) formulate the **spatial depth** (also L_1 -depth) as:

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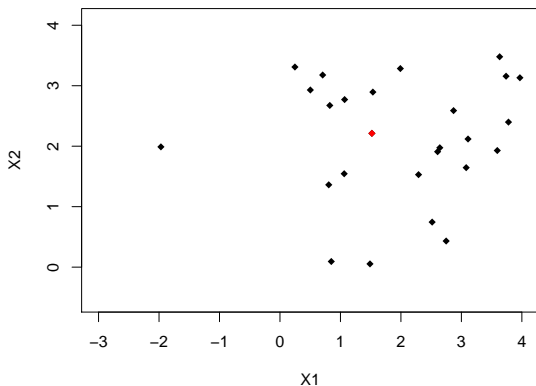
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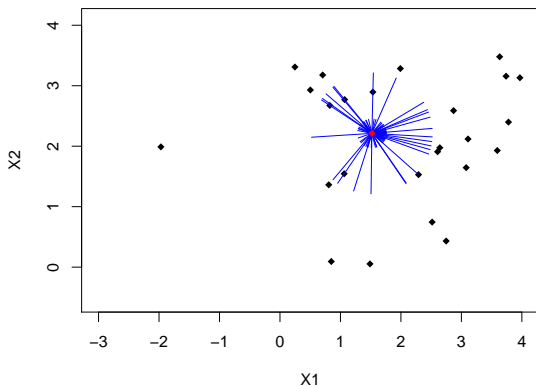
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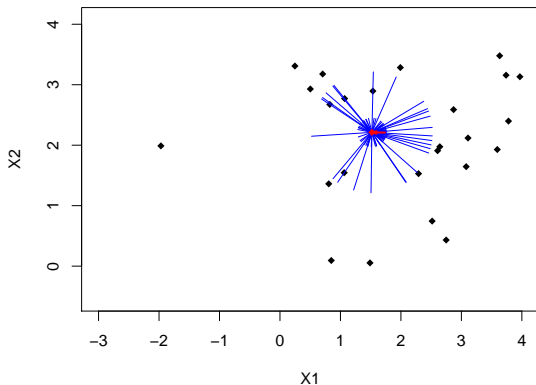
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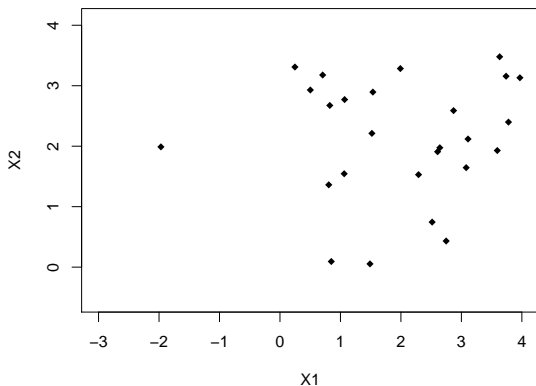
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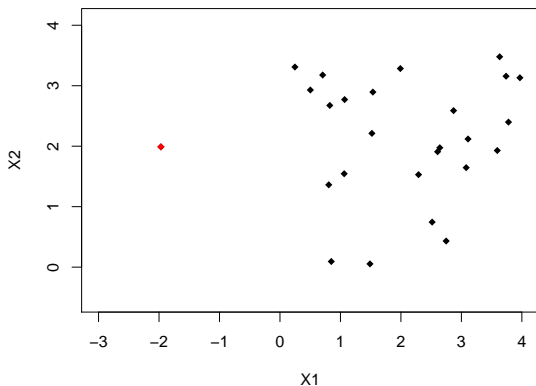
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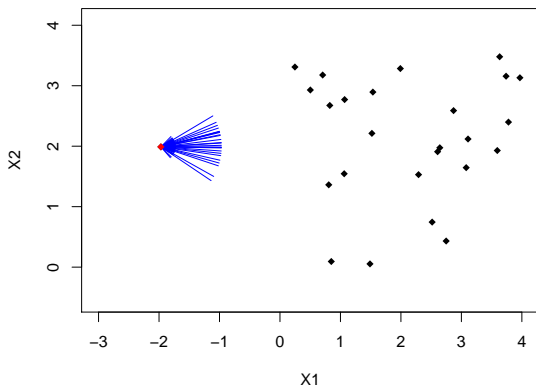
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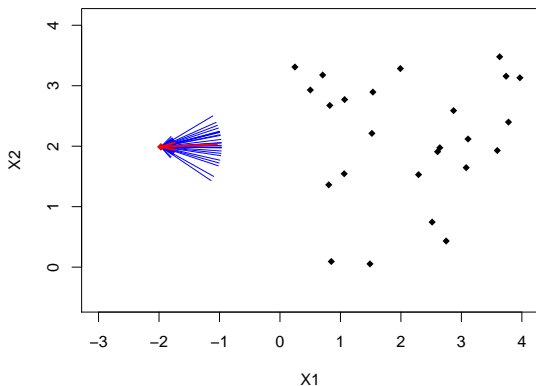
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$$D^{spt}(\mathbf{x}|X) = 1 - \left\| \mathbb{E} \left[\frac{\mathbf{x} - X}{\|\mathbf{x} - X\|} \right] \right\| \quad \text{with} \quad \frac{\mathbf{x} - X}{\|\mathbf{x} - X\|} = 0 \quad \text{if} \quad \mathbf{x} - X = \mathbf{0}.$$



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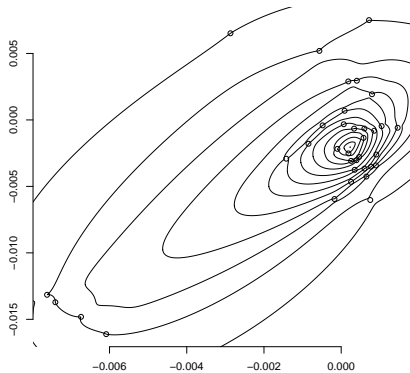
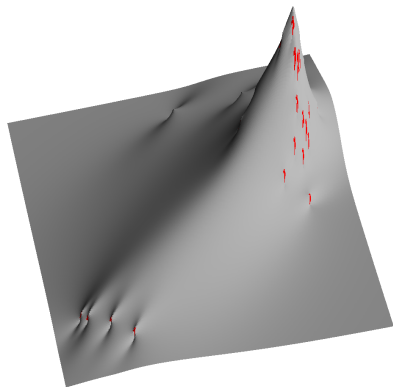
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- ▶ if $\boldsymbol{\Sigma}$ is orthogonal, satisfies **D2iso** only;
- ▶ with **D2iso** its maximum (say \mathbf{x}^*) is referred to as **spatial median**, a multivariate location estimator having asymptotic breakdown point of 0.5.

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



Contents

Introduction

Non-parametric approaches

- One-class support vector machines

- Local outlier factor

- Isolation forest

Systematic orderings: data depth

- The notion of data depth

- The Tukey depth function

- Central regions

- Further depth notions

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.
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- ▶ Mosler, K. (2013). Depth statistics. In: *Robustness and Complex Data Structures: Festschrift in Honour of Ursula Gather*, 17–34.

Practical session (part I)

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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