

Multivariate and functional anomaly detection

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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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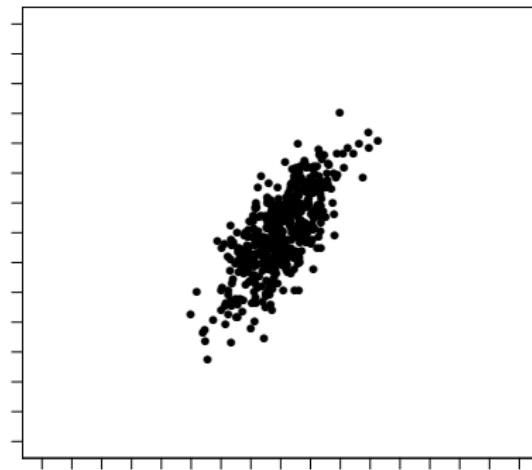
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- Integrated data depth
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Practical session

A real task

Regard two measurements during a test in a production process:

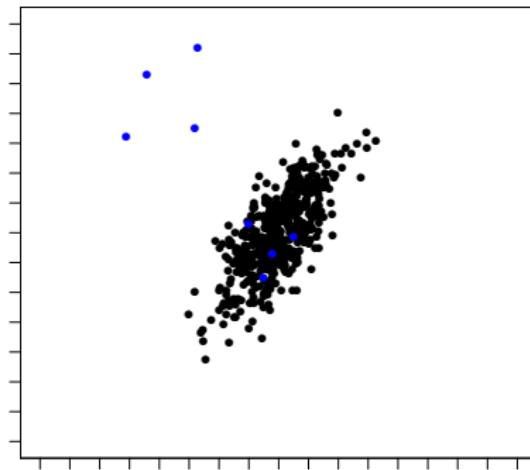


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- ▶ detect **anomalies** in the given data.

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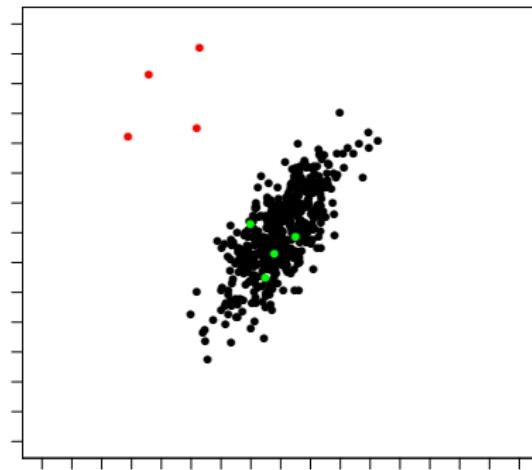
- ▶ detect **anomalies** in the given data.

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

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:

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

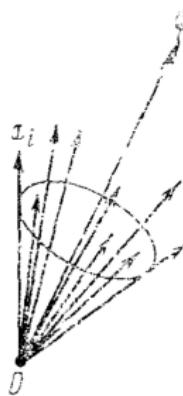


Рис. 24.

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

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

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Soft margin (Cortes, Vapnik; 1995):

- ▶ Allow for a portion of points from \mathcal{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

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

Idea 1: Separate points from the origin.

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This can be formulated as a quadratic programming problem

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

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

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The solution (ψ^*, ξ^*, ρ^*) yields the following decision function:

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

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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:

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

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

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

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The **decision function** is then:

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

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.

$$\min_{R \in \mathbb{R}, \xi \in \mathbb{R}^n, \mathbf{c} \in \mathcal{H}} R^2 + \frac{1}{\nu n} \sum_{i=1}^n \xi_i$$

subject to $\|\Phi(\mathbf{x}_i) - \mathbf{c}\| \leq R^2 + \xi_i, \quad \xi_i \geq 0 \text{ for } i = 1, \dots, n.$

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This leads to the dual:

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

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

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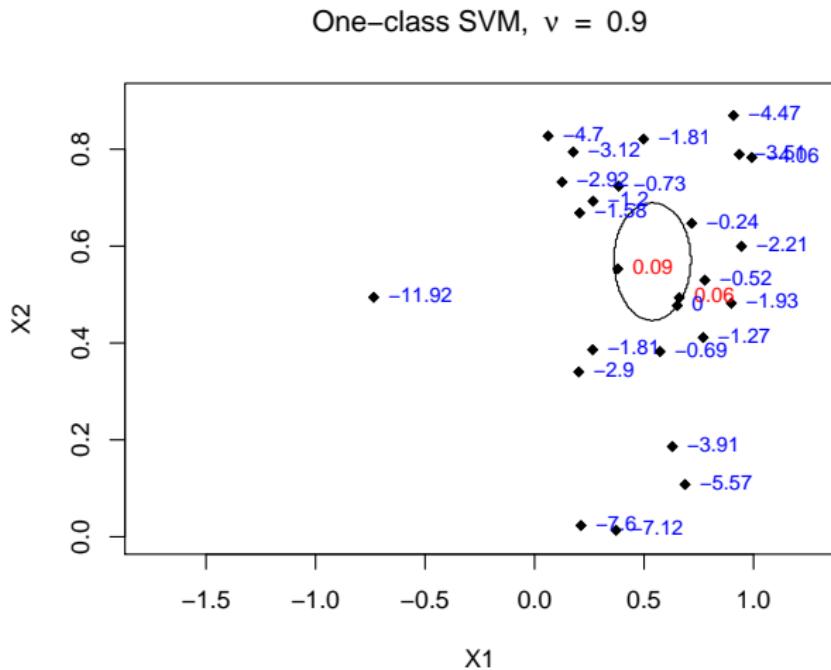
which leads to the **decision function**:

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

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 $0 < \alpha_k < 1/(\nu n)$.

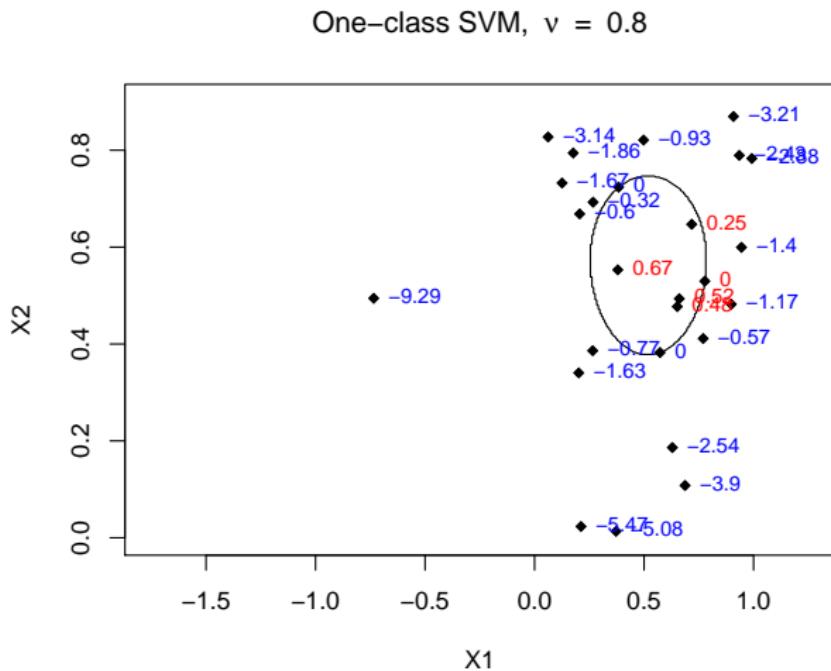
One-class support vector machines (Schölkopf, Platt, Shawe-Taylor, Smola, Williamson; 1999)

Illustration: Case 1



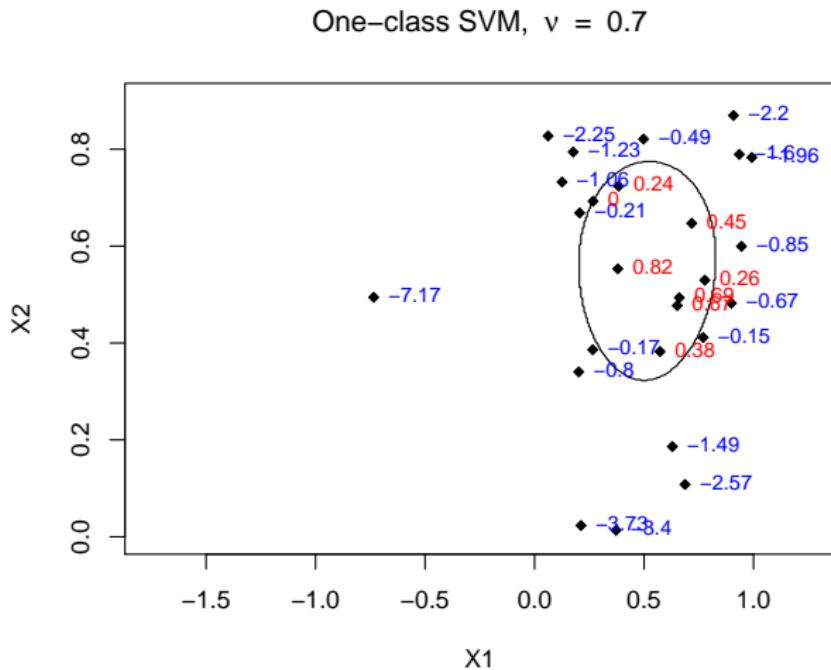
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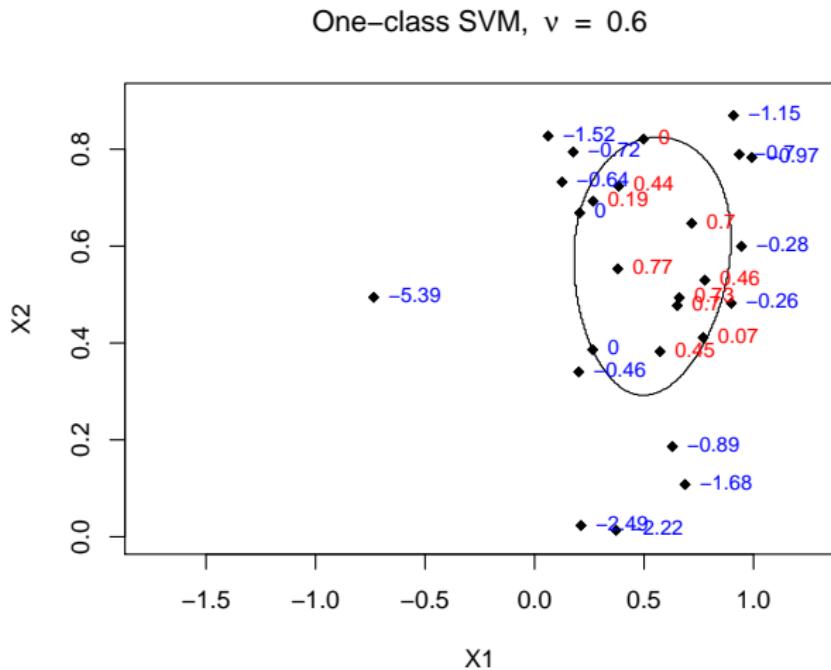
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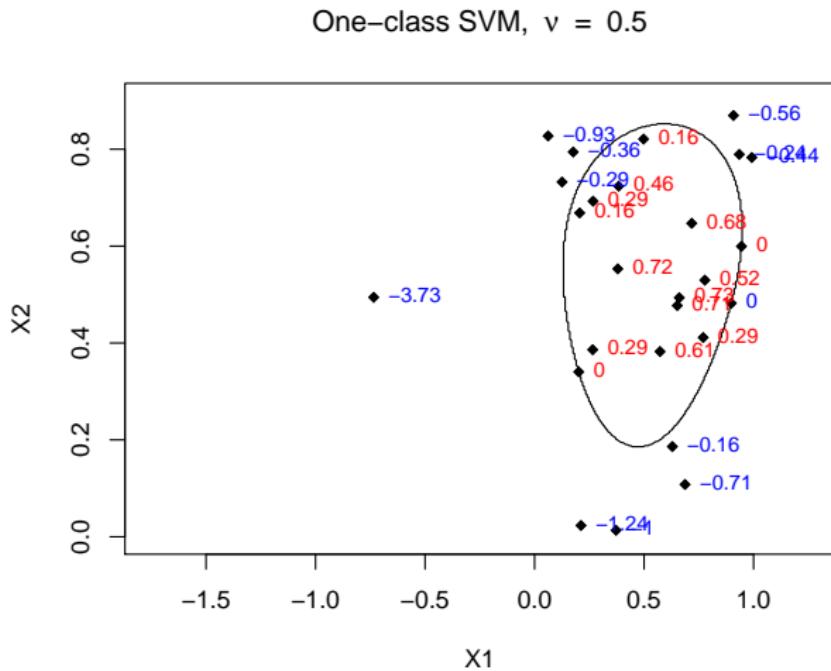
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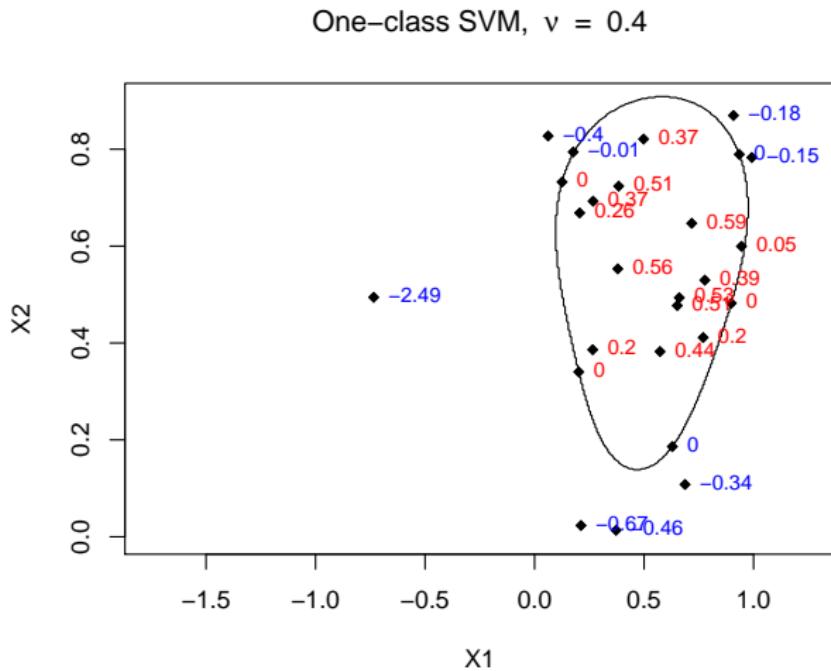
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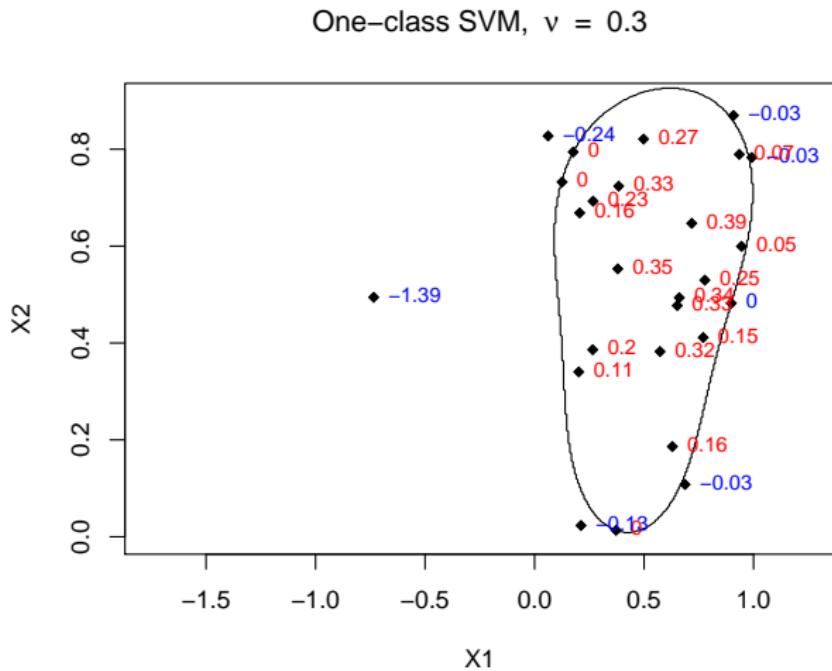
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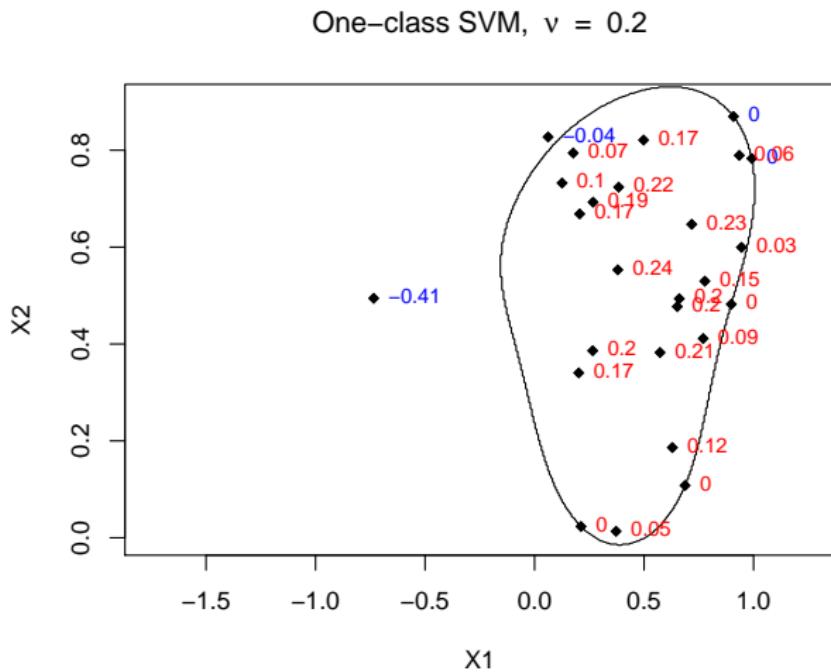
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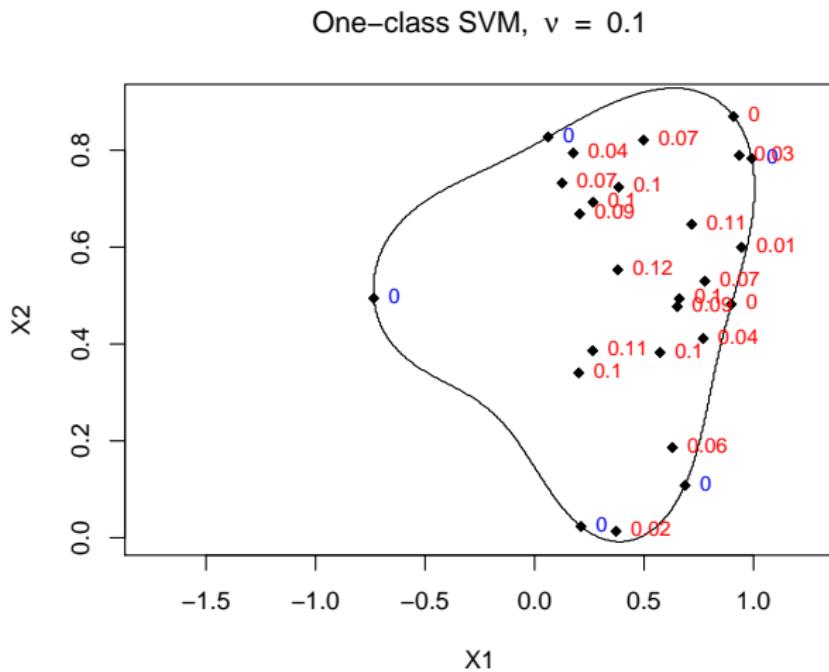
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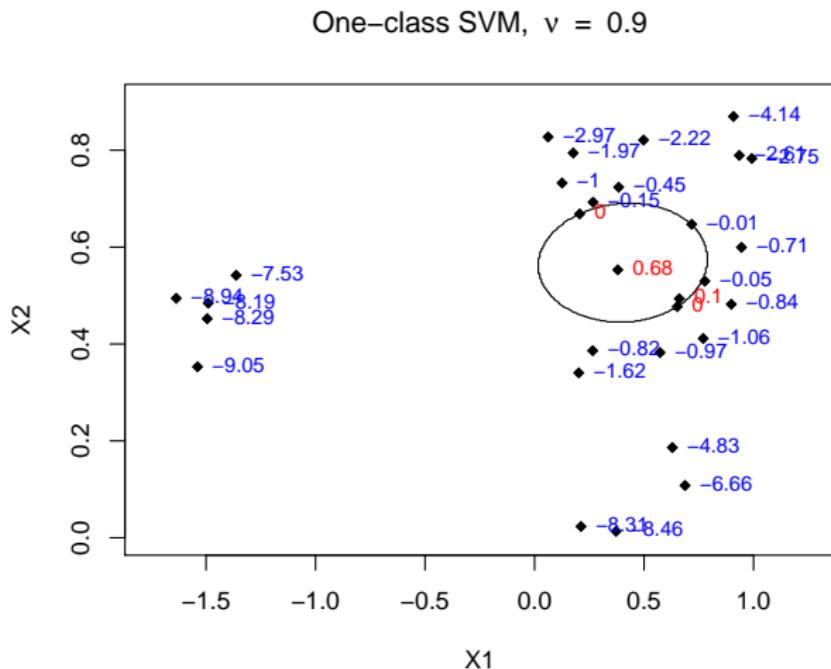
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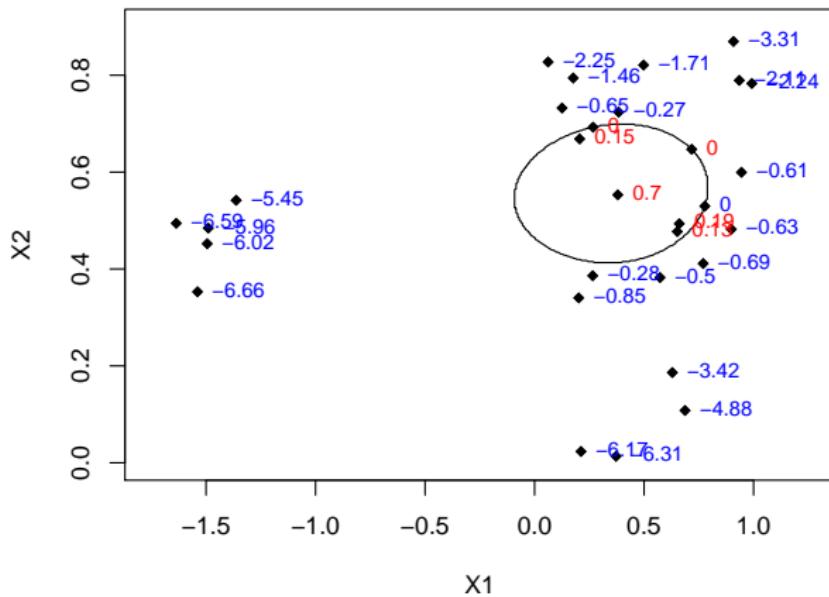
Illustration: Case 2



One-class support vector machines (Schölkopf, Platt, Shawe-Taylor, Smola, Williamson; 1999)

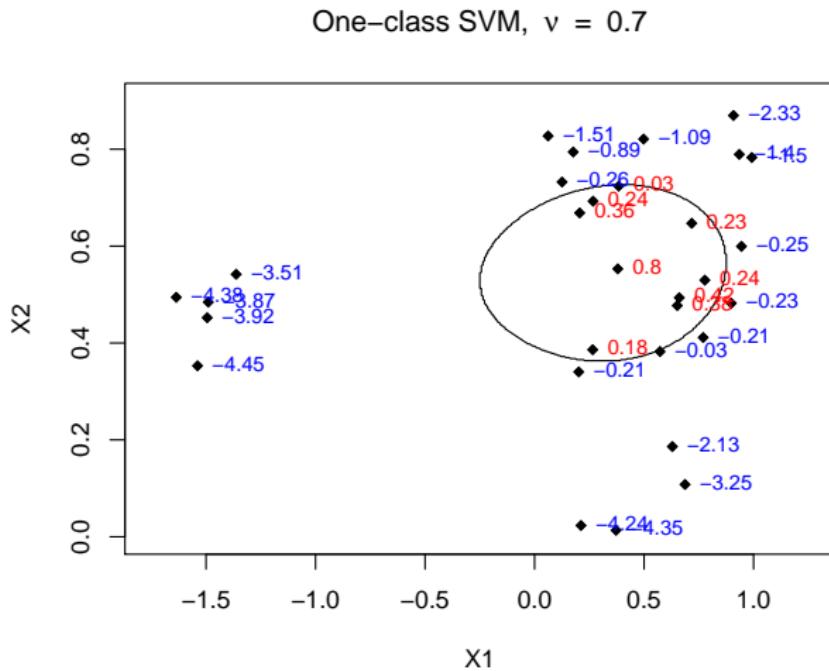
Illustration: Case 2

One-class SVM, $\nu = 0.8$



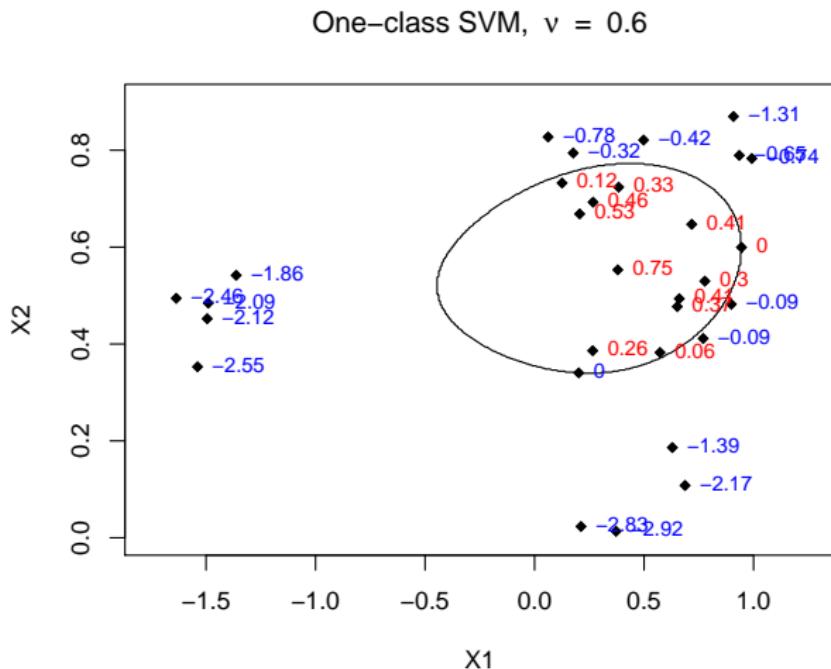
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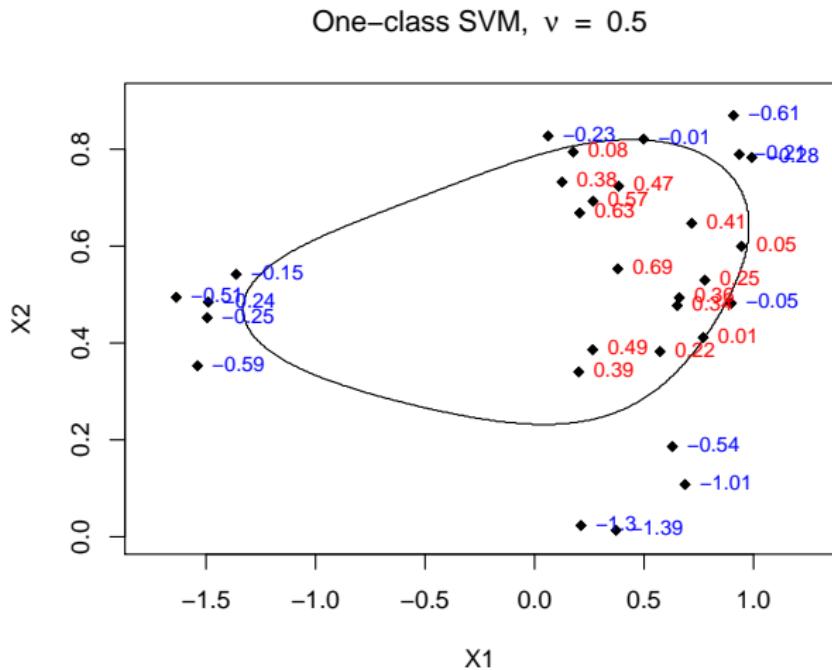
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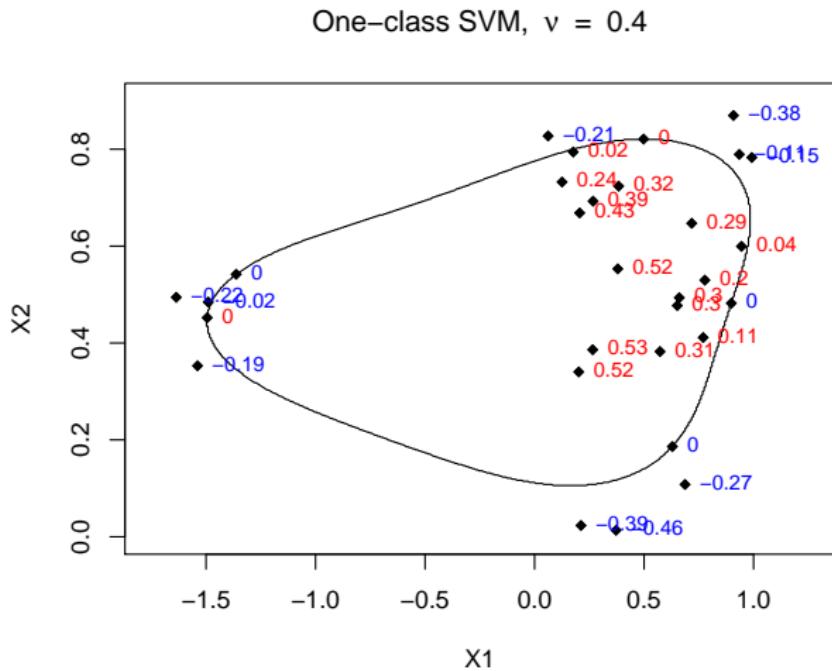
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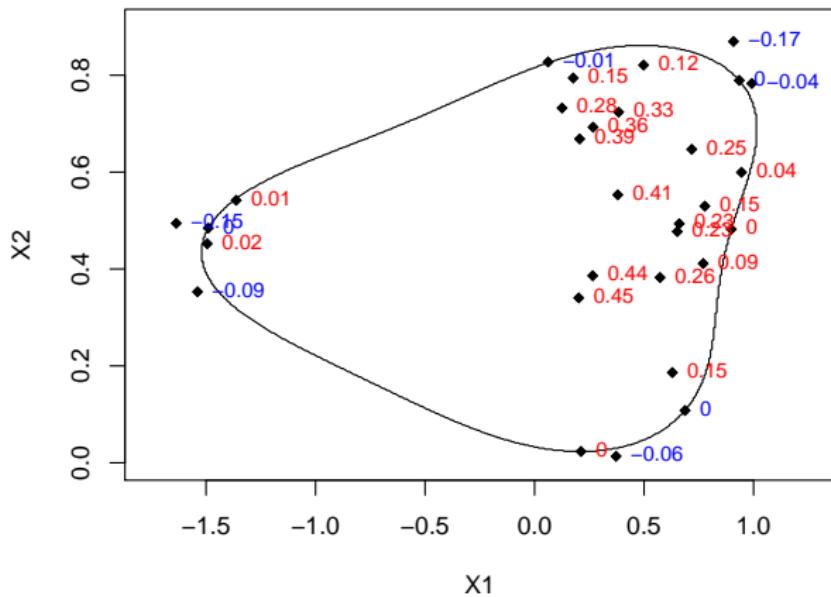
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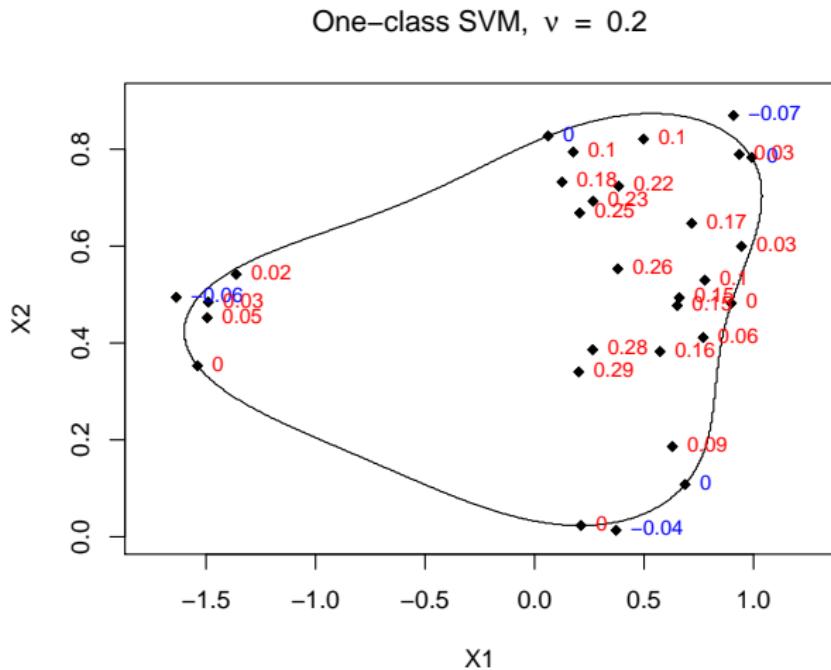
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One-class SVM, $\nu = 0.3$



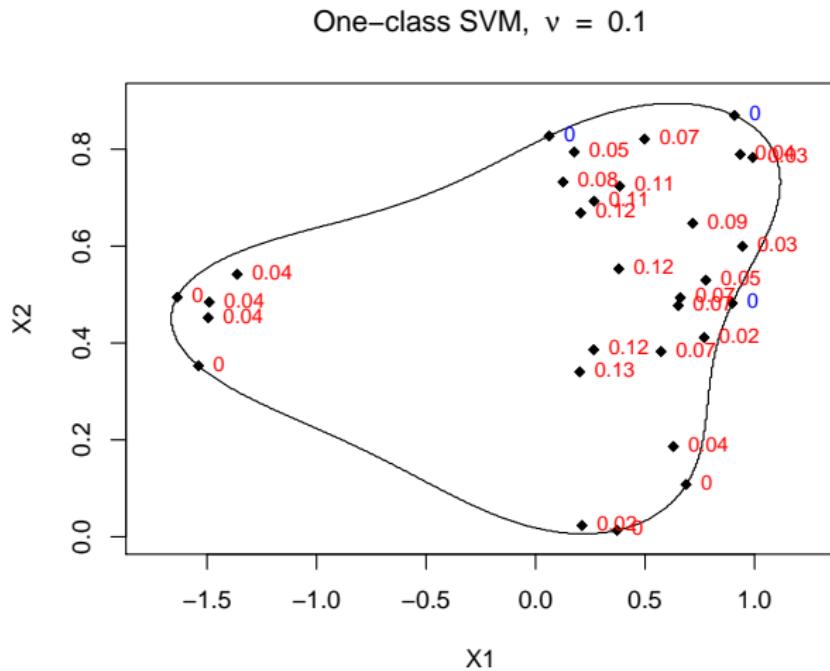
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Local outlier factor (Breunig, Kriegel, Ng, Sander; 2000)

k -distance of a point x :

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

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

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(=Distance from x to its k th neighbor.)

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(=Distance from x to its k th neighbor.)

k -neighborhood of a point x :

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

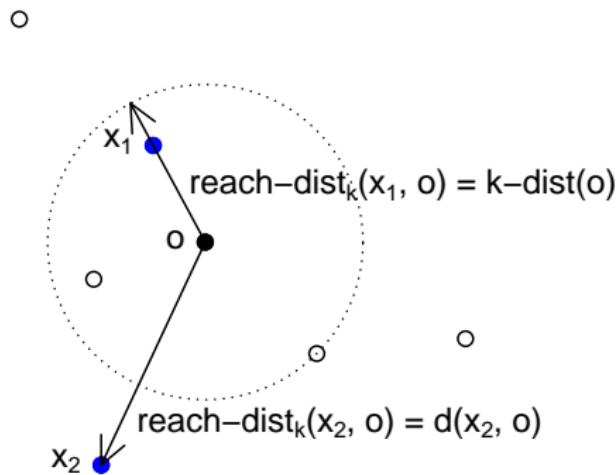
$$N_k(x) = \{q \in X \setminus \{x\} \mid d(x, q) \leq k\text{-dist}(x)\}.$$

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

Reachability distance of order k of point x w.r.t. point o :

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

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



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Local reachability density of a point x :

The local reachability density of x is defined as:

$$lrd_k(x) = \frac{|N_k(x)|}{\sum_{o \in N_k(x)} \text{reach-dist}_k(x, o)}.$$

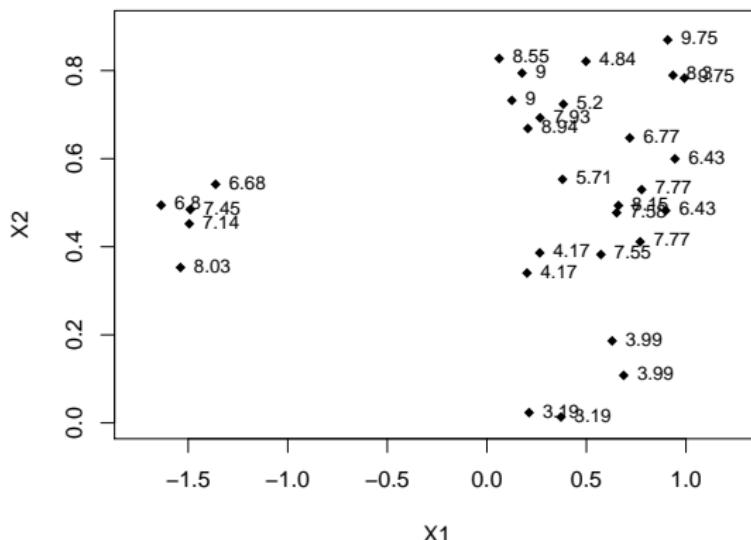
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Local reachability density, $k = 2$



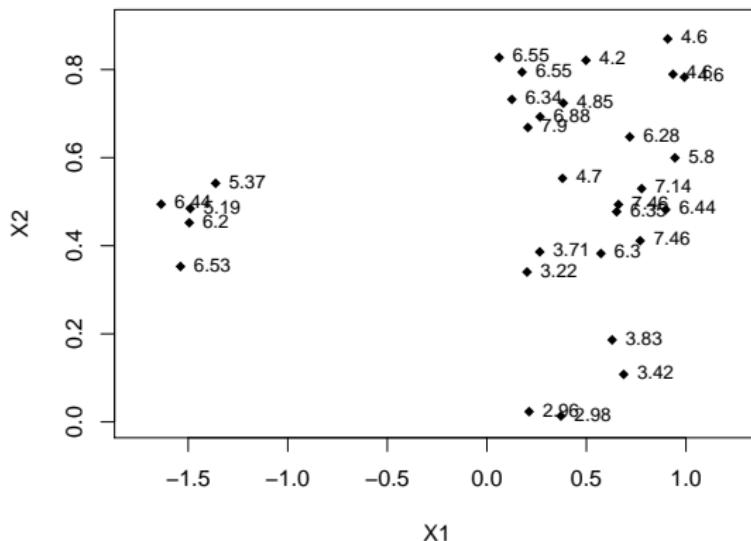
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Local reachability density, $k = 3$



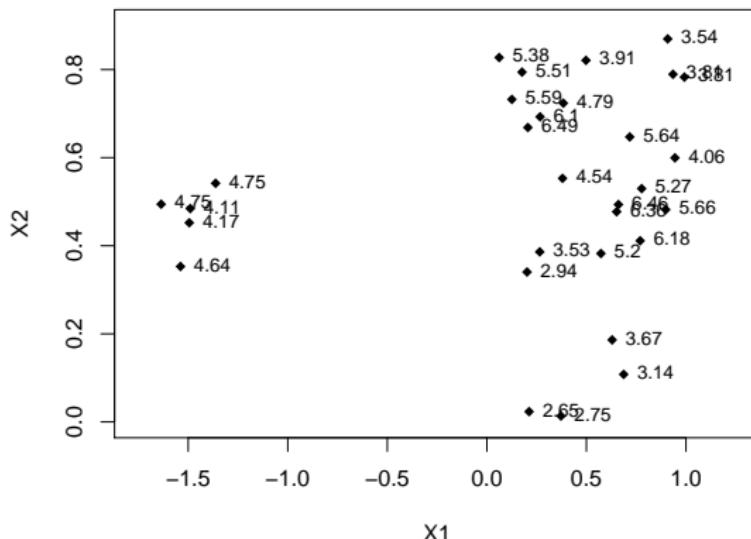
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Local reachability density, $k = 4$



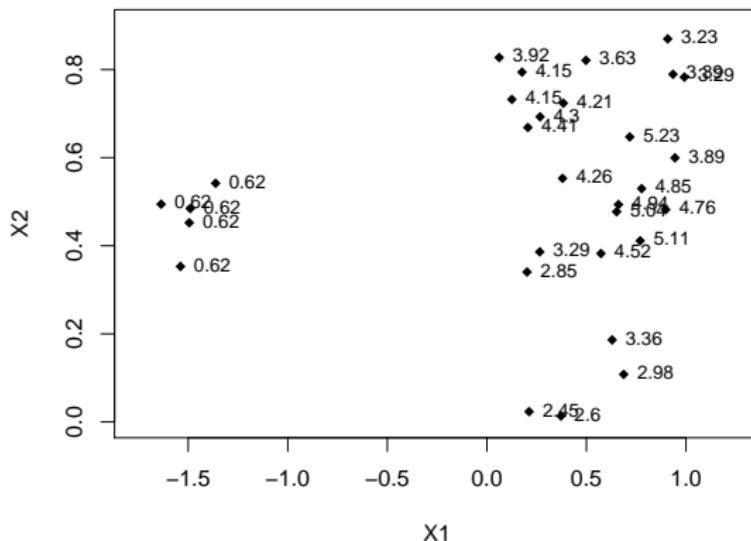
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Local reachability density, $k = 5$



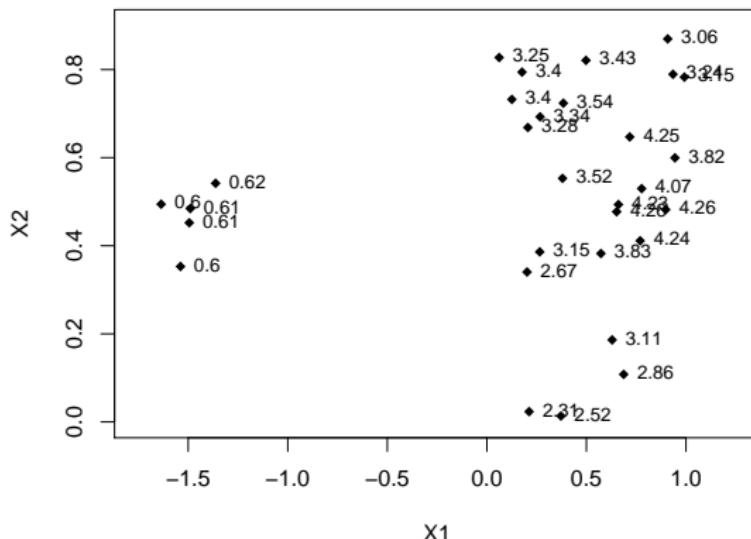
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Local reachability density, $k = 6$



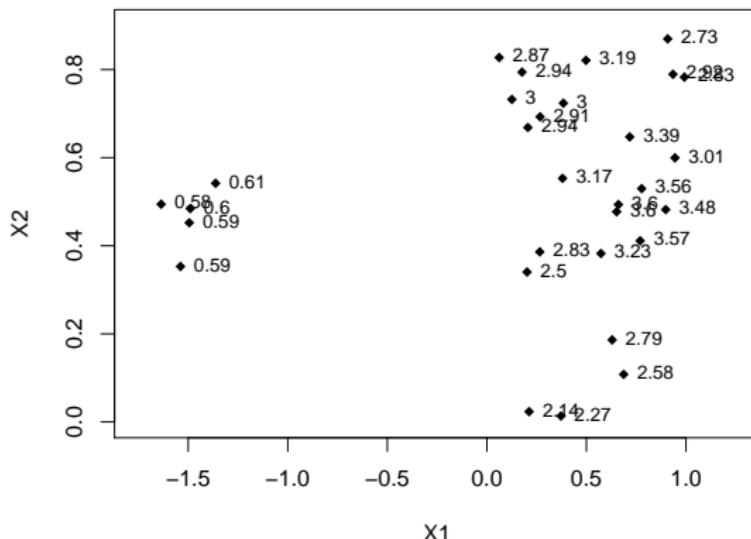
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Local reachability density, $k = 7$



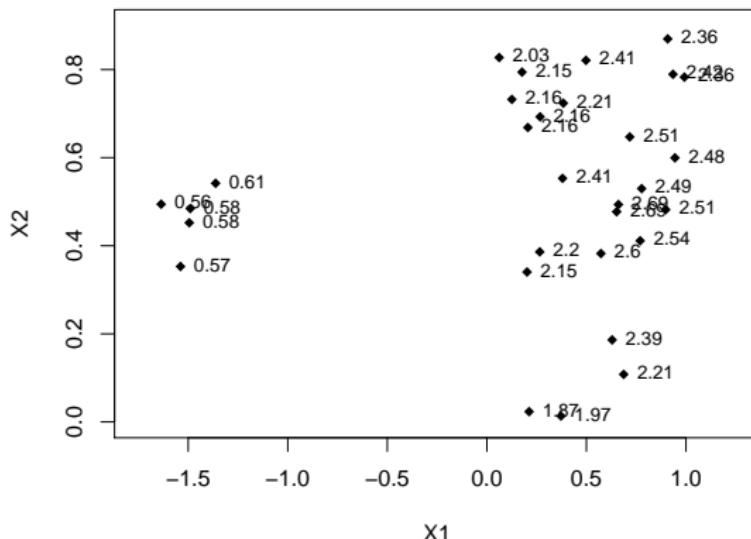
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Local reachability density, k = 10



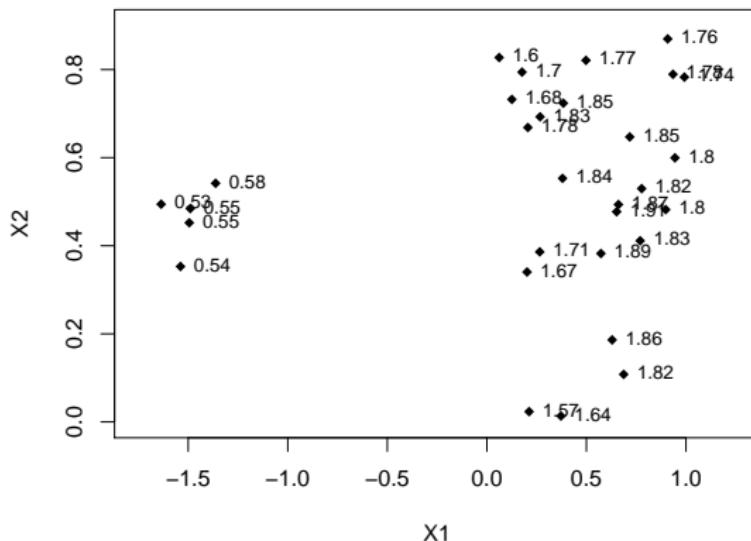
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Local reachability density, k = 15



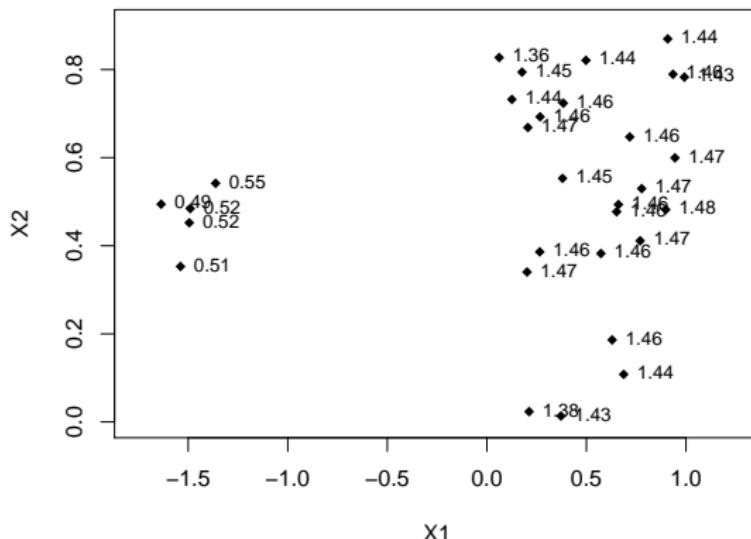
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Local reachability density, k = 20



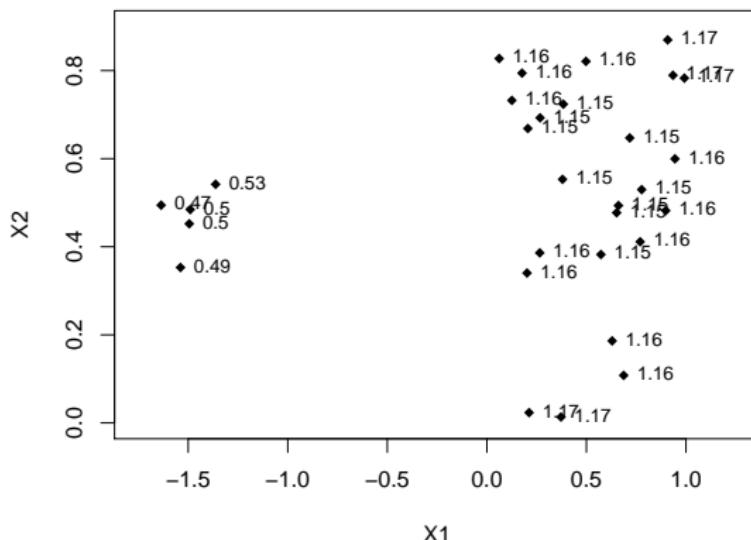
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Local reachability density, k = 24



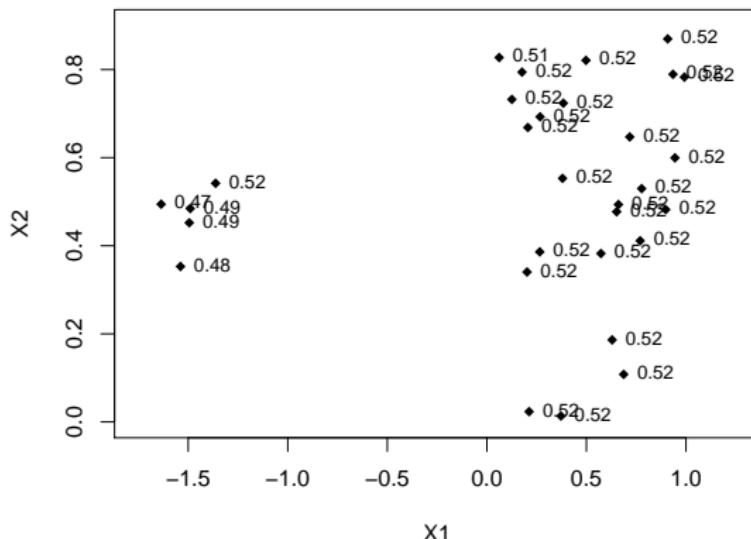
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Local reachability density, k = 25



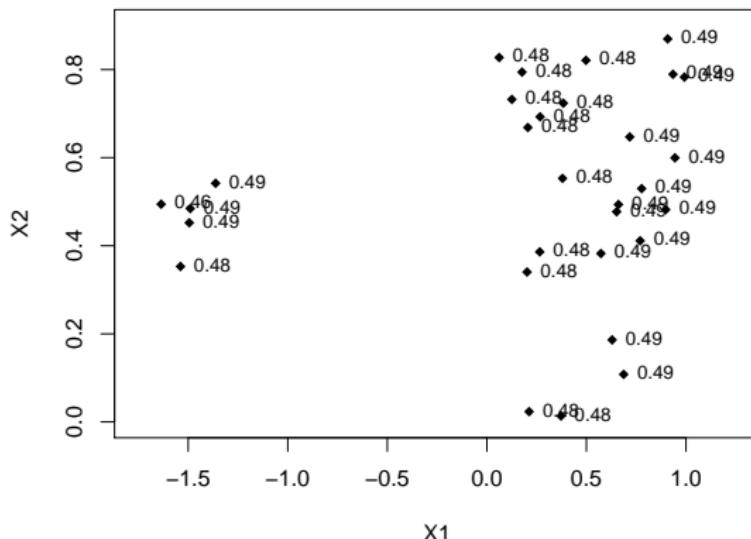
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Local reachability density, k = 26



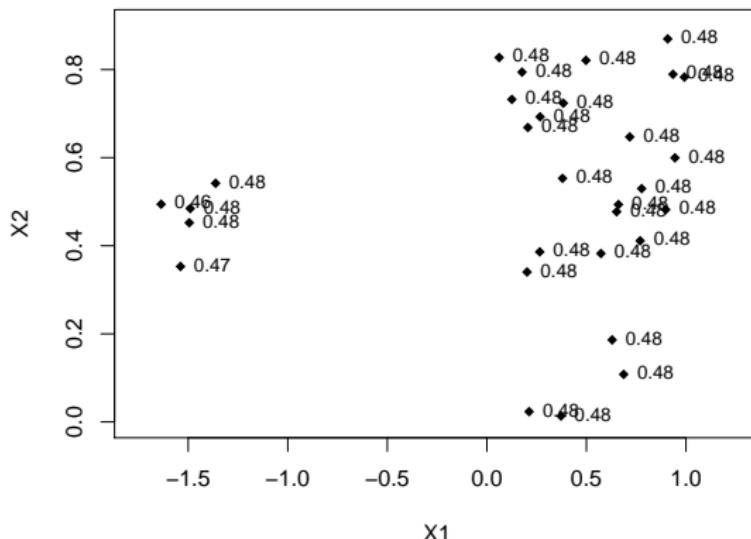
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Local reachability density, k = 27



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

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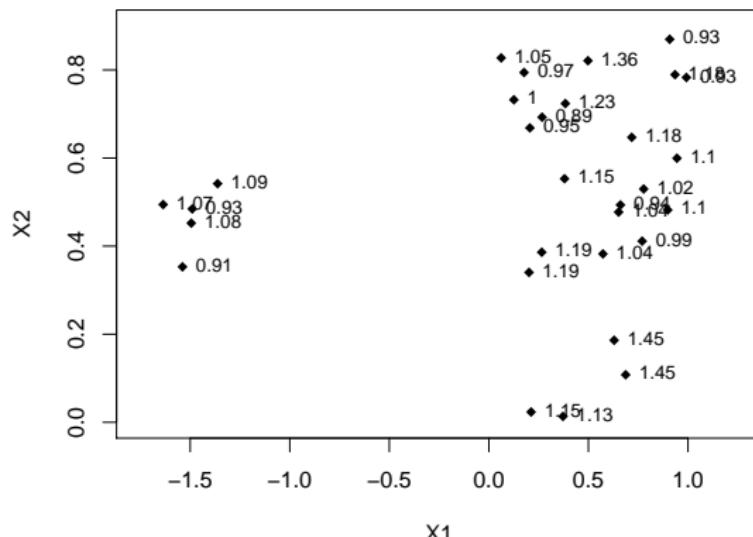
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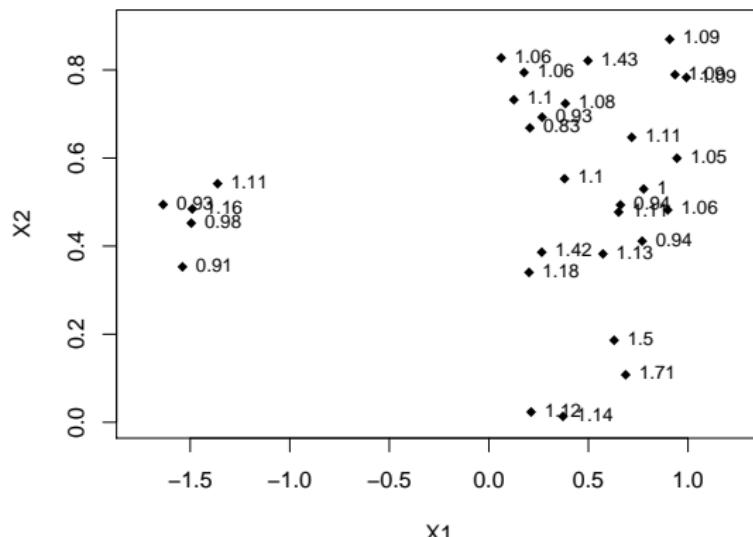
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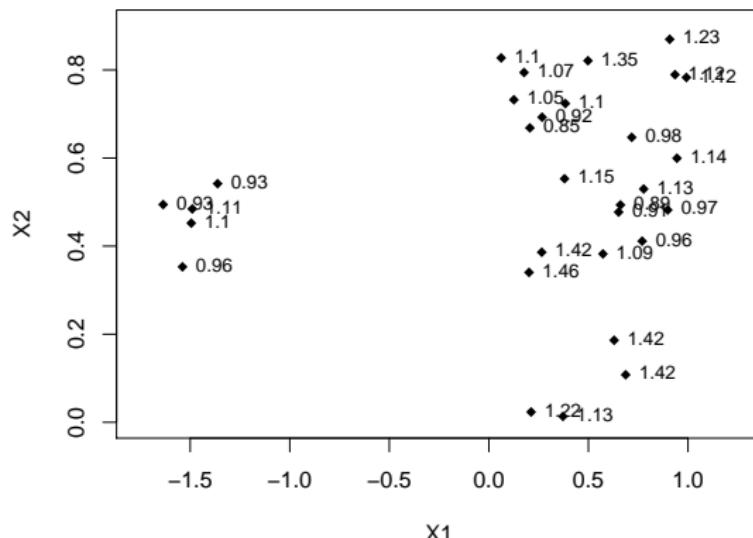
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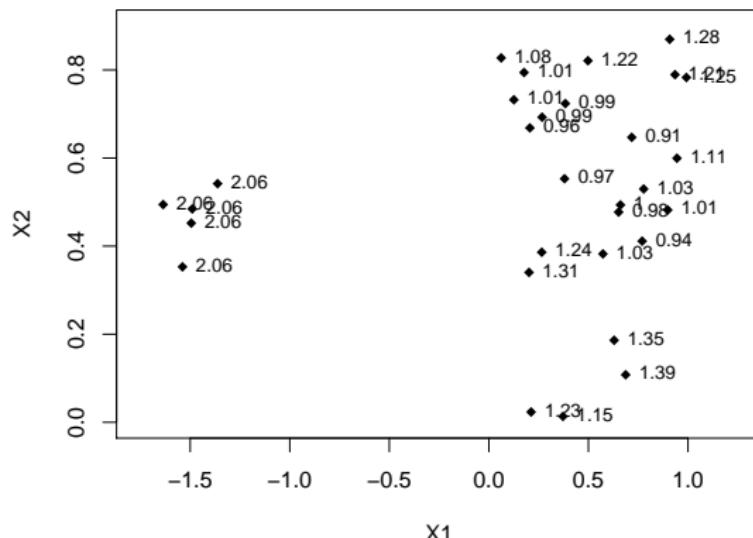
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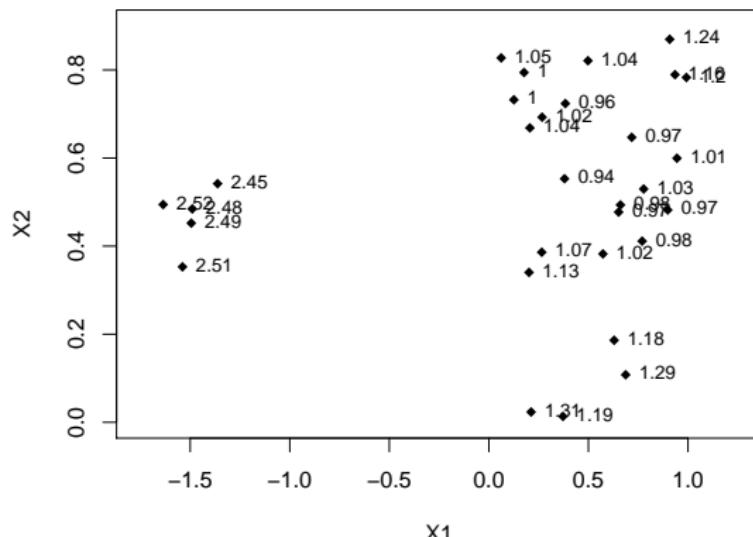
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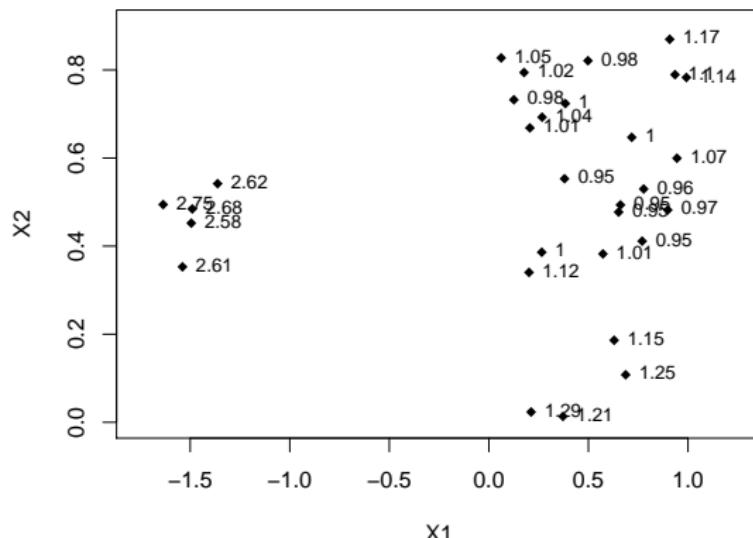
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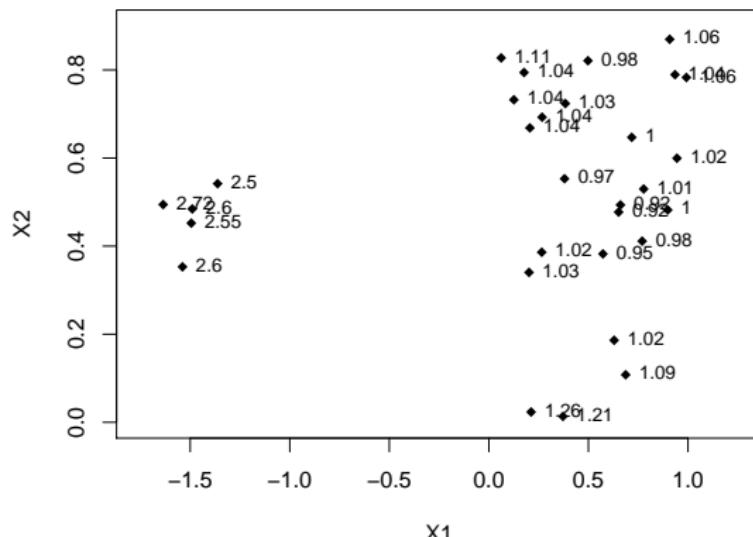
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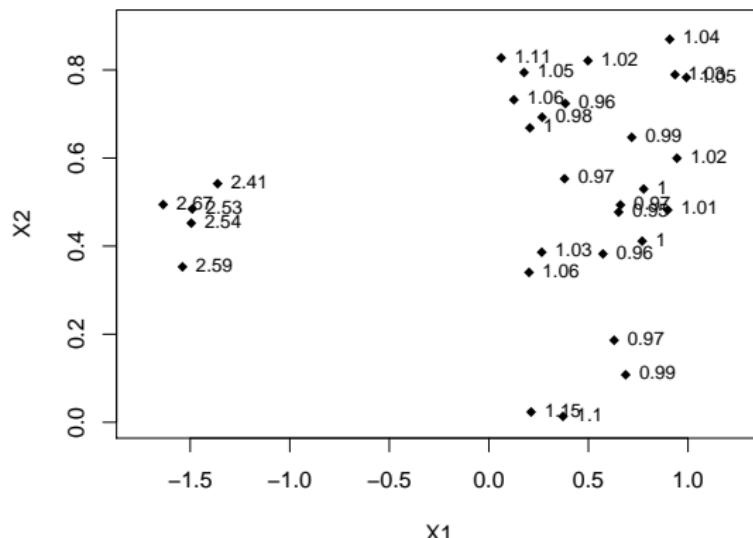
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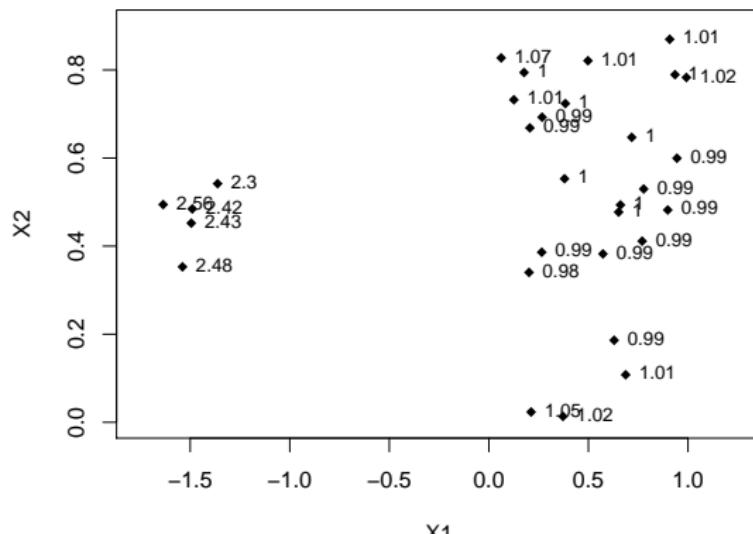
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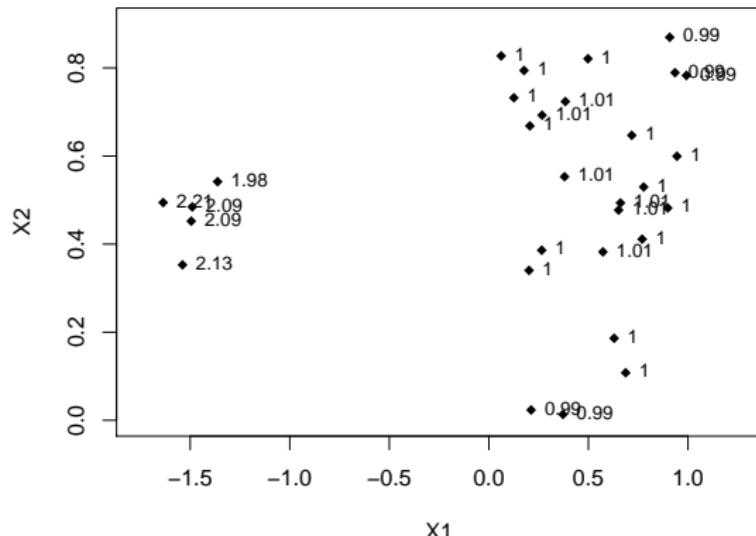
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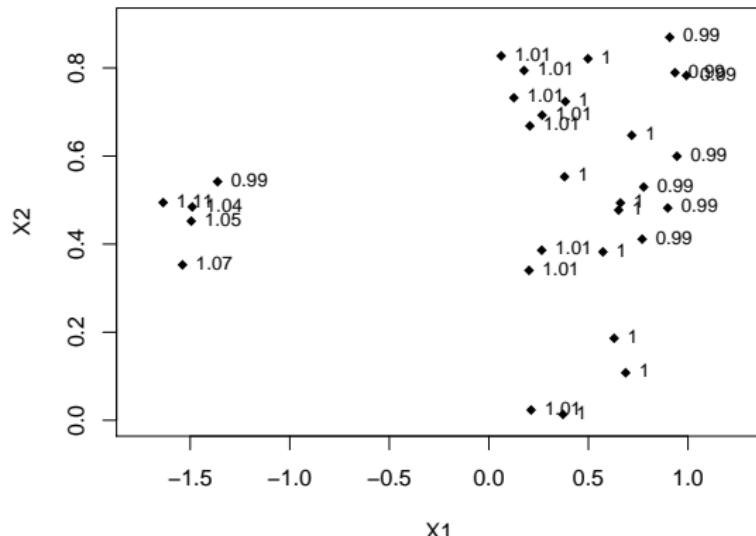
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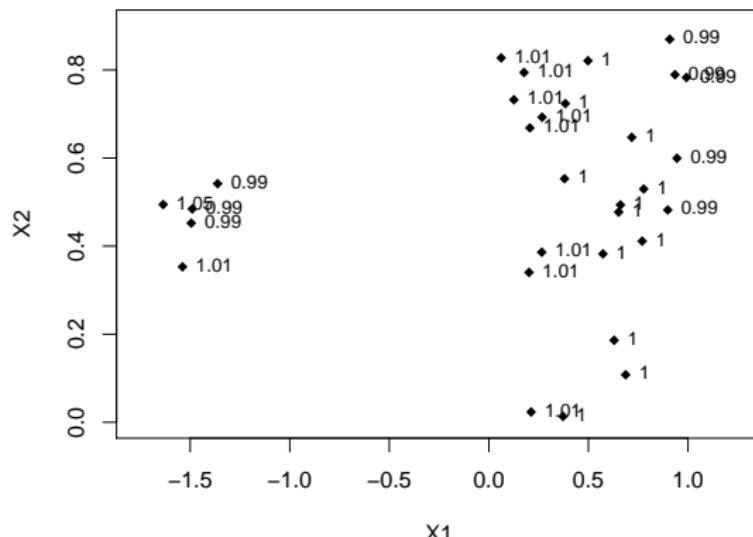
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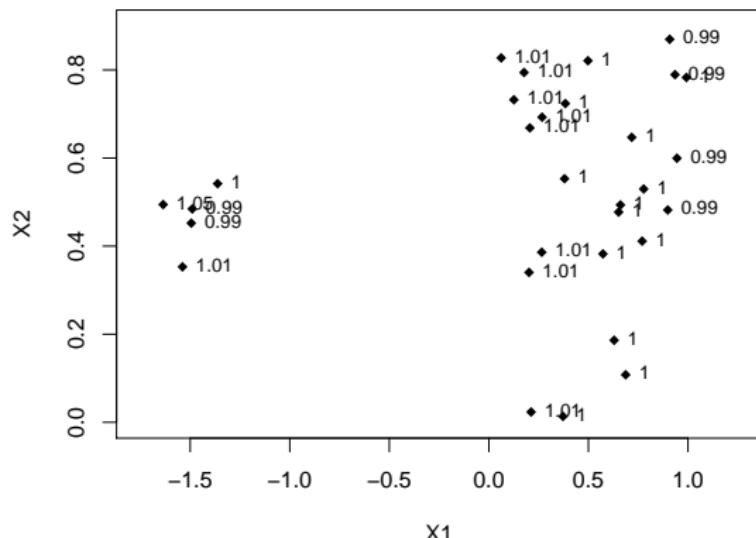
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Local outlier factor, k = 27



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Non-parametric approaches

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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).
- ▶ Since no supervised feedback is given, isolation forest is based on **purely random** (uniform) variable-based partitioning.

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- ▶ Since no supervised feedback is given, isolation forest is based on **purely random** (uniform) variable-based partitioning.
- ▶ **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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2. Choose randomly and uniformly a **split value** κ in the interval

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

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3. Form the children subsets

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

as well as the children training datasets

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

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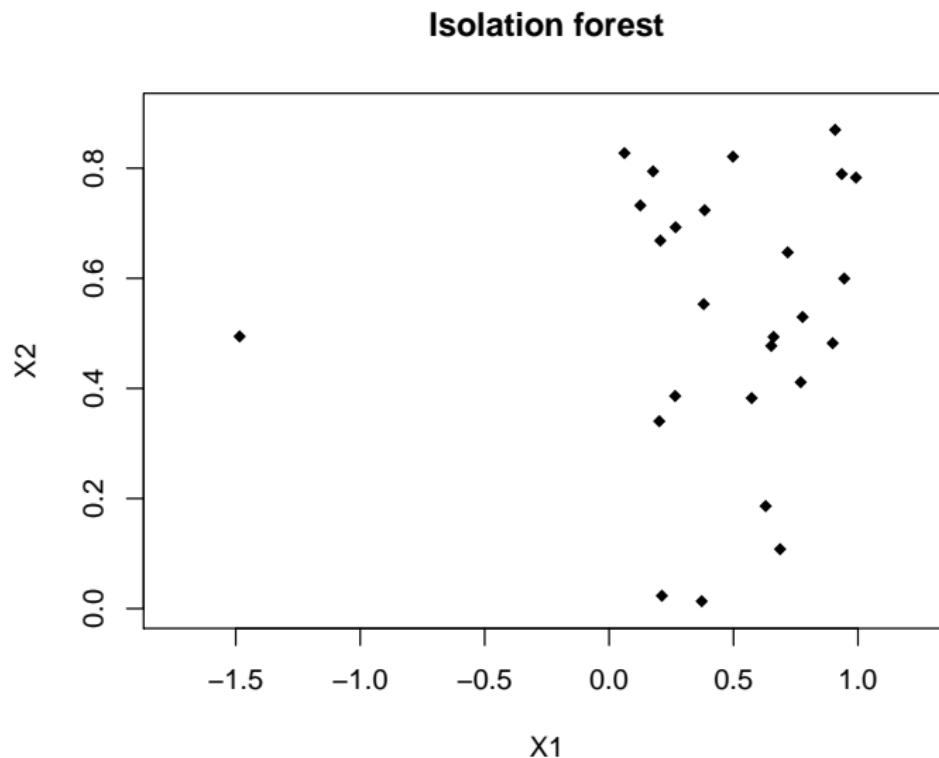
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Stop when only one observation is in each node: **isolation**.

Isolation forest (Liu, Ting, Zhou; 2008)

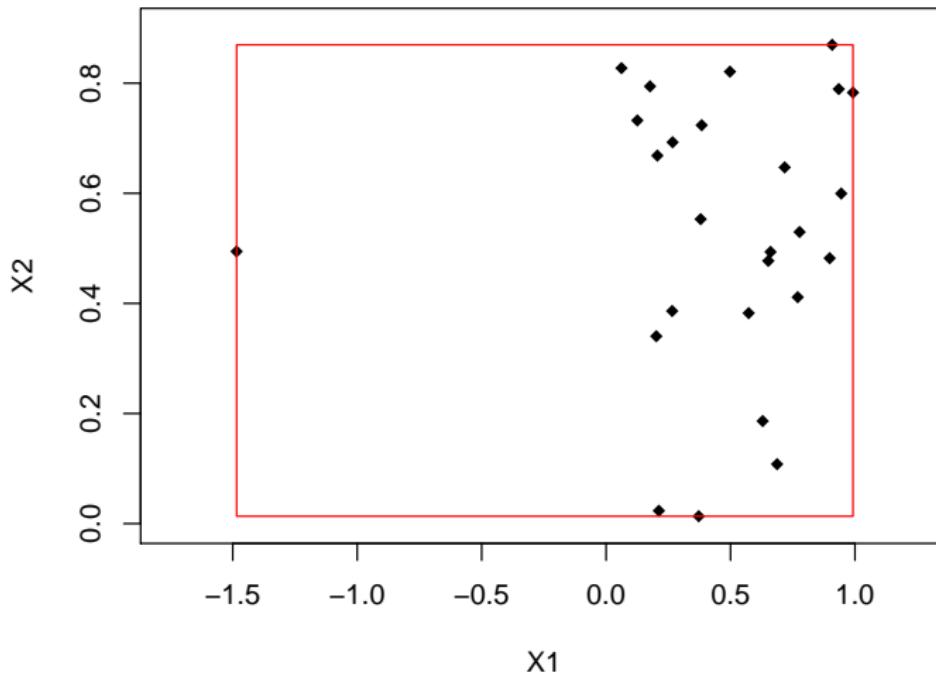
Illustration: Isolation tree



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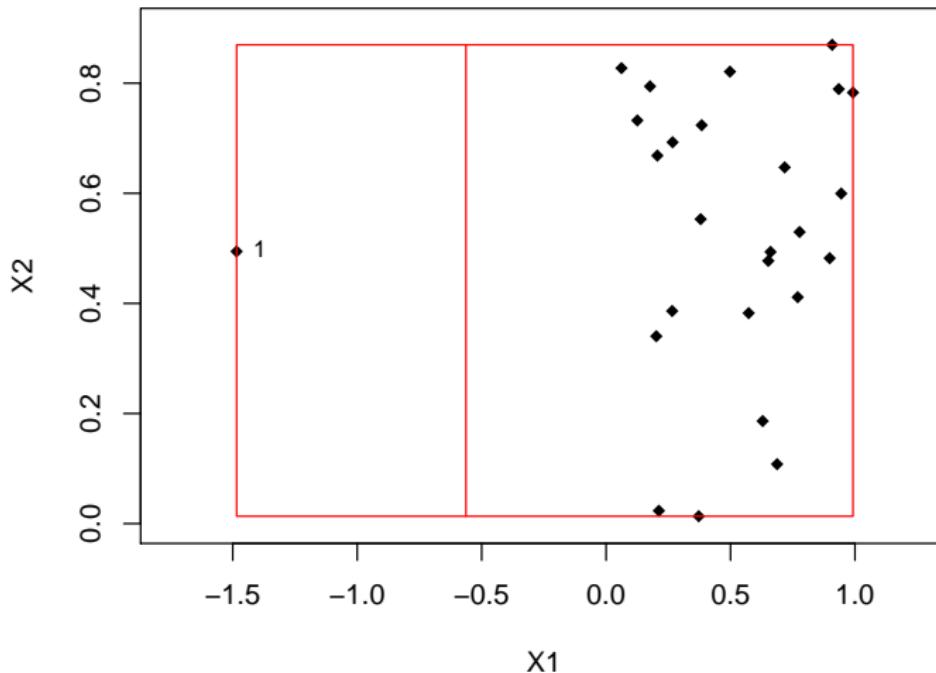
Isolation tree, split 0



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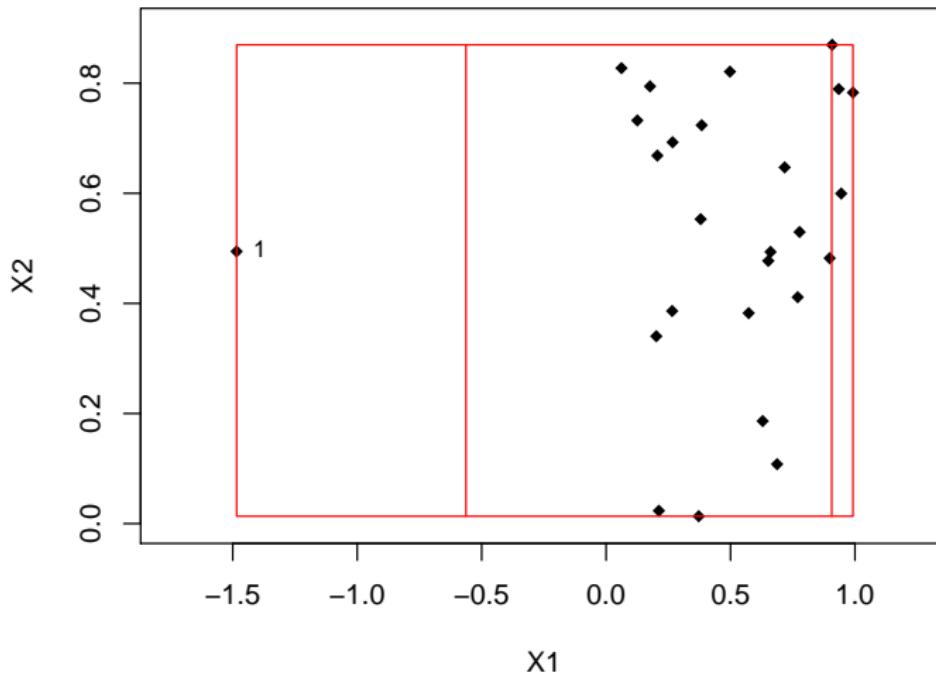
Isolation tree, split 1



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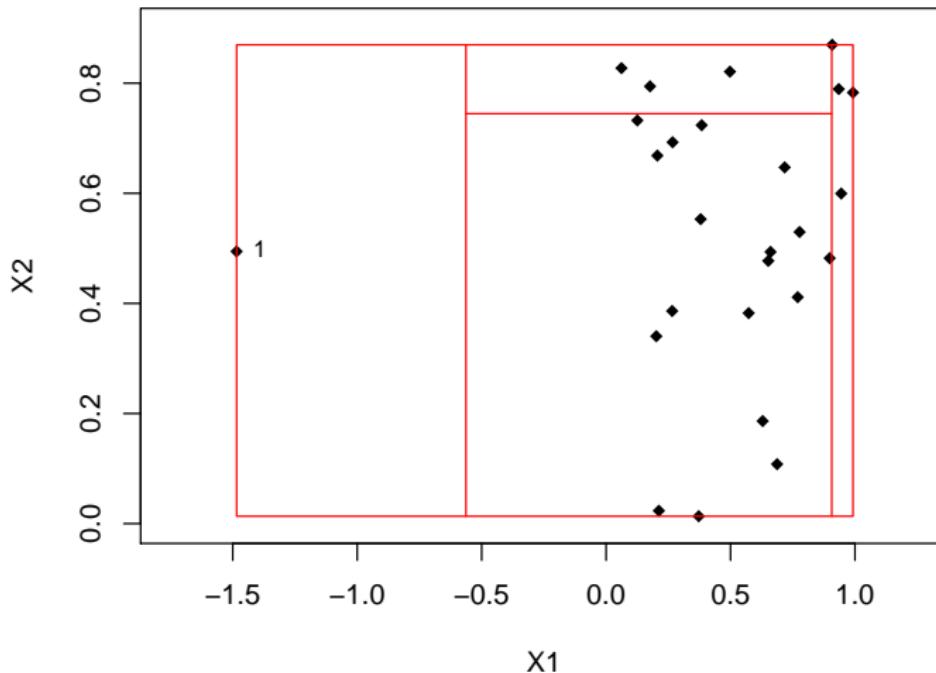
Isolation tree, split 2



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

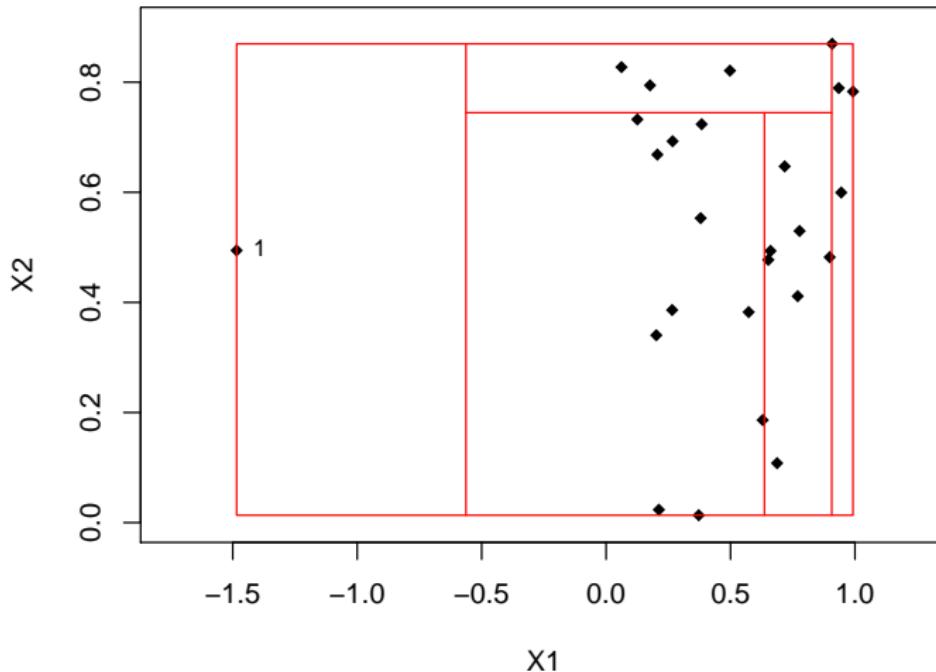
Isolation tree, split 3



Isolation forest (Liu, Ting, Zhou; 2008)

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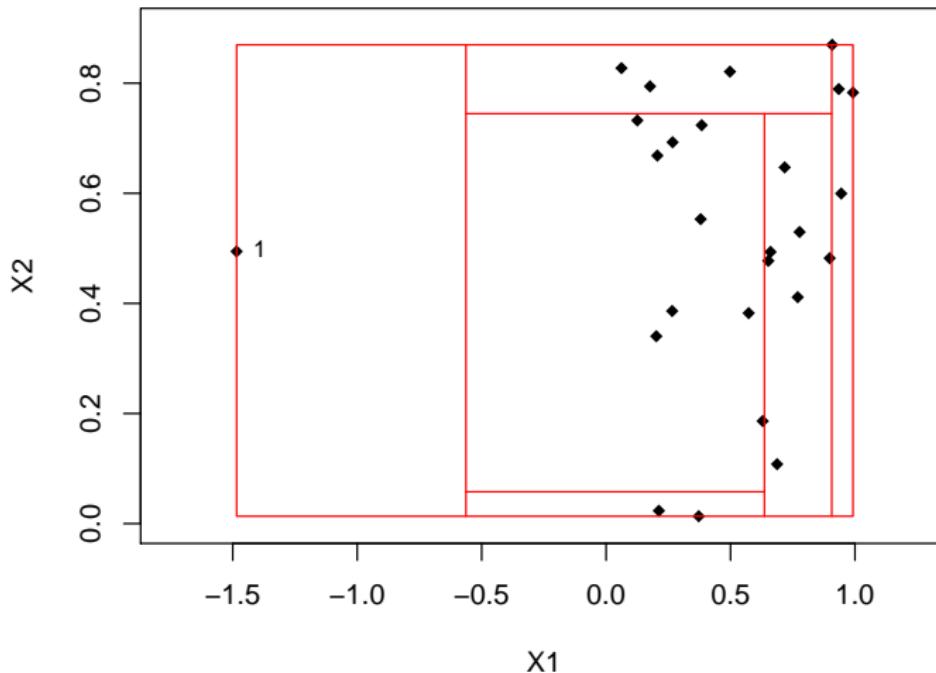
Isolation tree, split 4



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

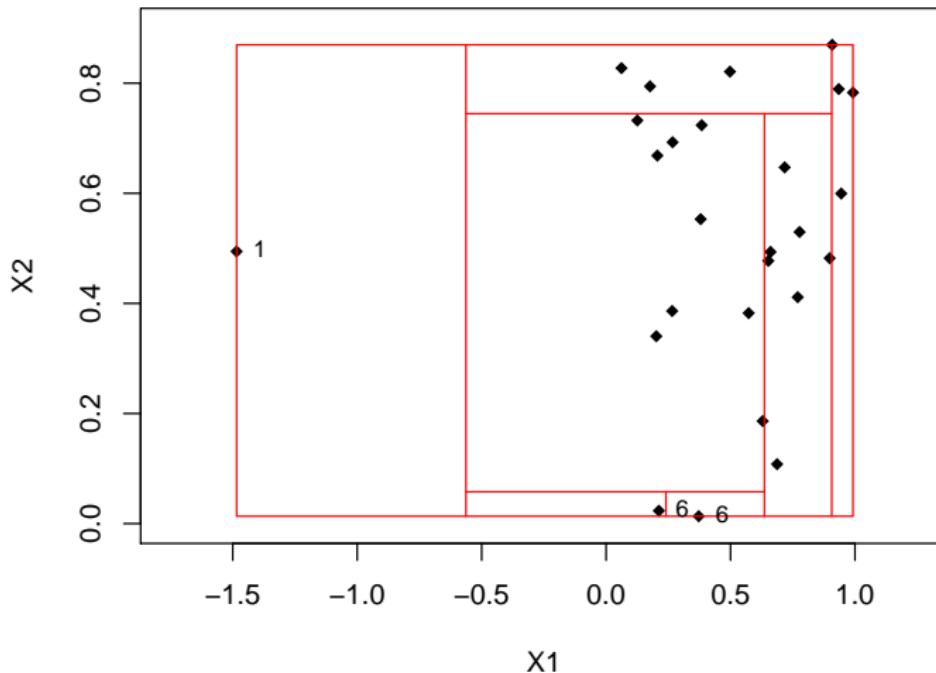
Isolation tree, split 5



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

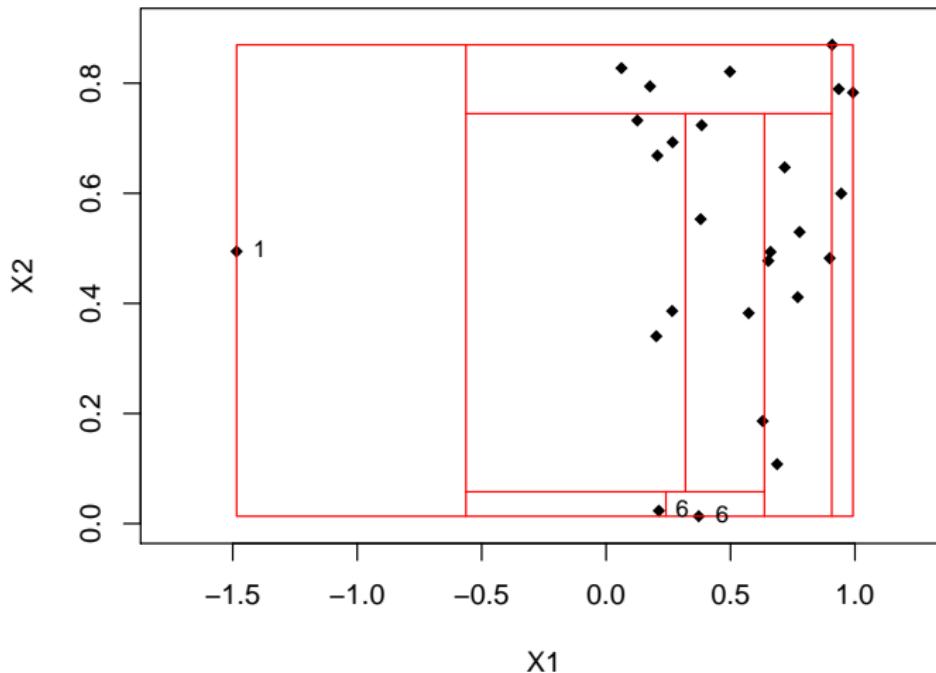
Isolation tree, split 6



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

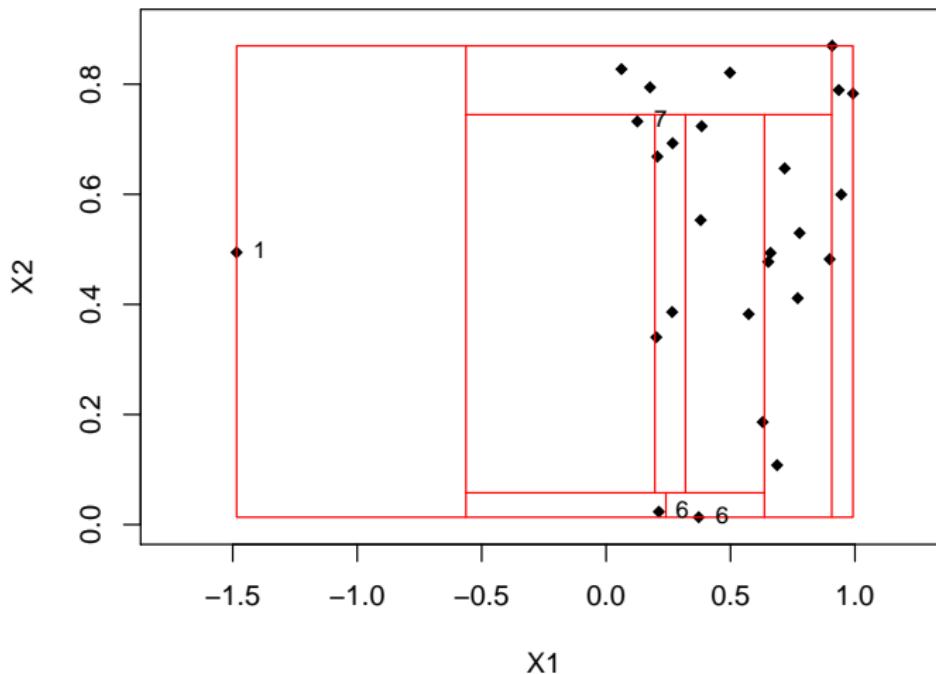
Isolation tree, split 7



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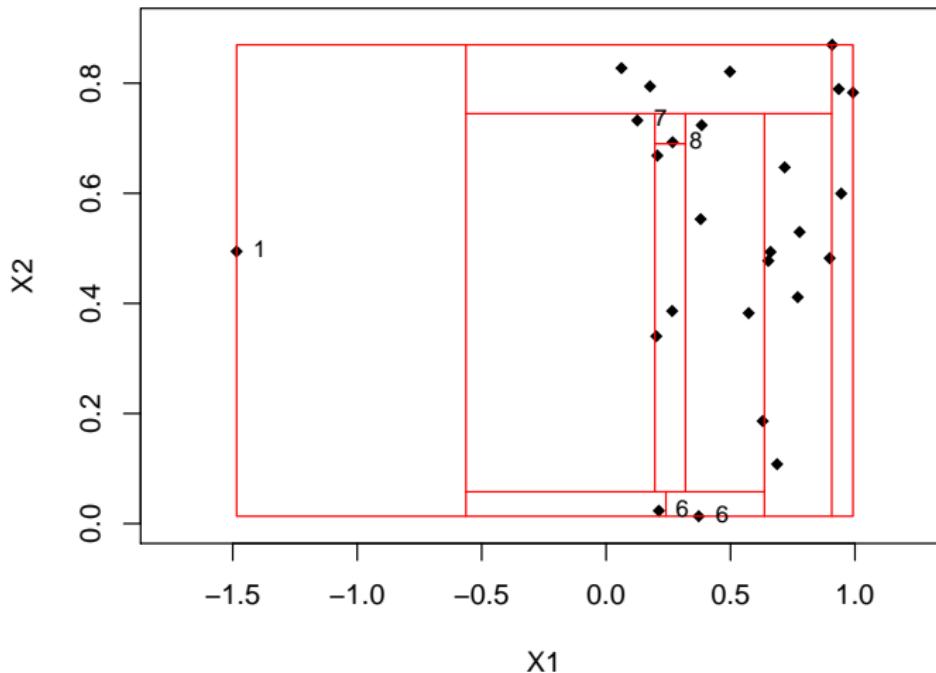
Isolation tree, split 8



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

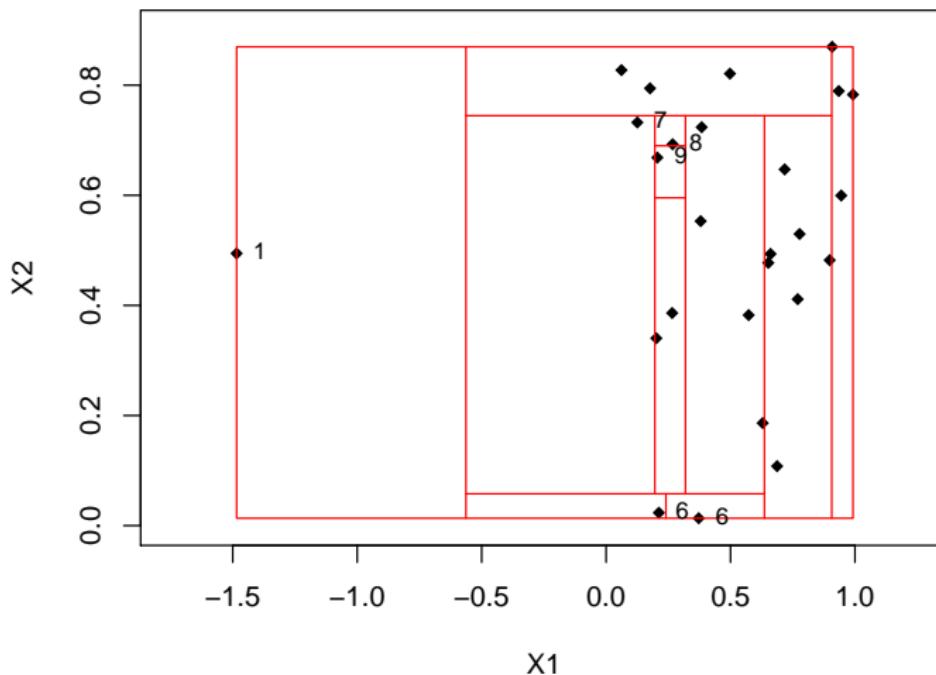
Isolation tree, split 9



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

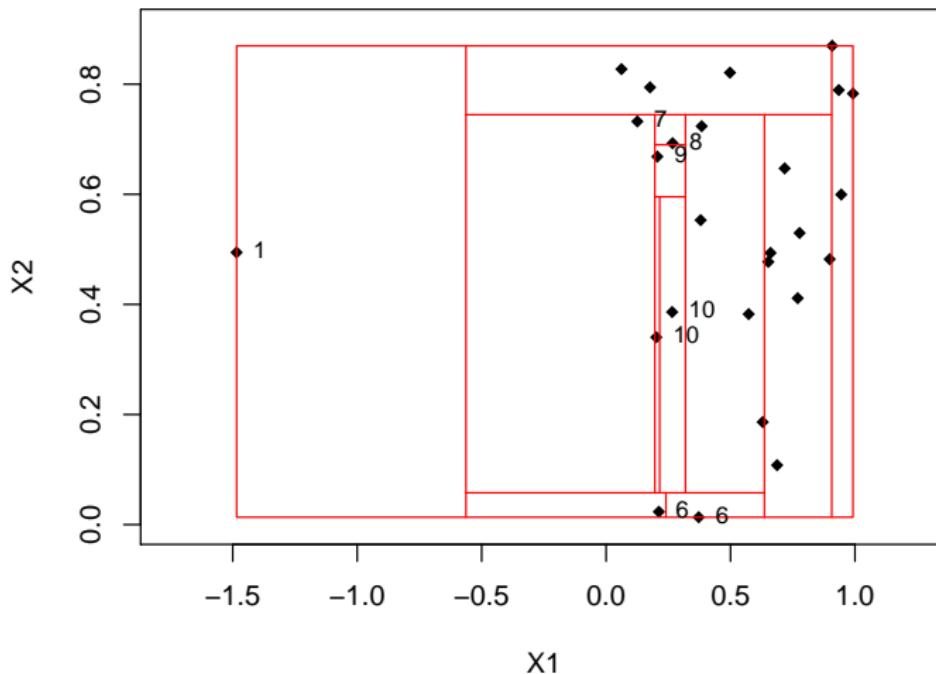
Isolation tree, split 10



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

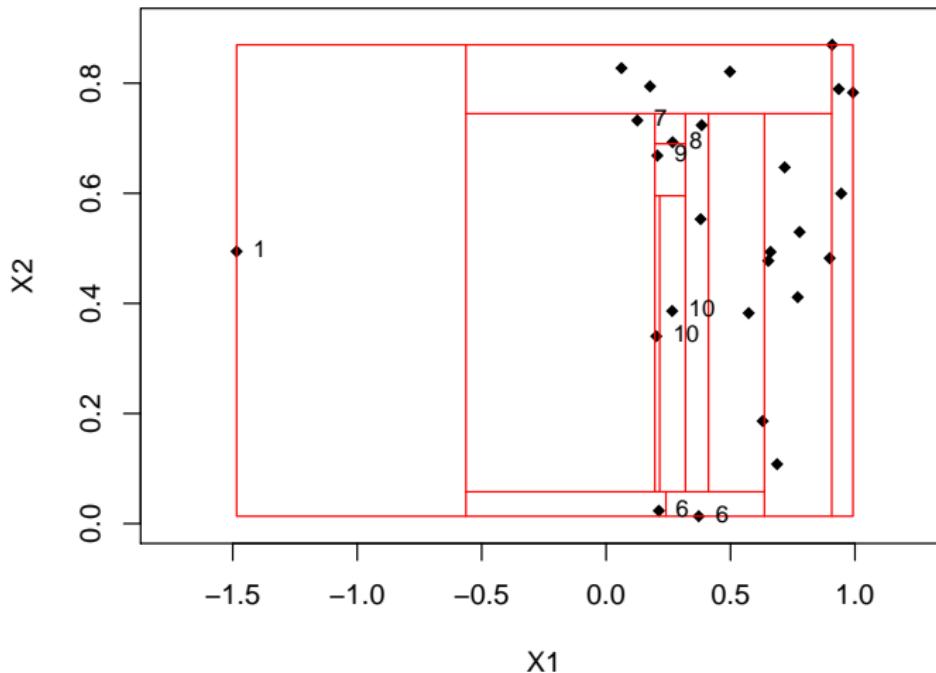
Isolation tree, split 11



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

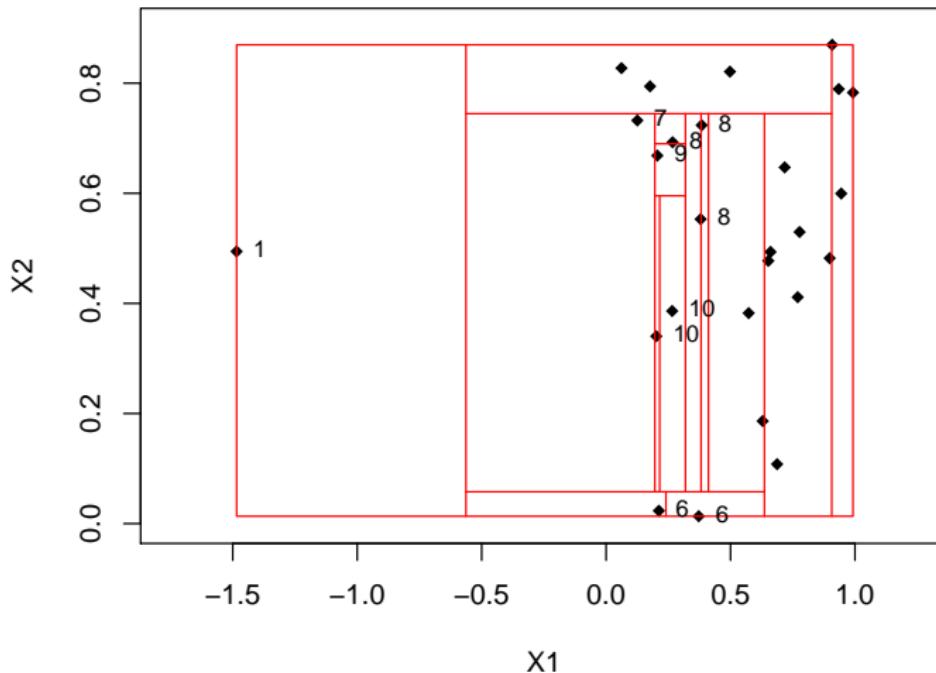
Isolation tree, split 12



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

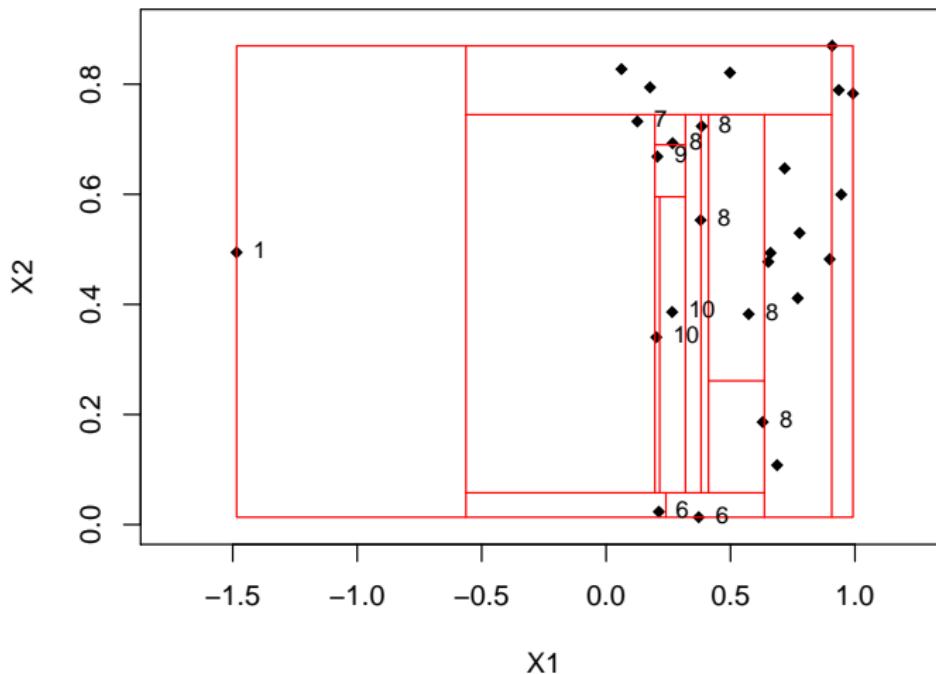
Isolation tree, split 13



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

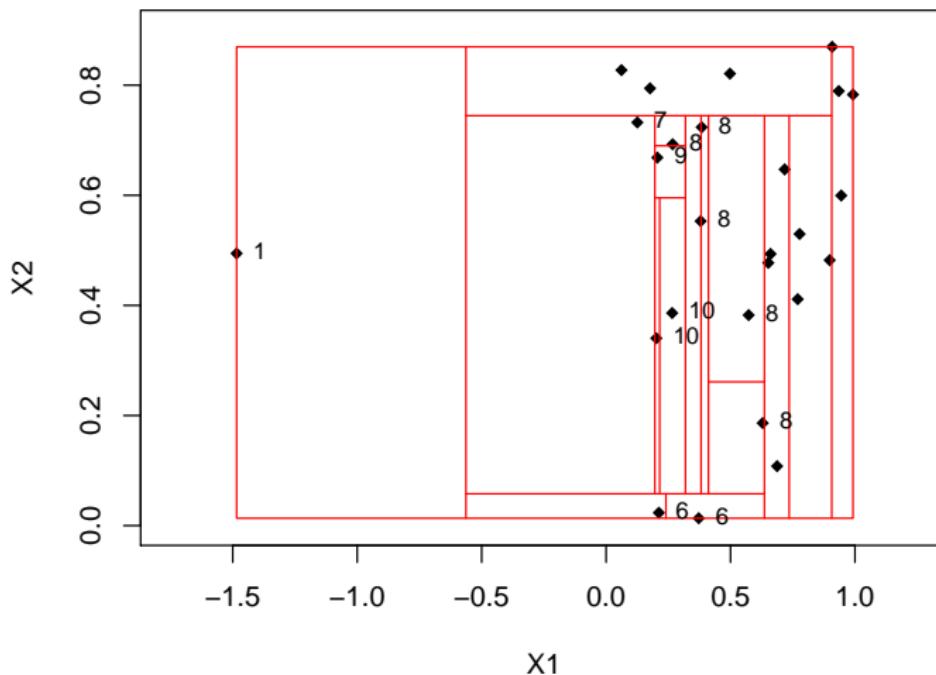
Isolation tree, split 14



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

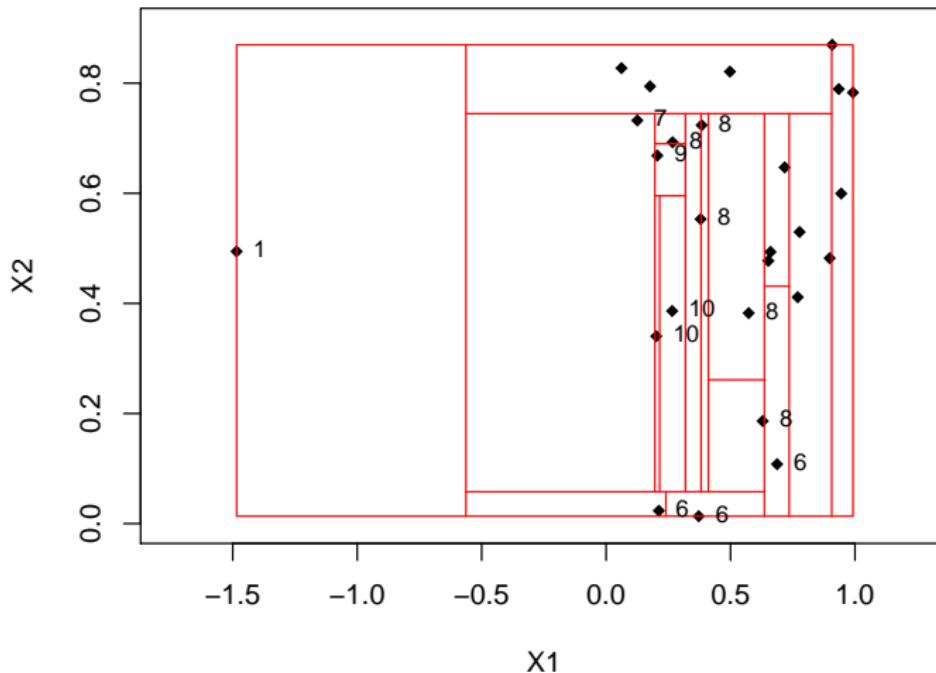
Isolation tree, split 15



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

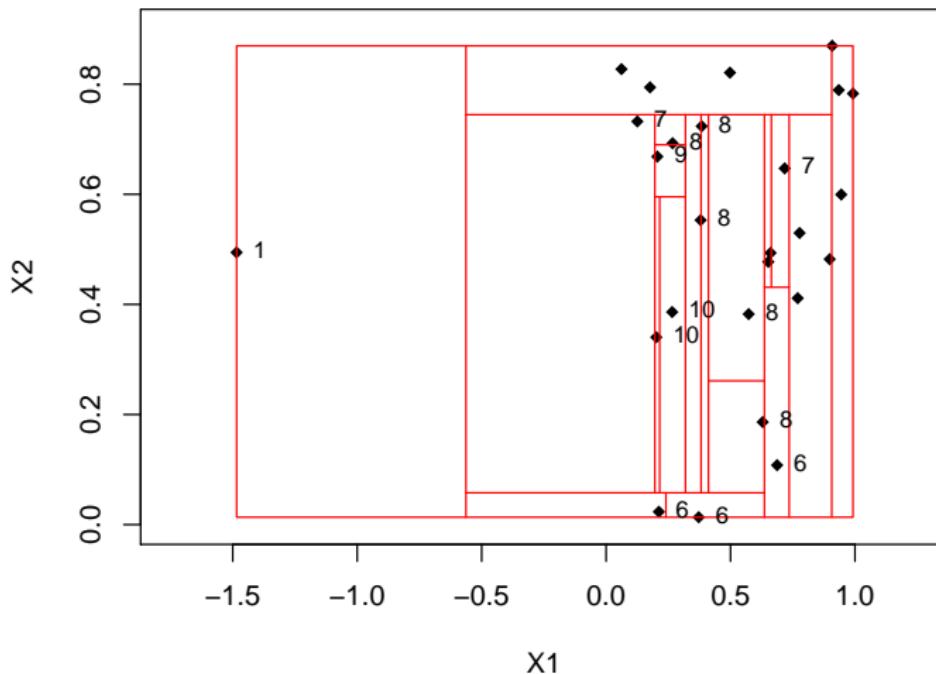
Isolation tree, split 16



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

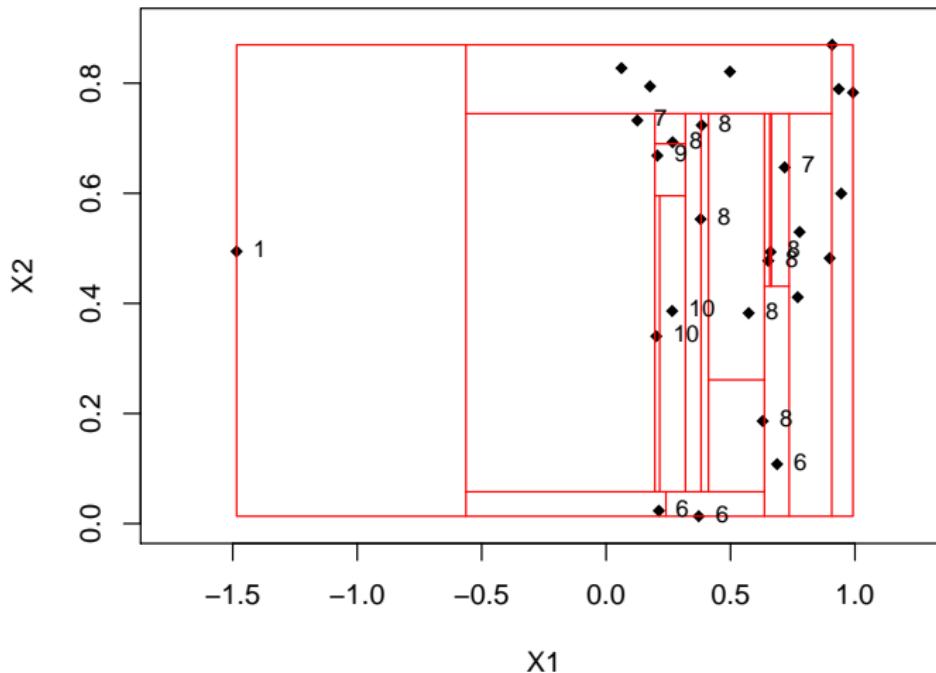
Isolation tree, split 17



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

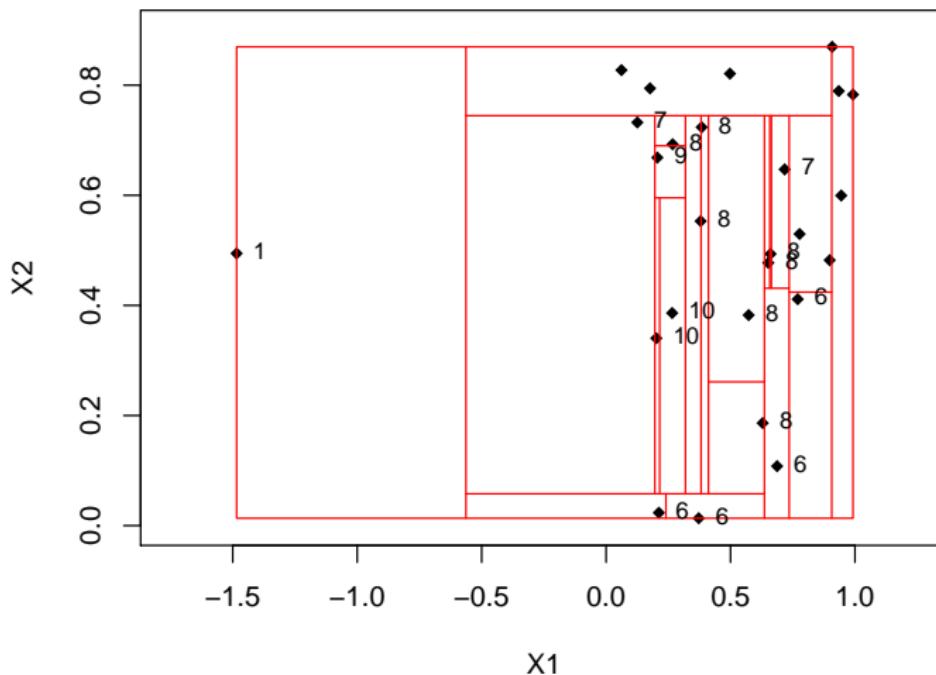
Isolation tree, split 18



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

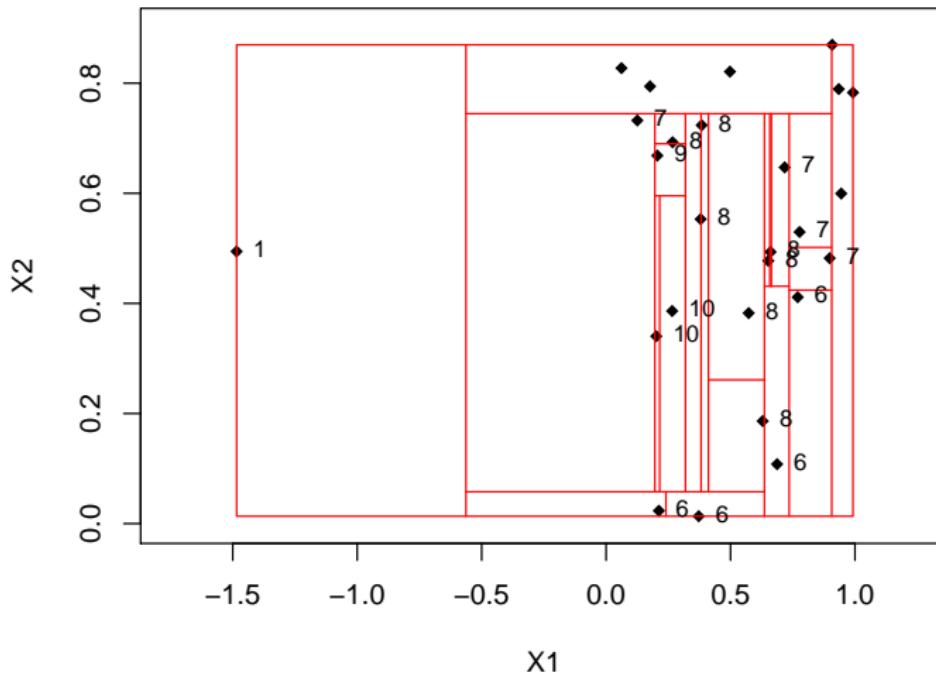
Isolation tree, split 19



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

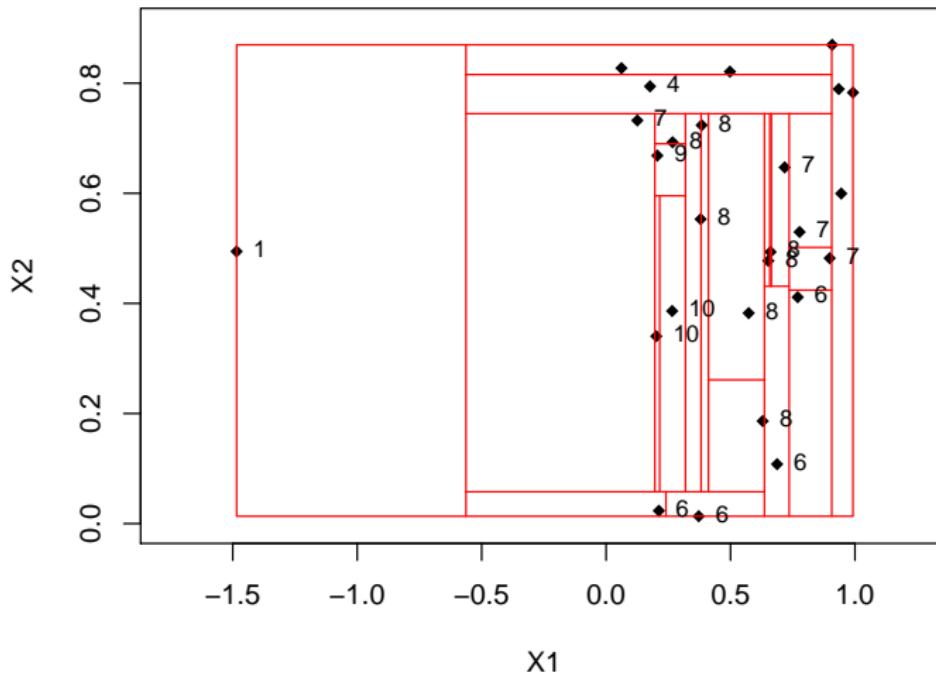
Isolation tree, split 20



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

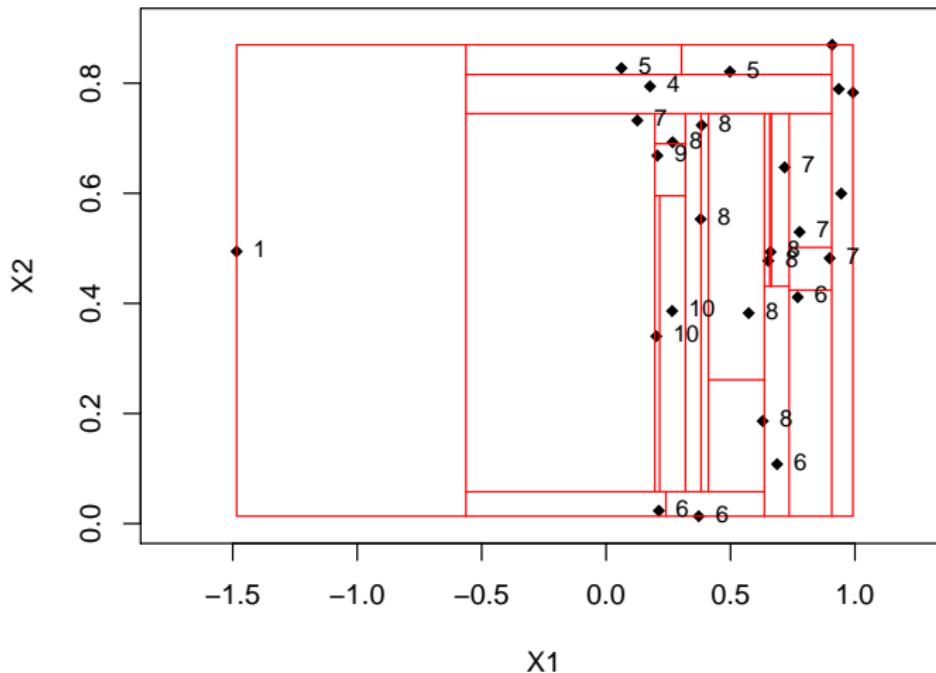
Isolation tree, split 21



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

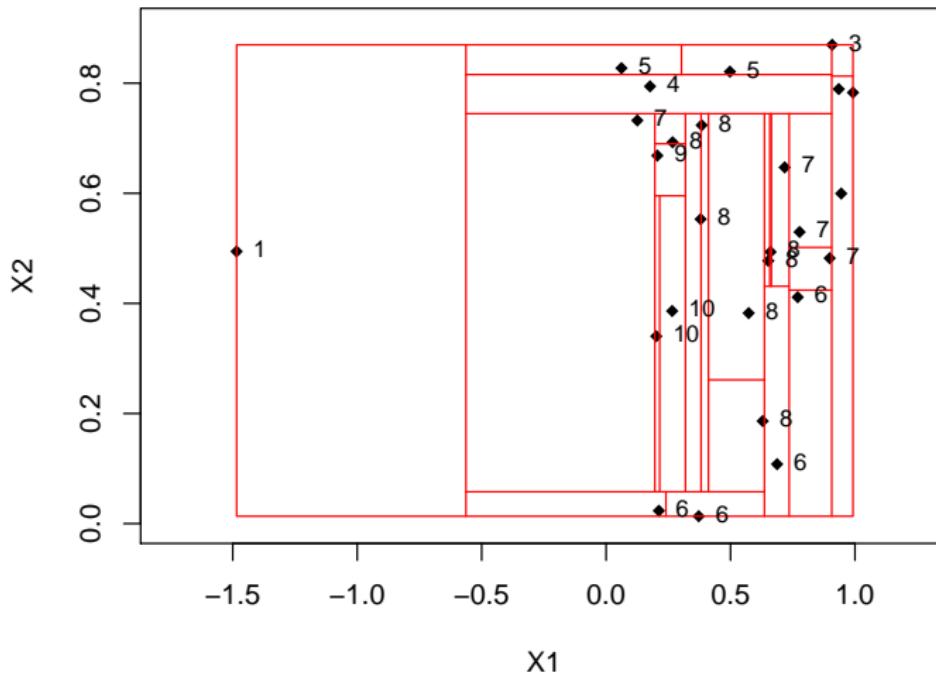
Isolation tree, split 22



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

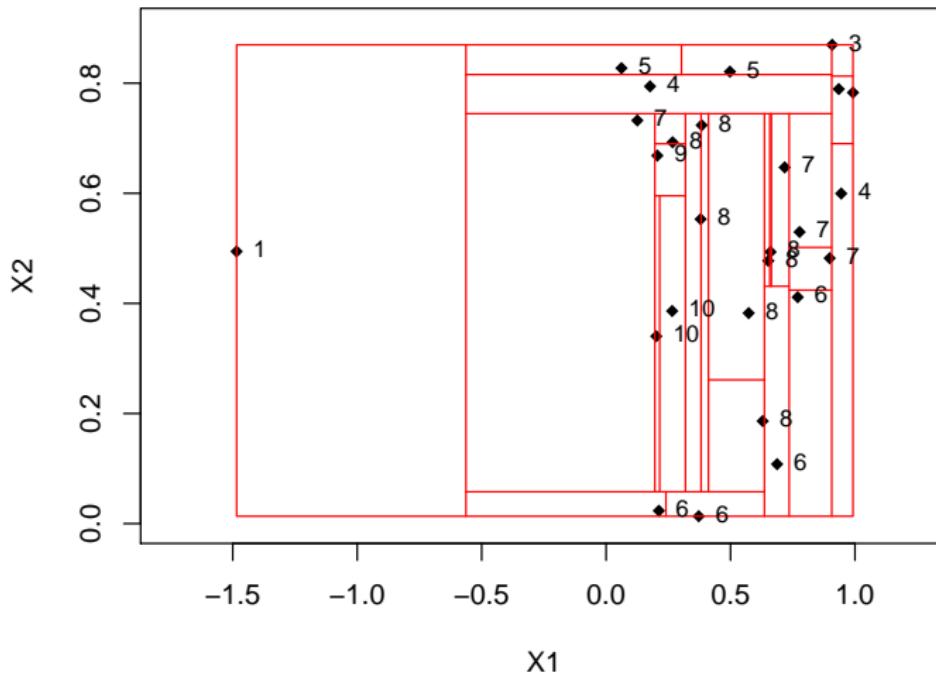
Isolation tree, split 23



Isolation forest (Liu, Ting, Zhou; 2008)

Illustration: Isolation tree

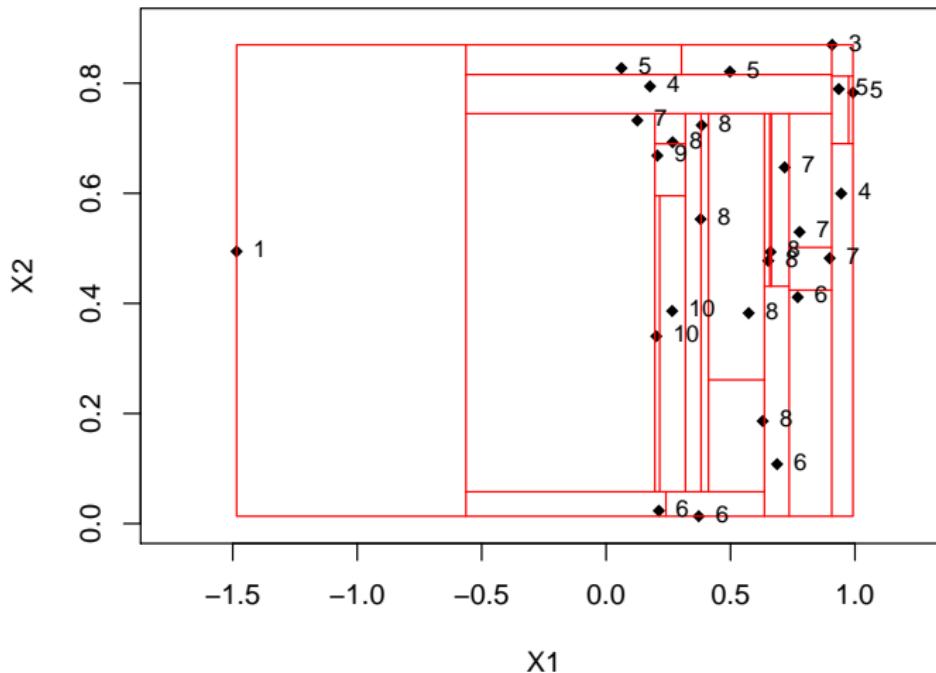
Isolation tree, split 24



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:

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

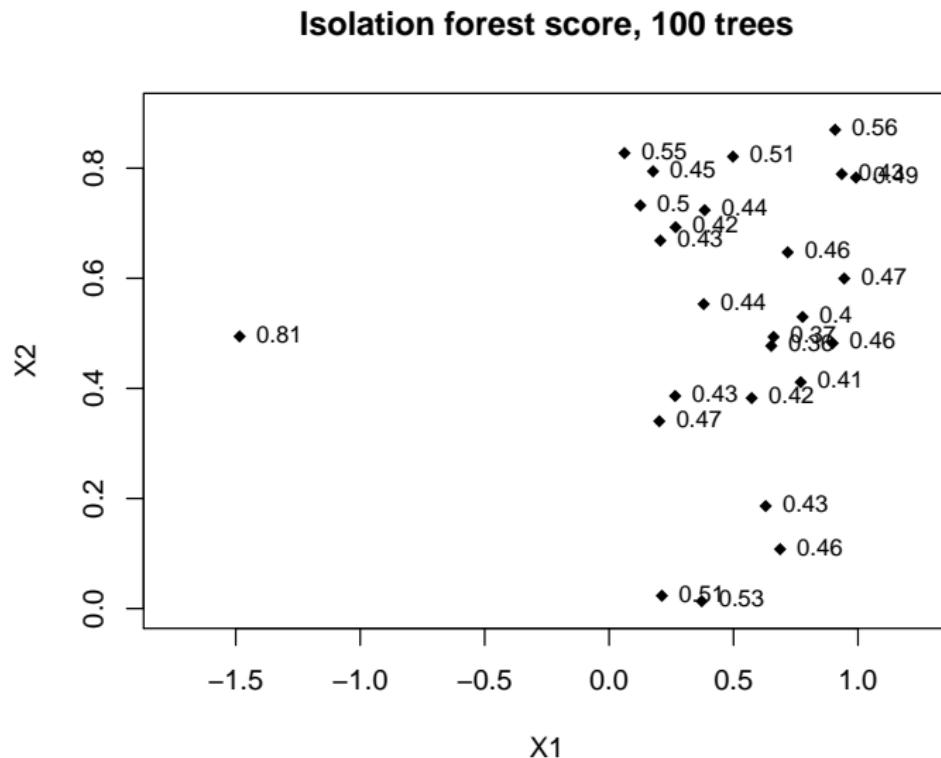
with $c(n) = 2H(n-1) - \frac{2(n-1)}{n}$ where $H(k)$ is the harmonic number and can be estimated by $\ln(k) + 0.5772156649$.

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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- Local outlier factor

- Isolation forest

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- Further depth notions

Functional anomaly detection

- Integrated data depth

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- Depth for curve data

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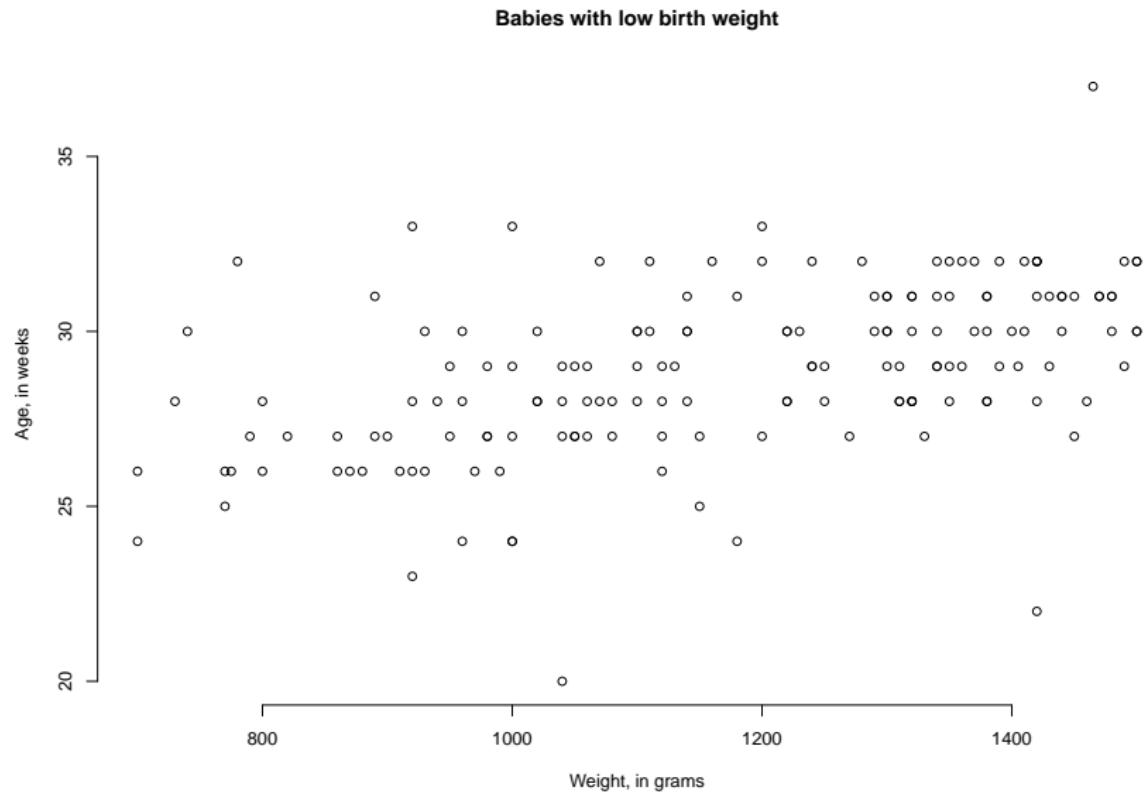
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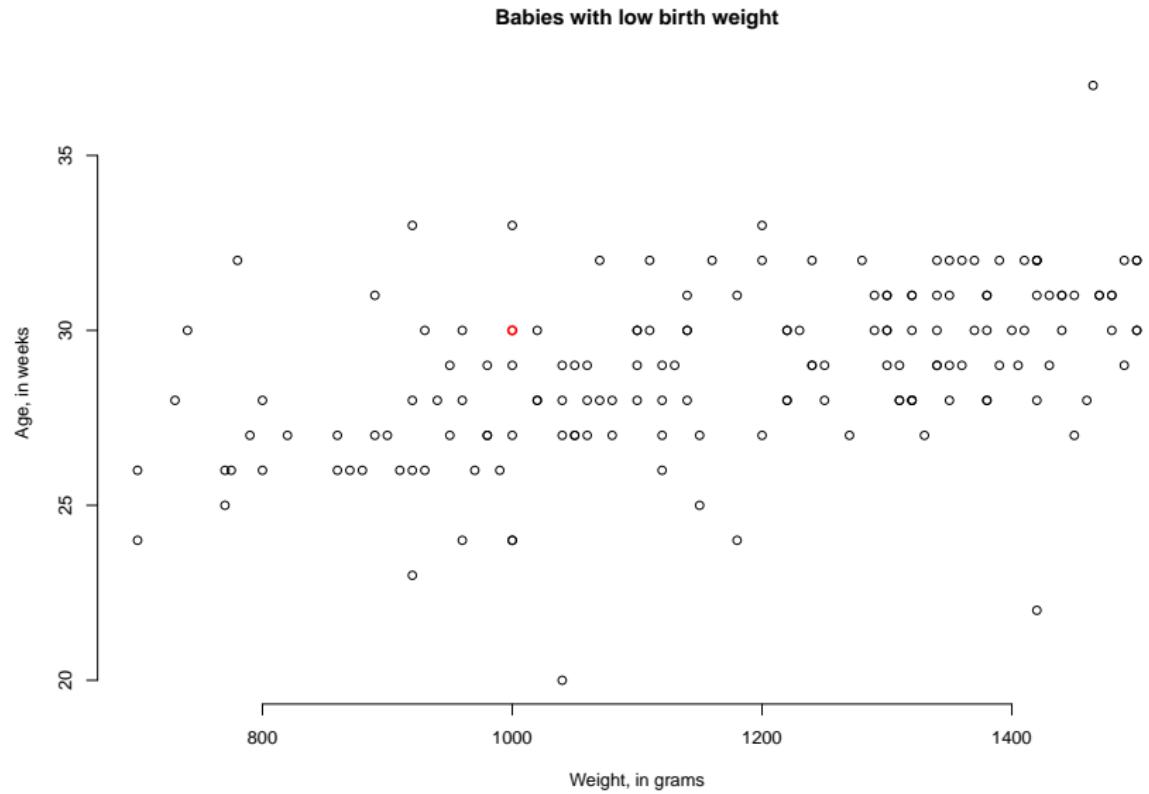
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Data depth



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

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- D5 **upper semicontinuous in \mathbf{x} :** the upper-level sets
$$D_\alpha(X) = \{\mathbf{x} \in \mathbb{R}^p : D(\mathbf{x}|X) \geq \alpha\}$$
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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** (Cascos, 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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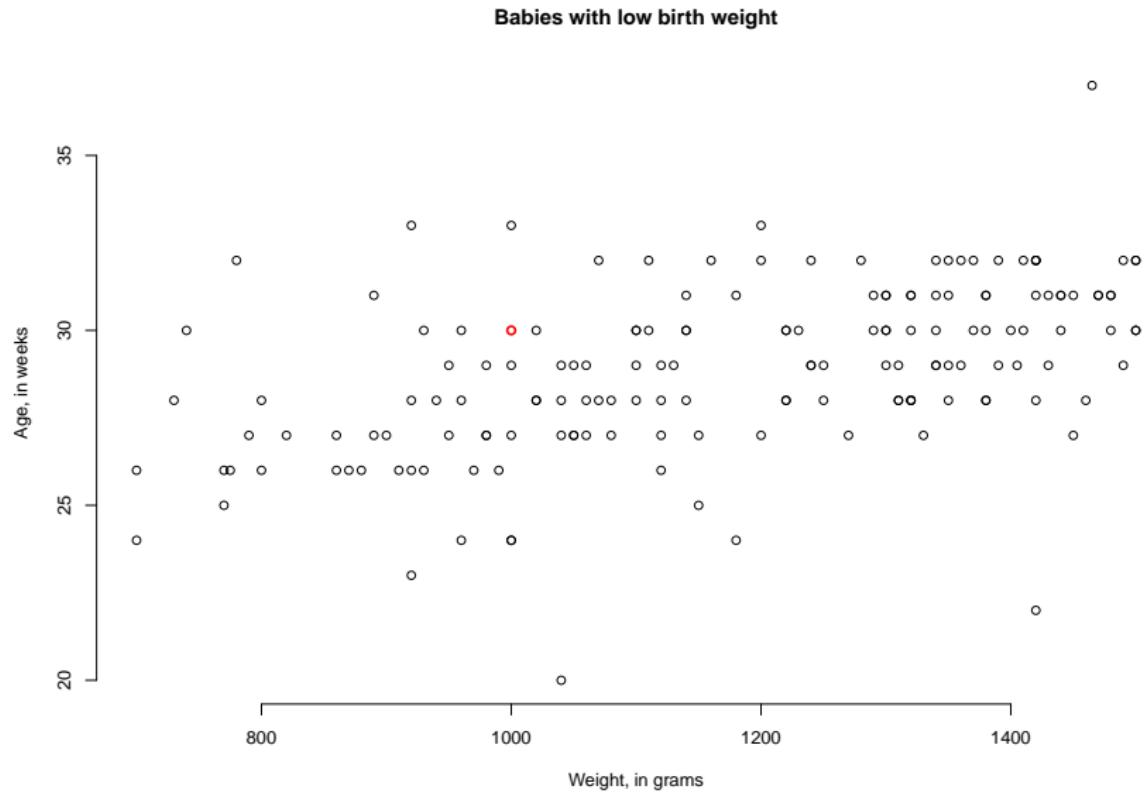
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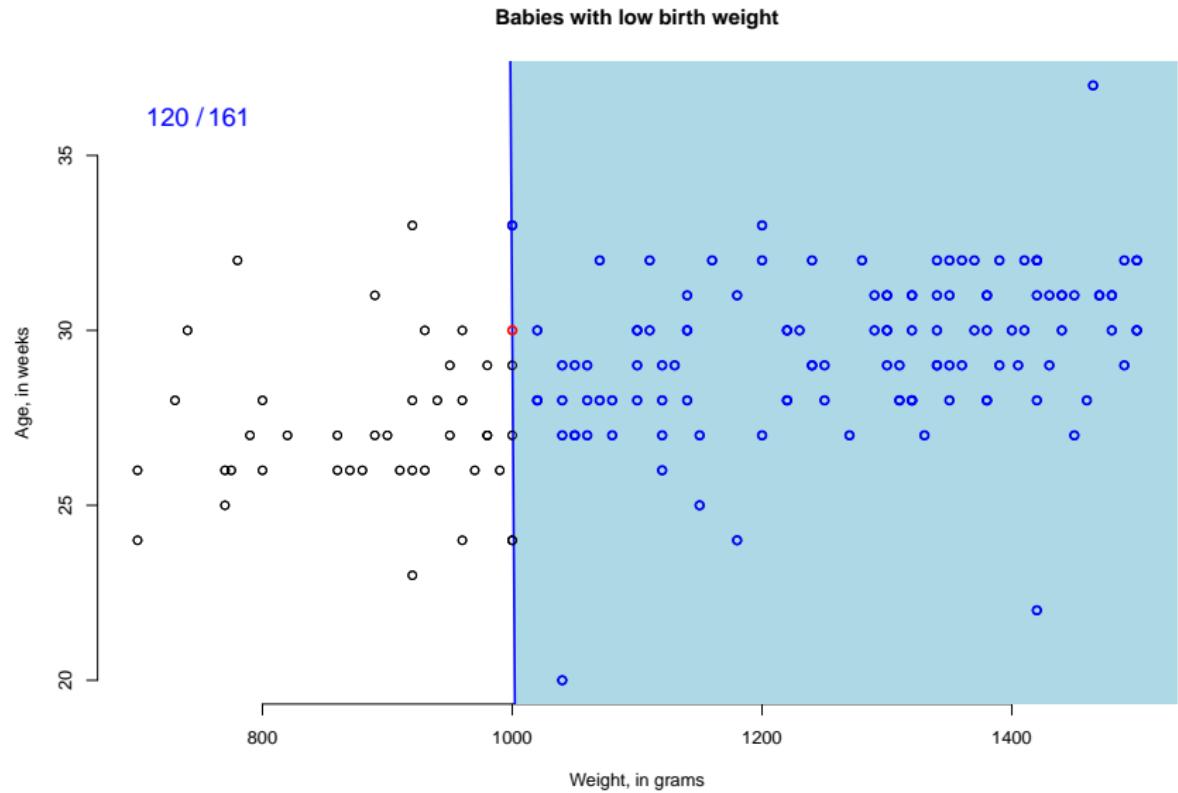
Tukey depth

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

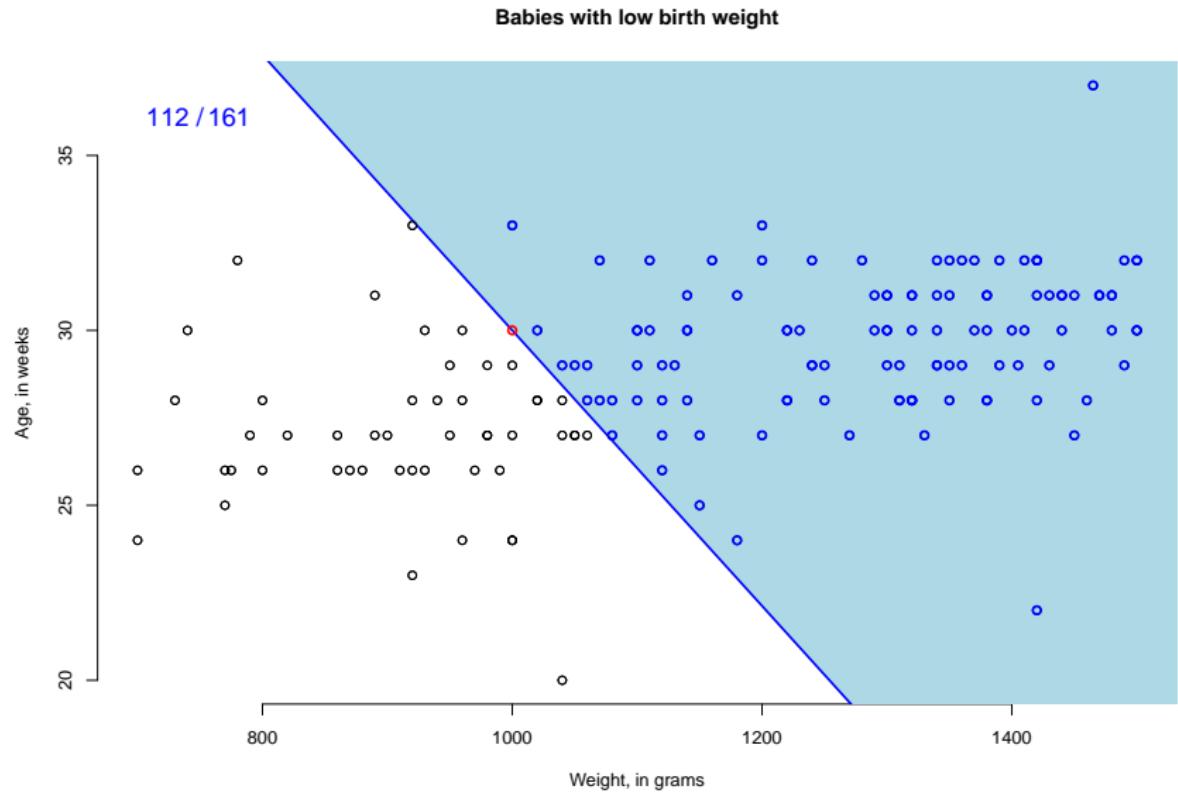
Tukey (=halfspace, location) data depth



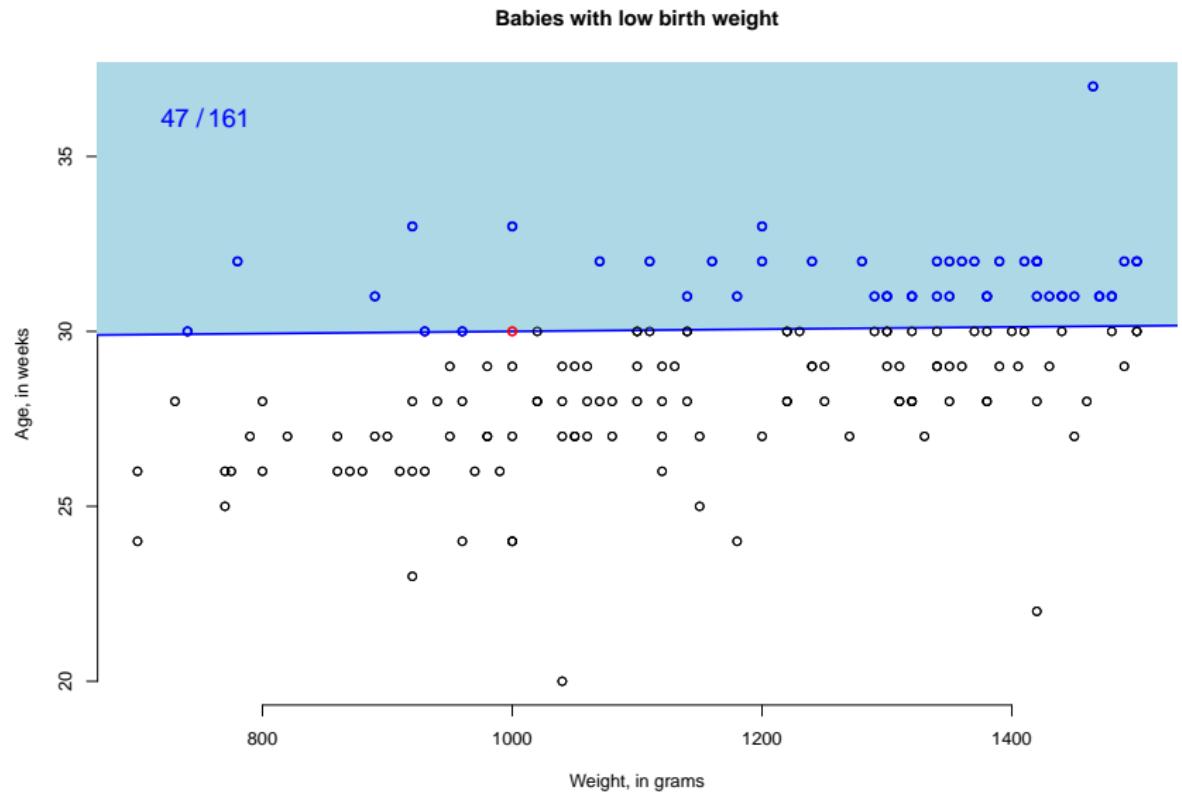
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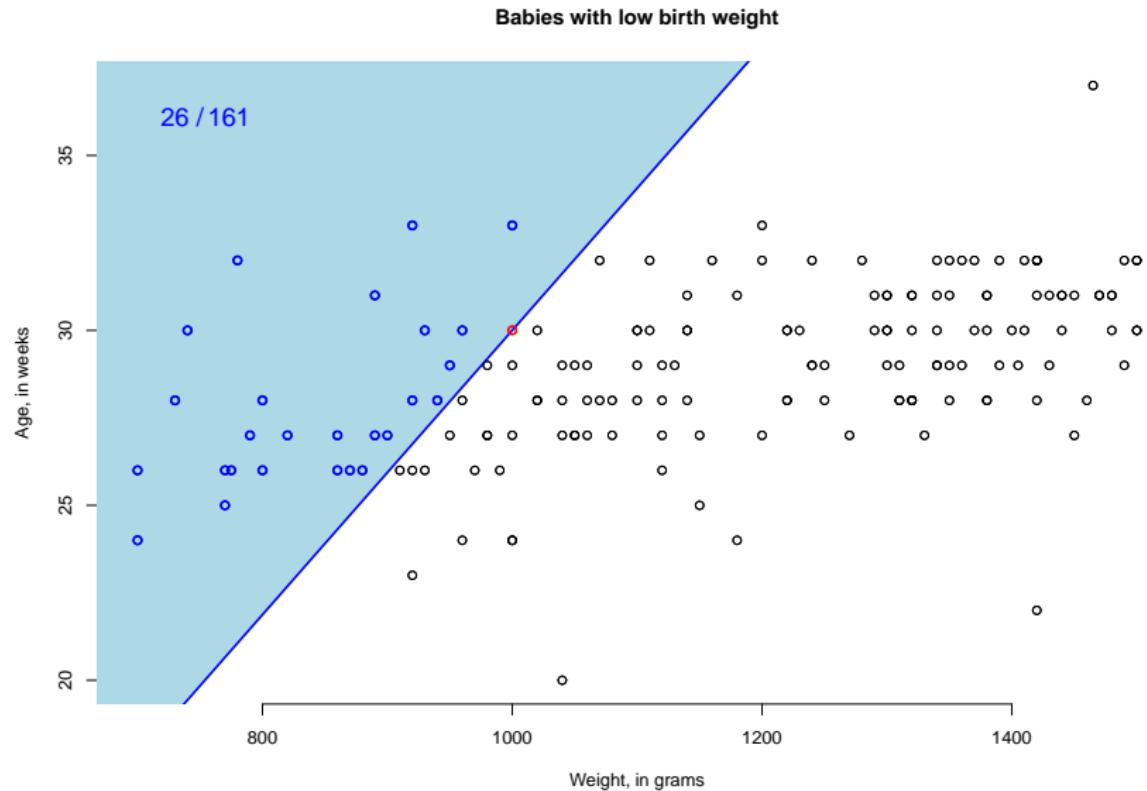
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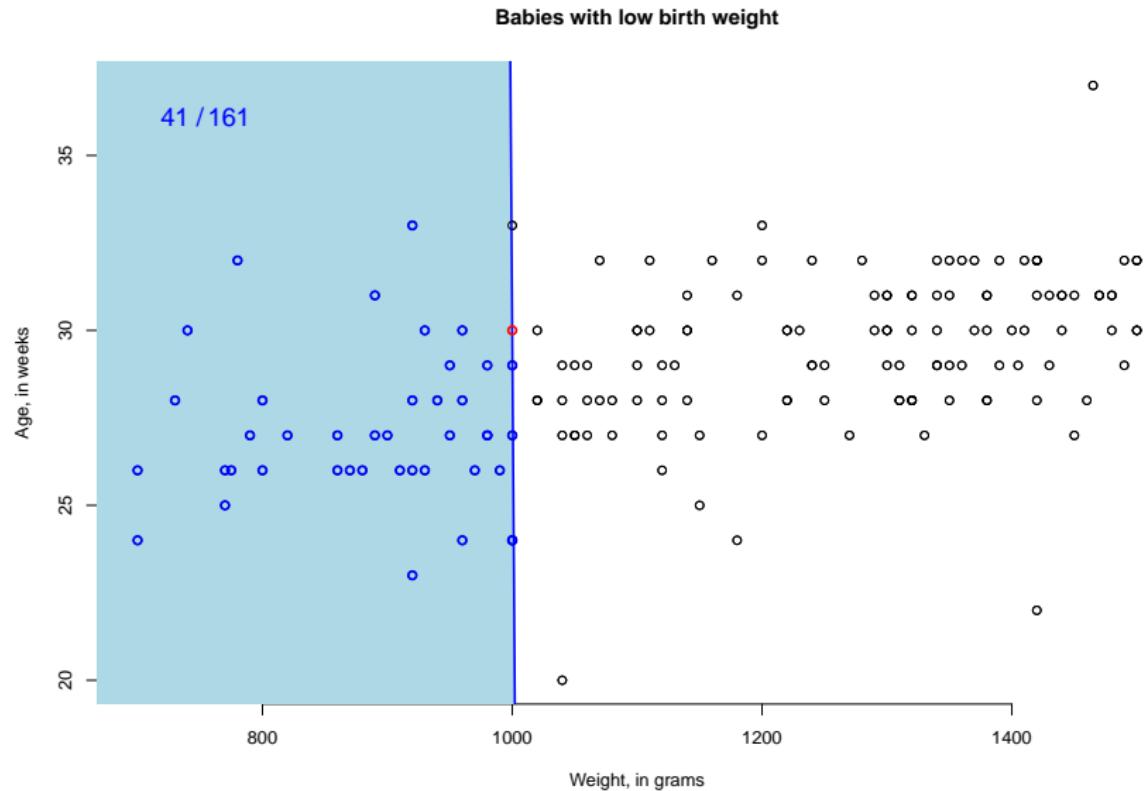
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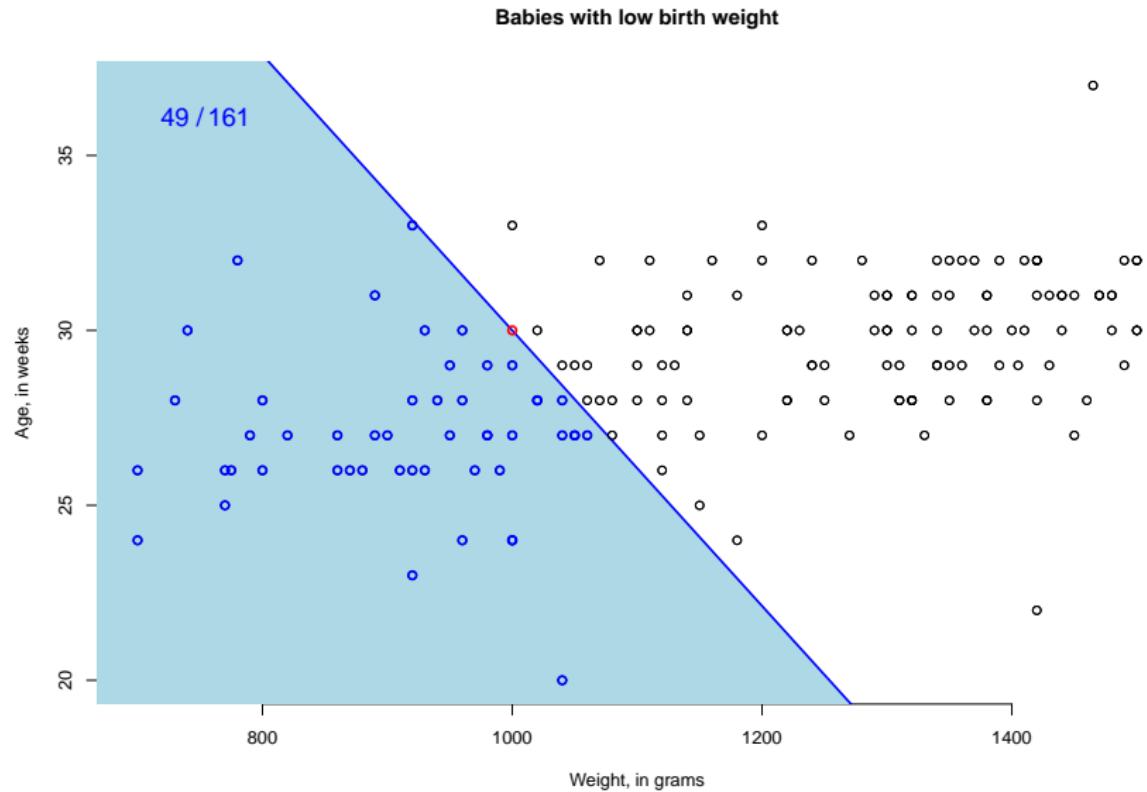
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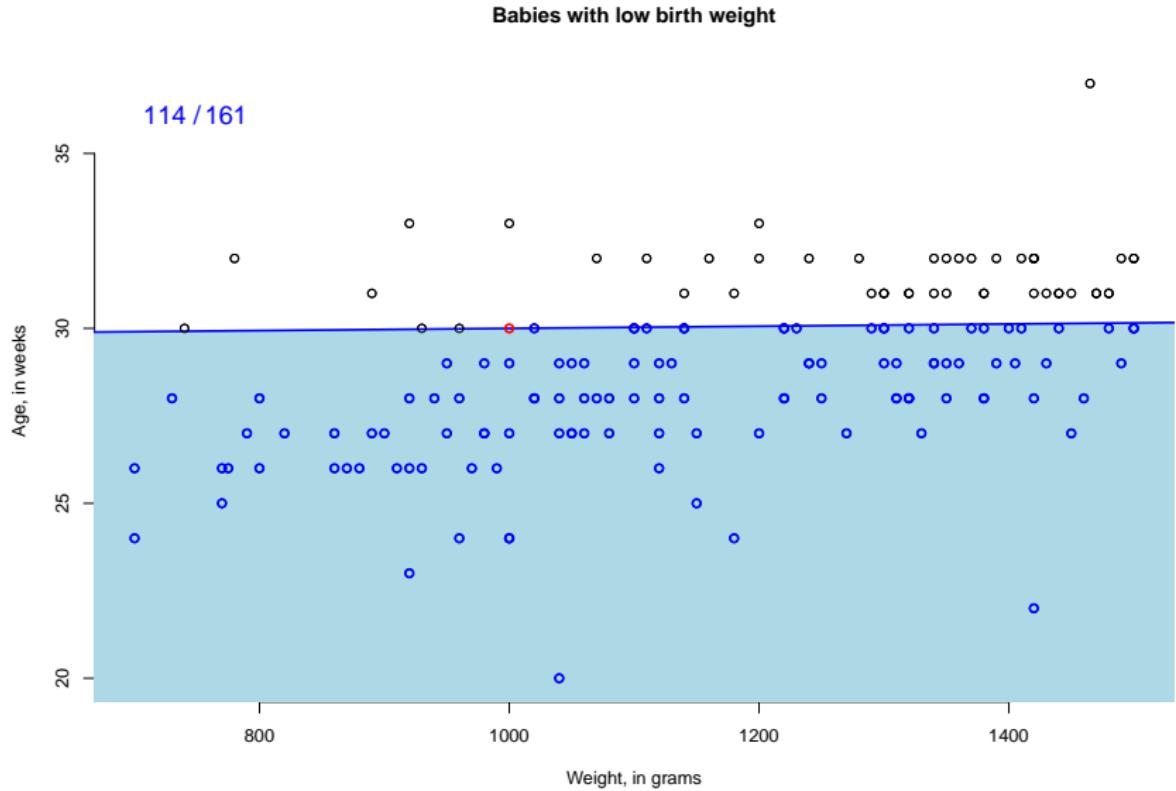
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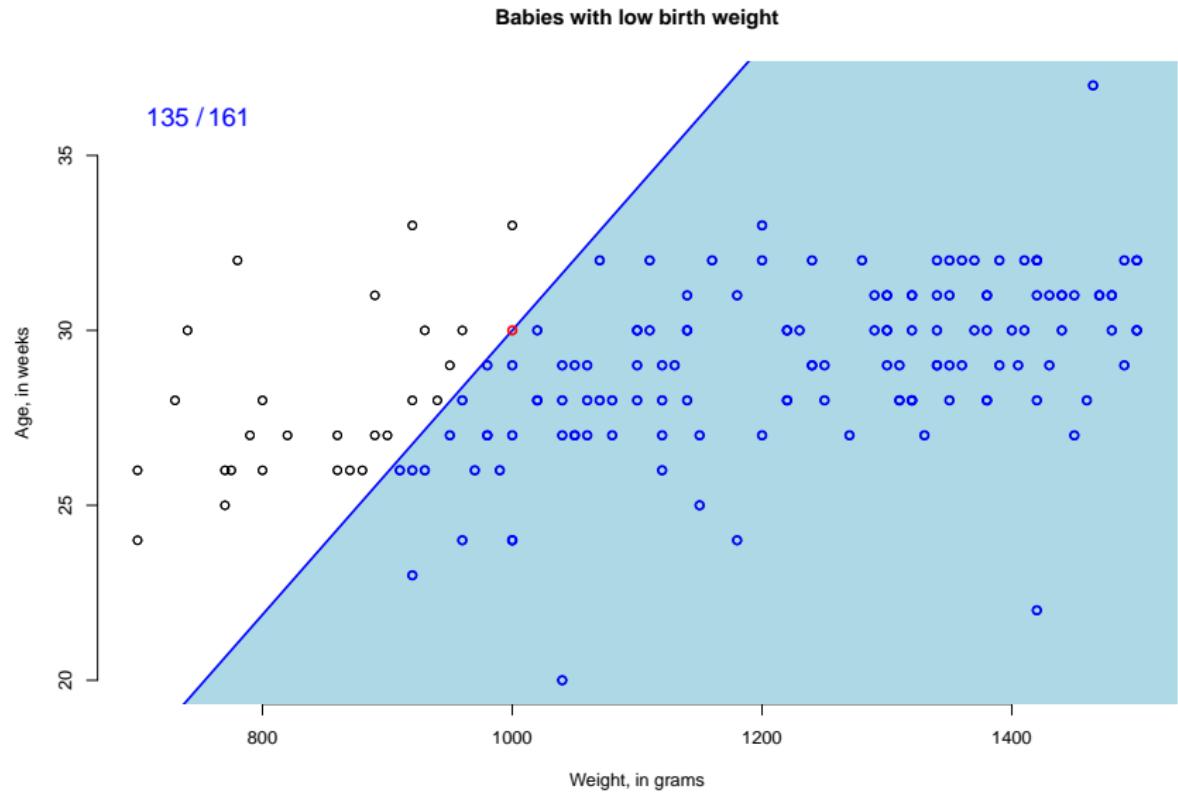
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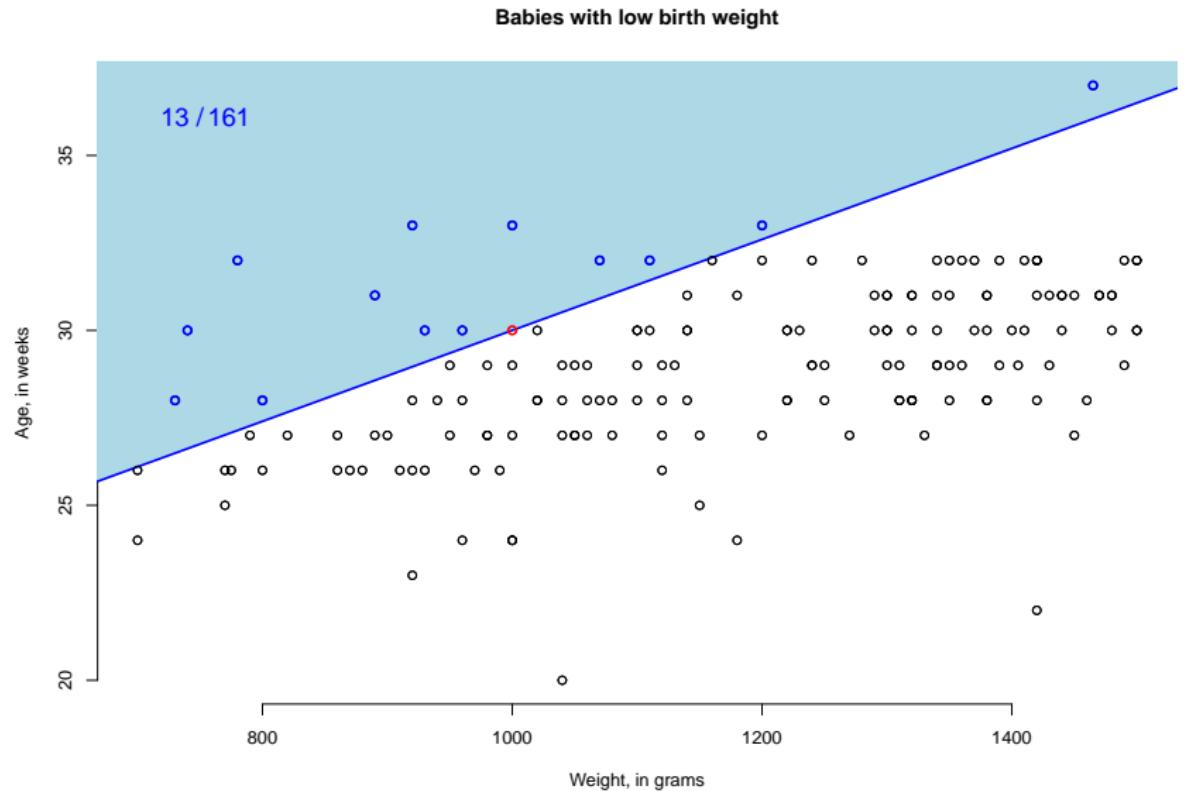
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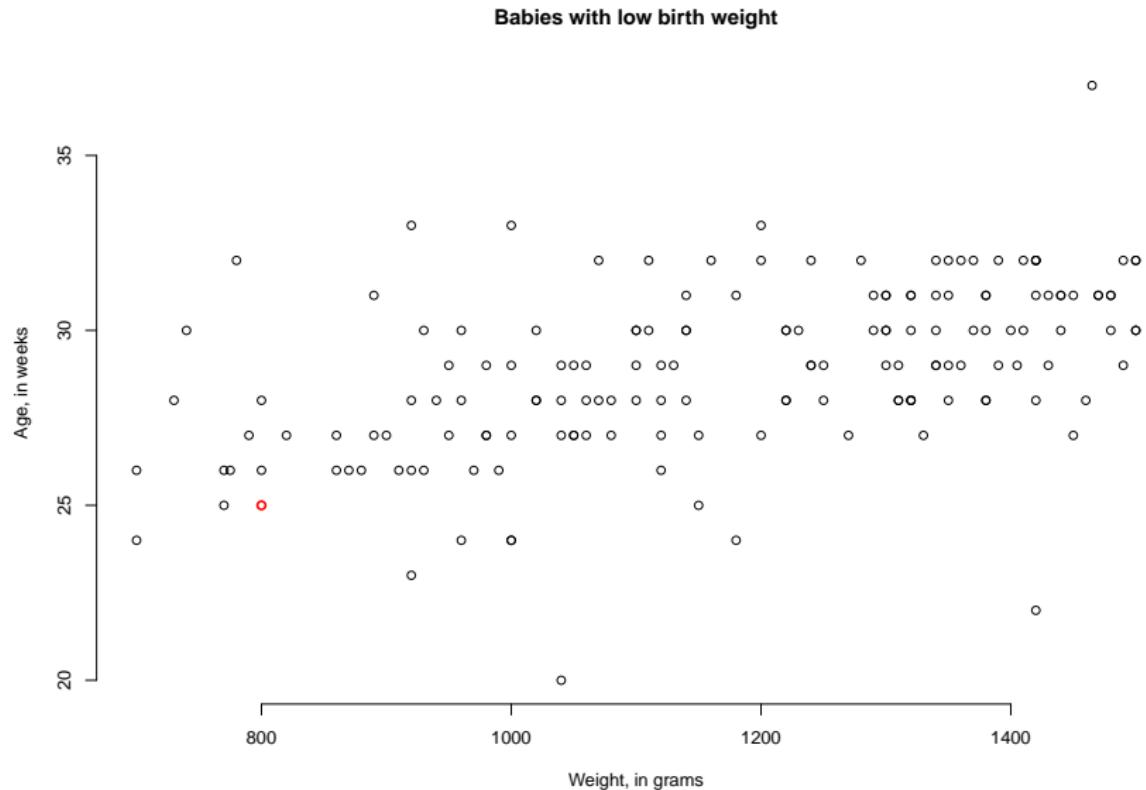
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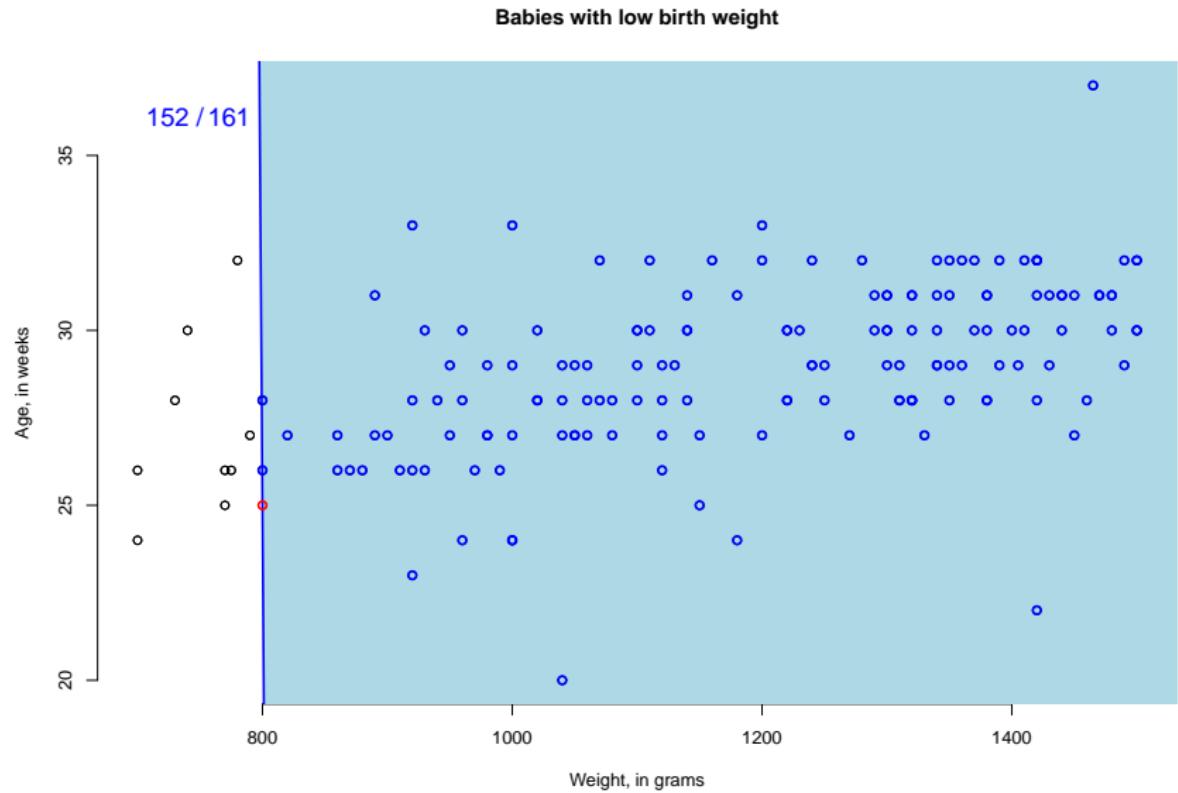
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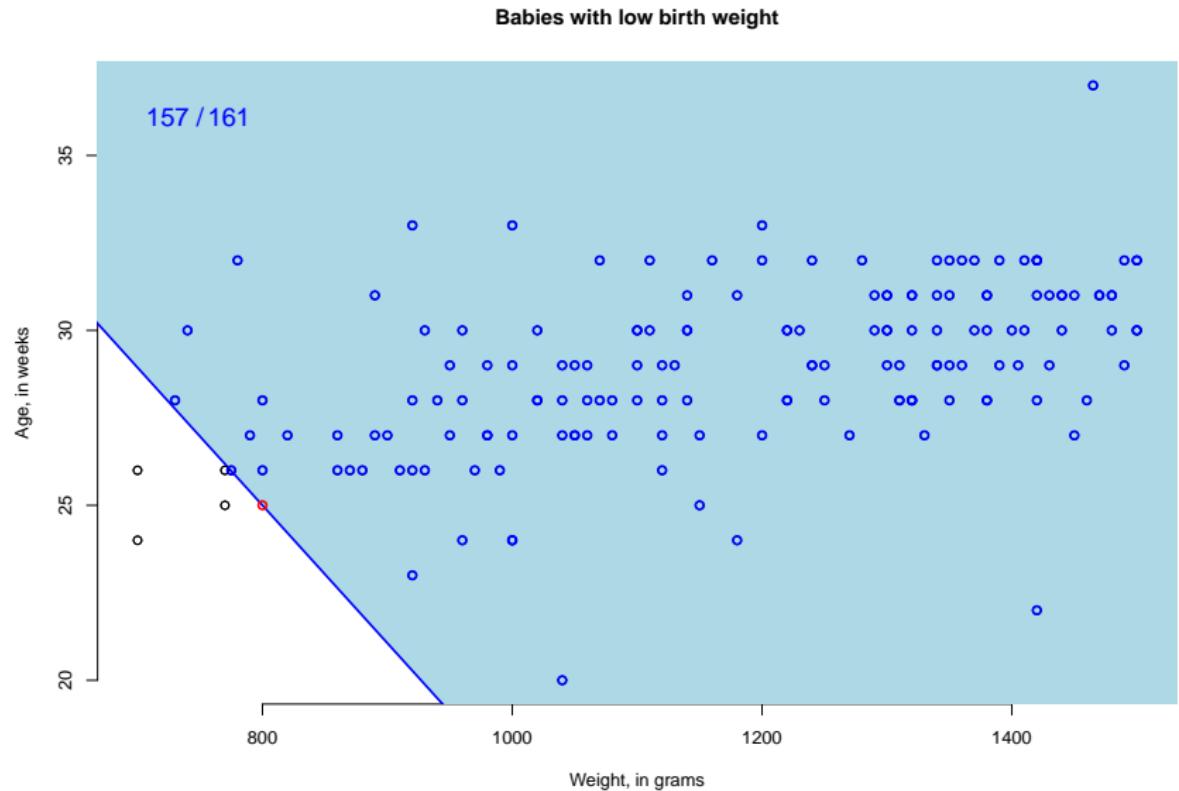
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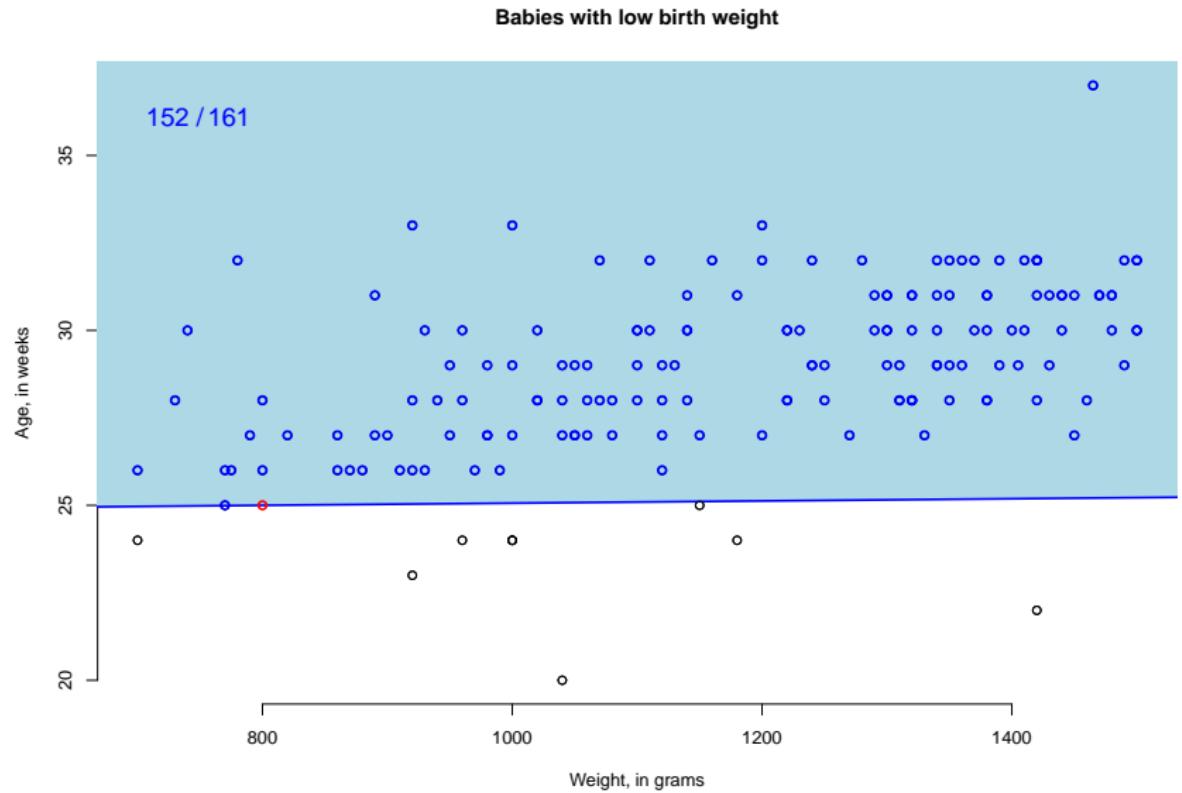
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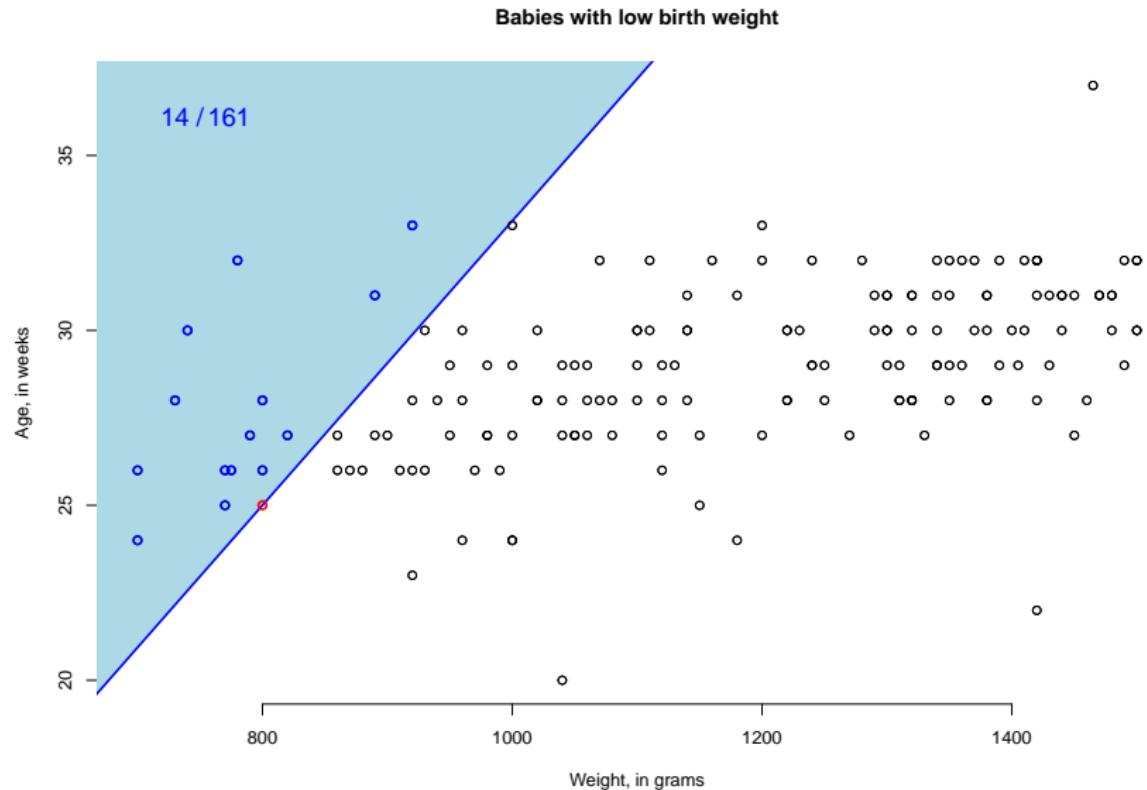
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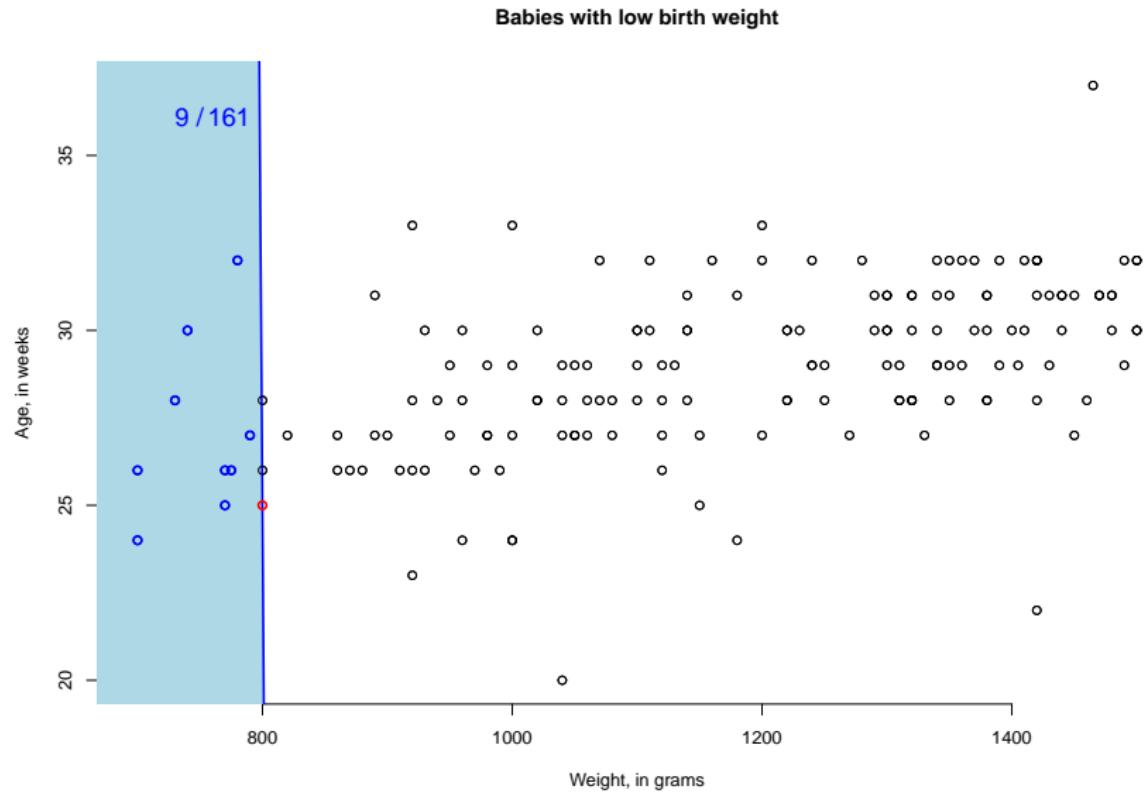
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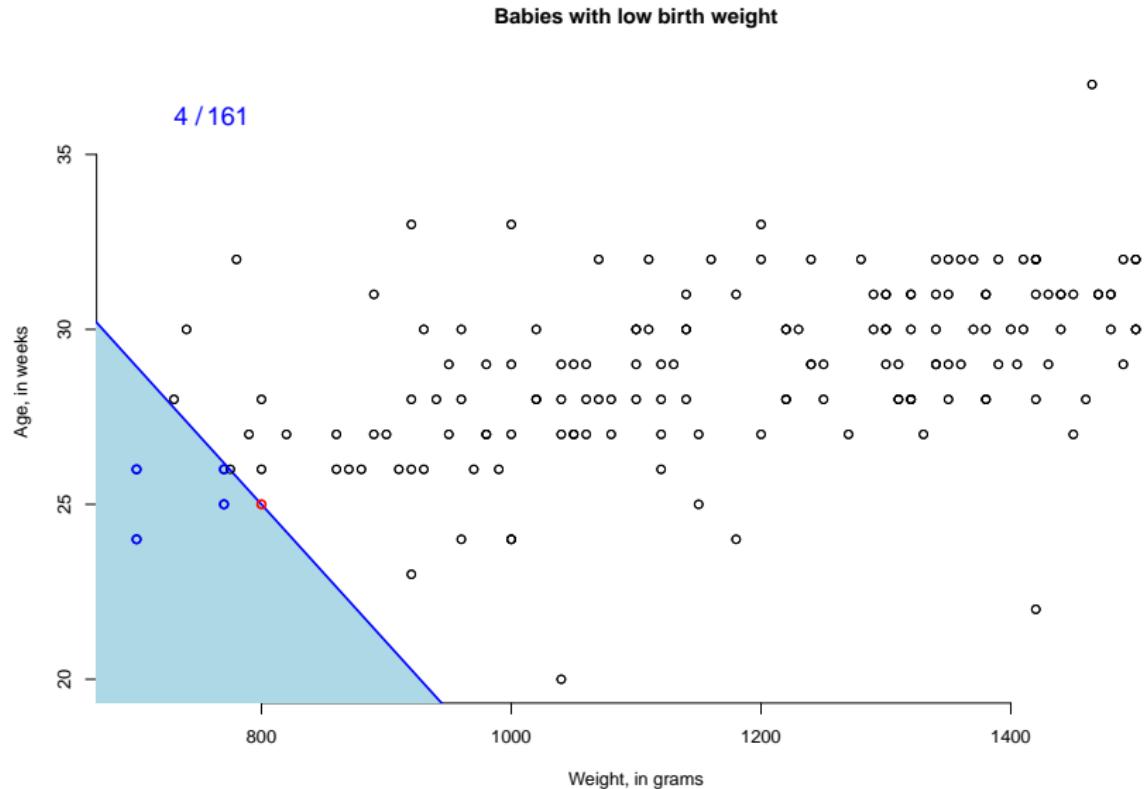
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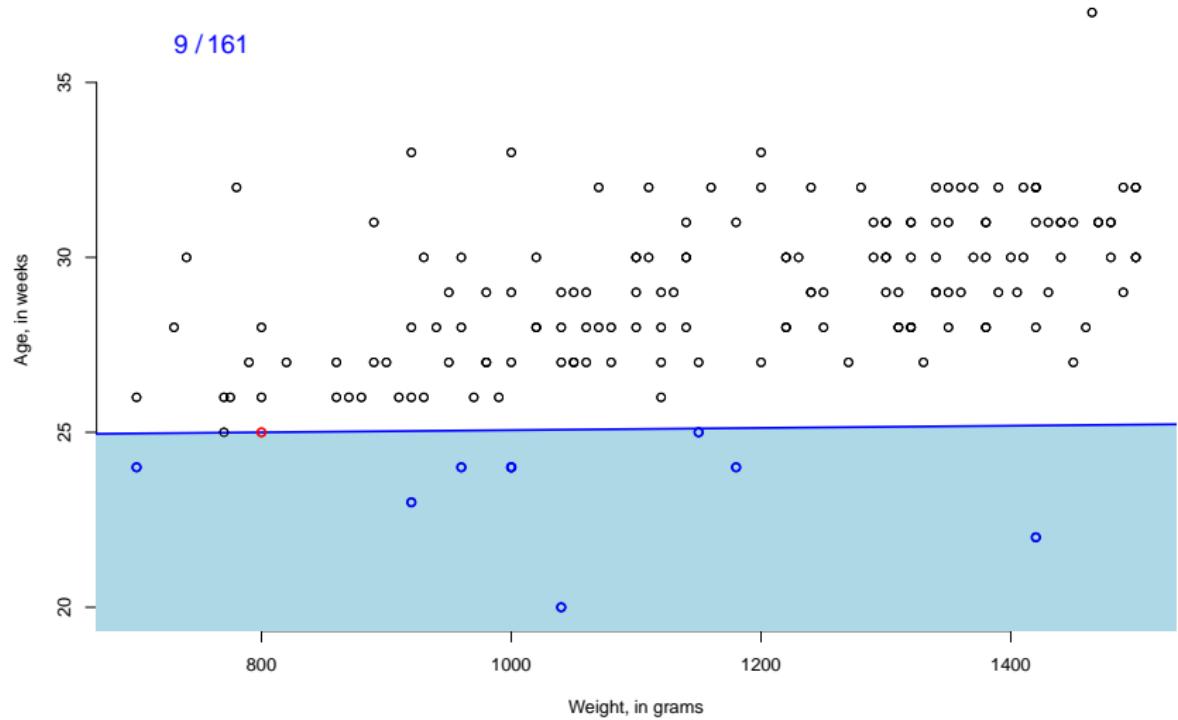


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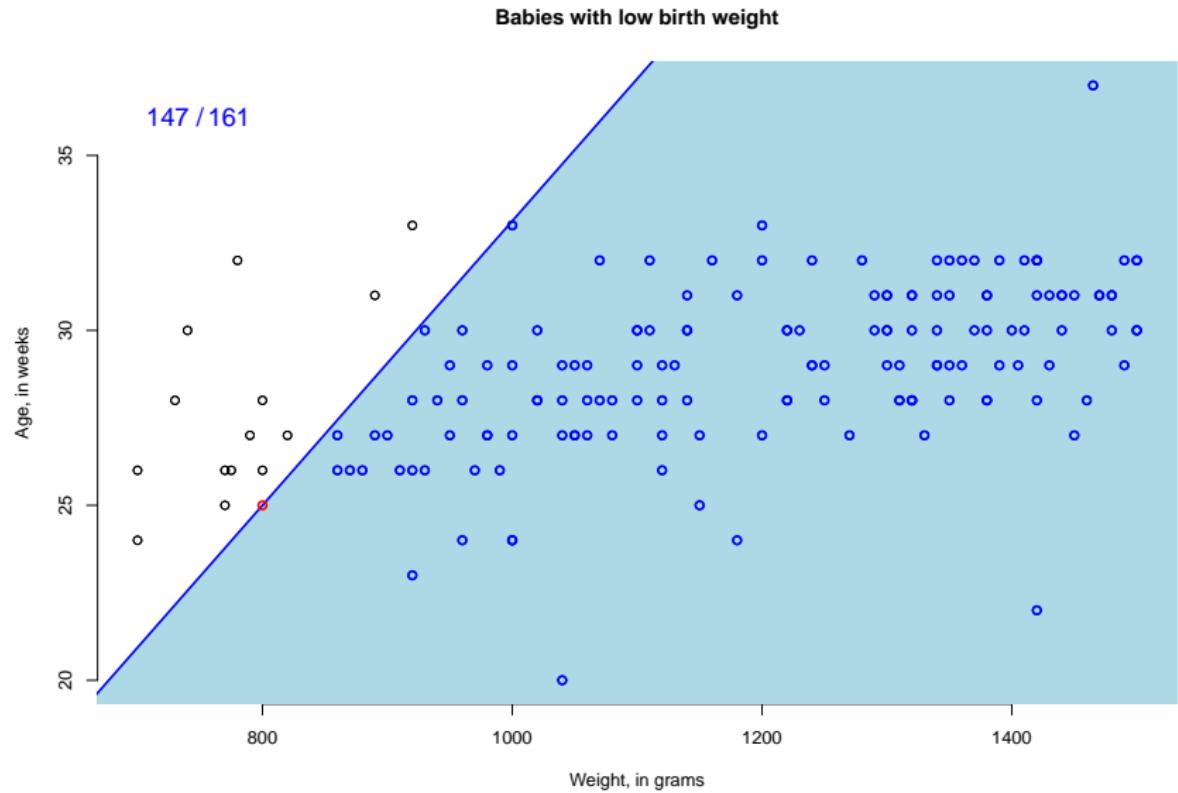


Tukey (=halfspace, location) data depth

Babies with low birth weight

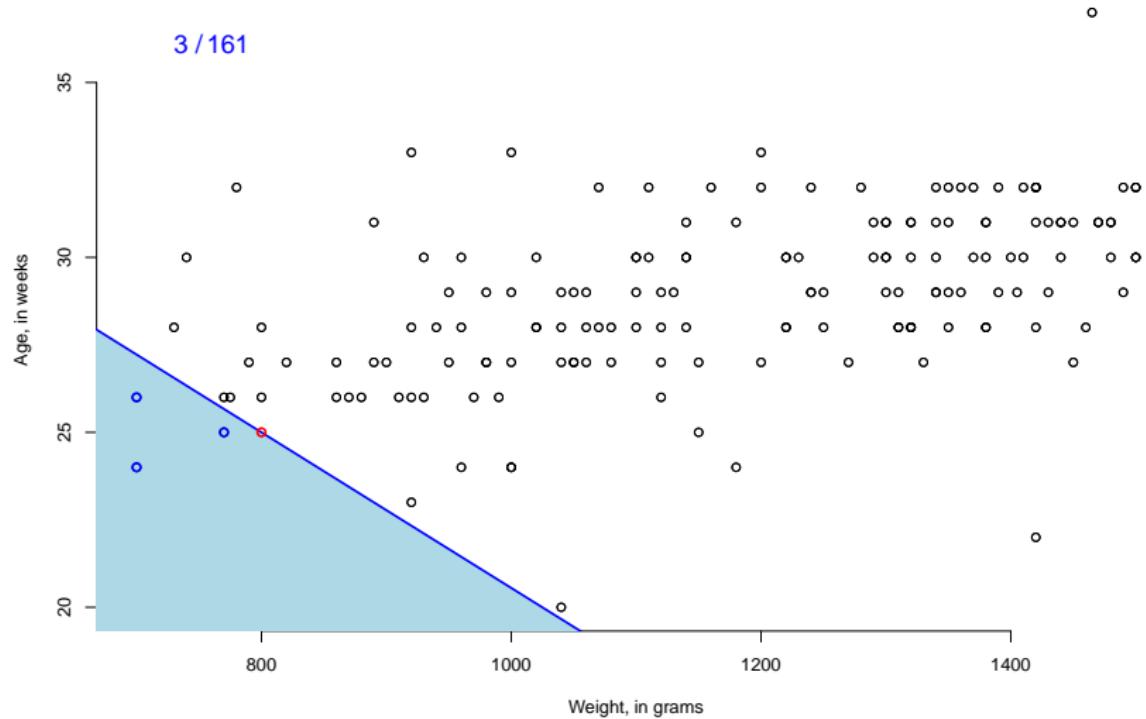


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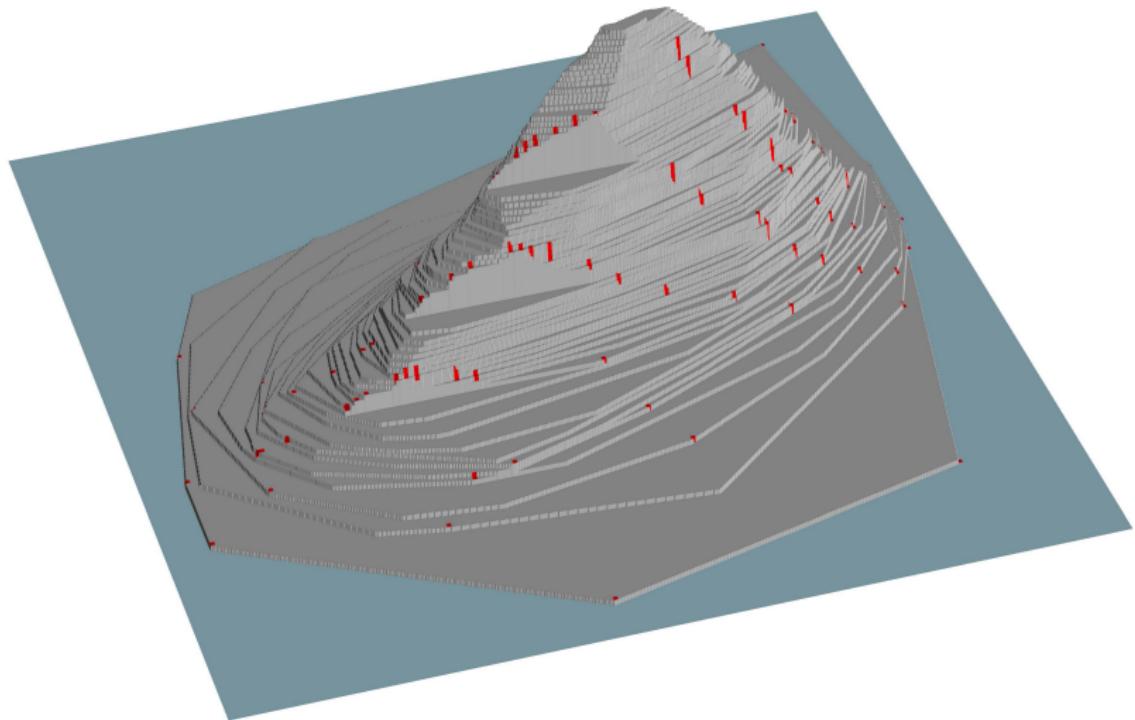


Tukey (=halfspace, location) data depth

Babies with low birth weight



Tukey (=halfspace, location) data depth



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- ▶ 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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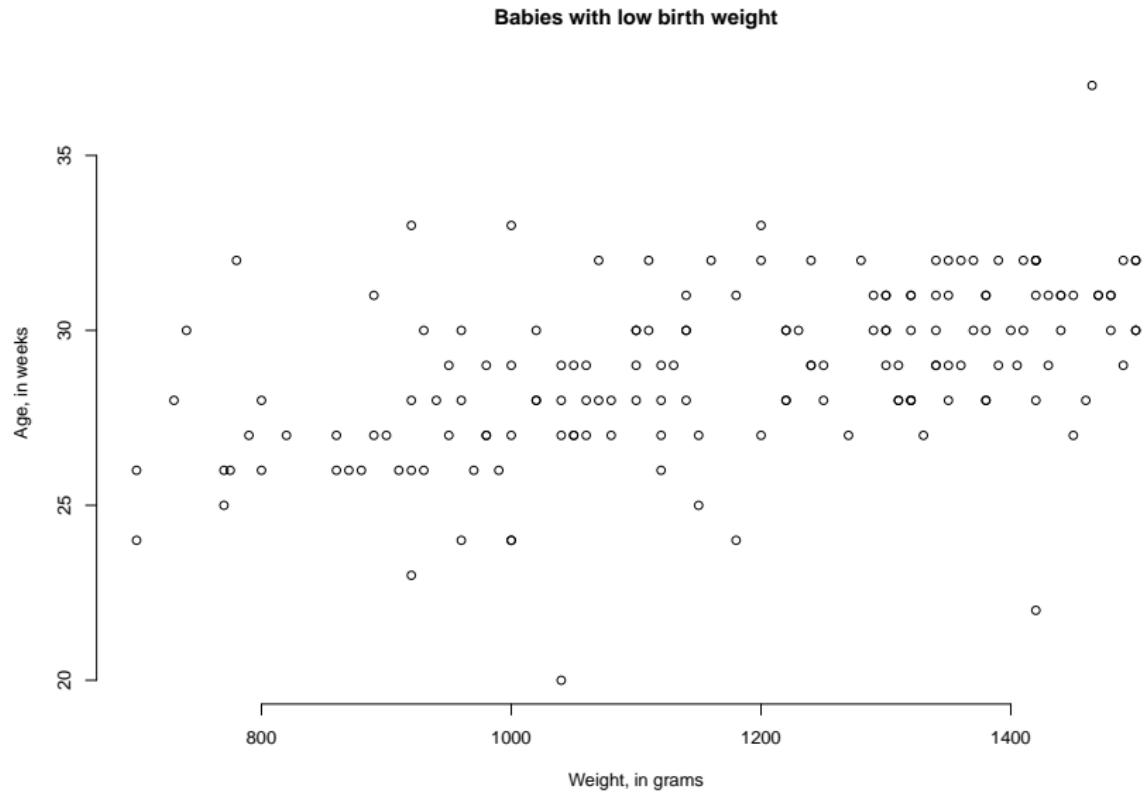
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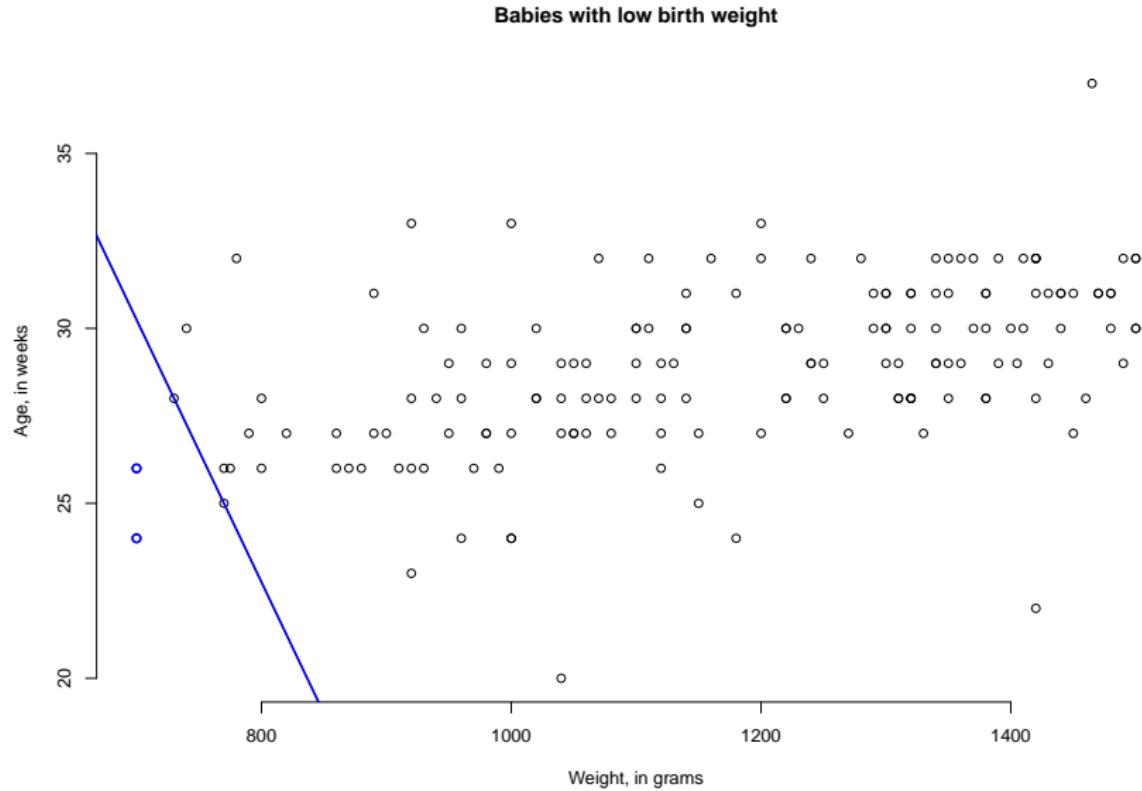
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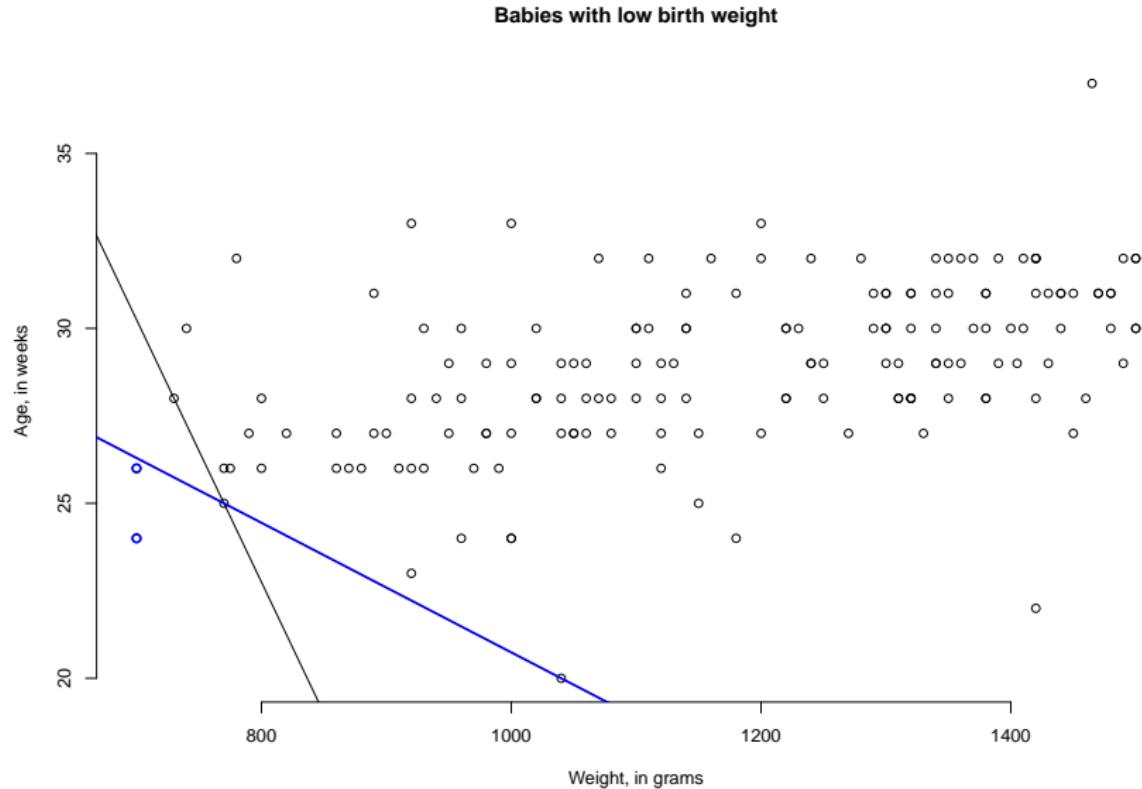
Tukey (=halfspace, location) depth-trimmed regions



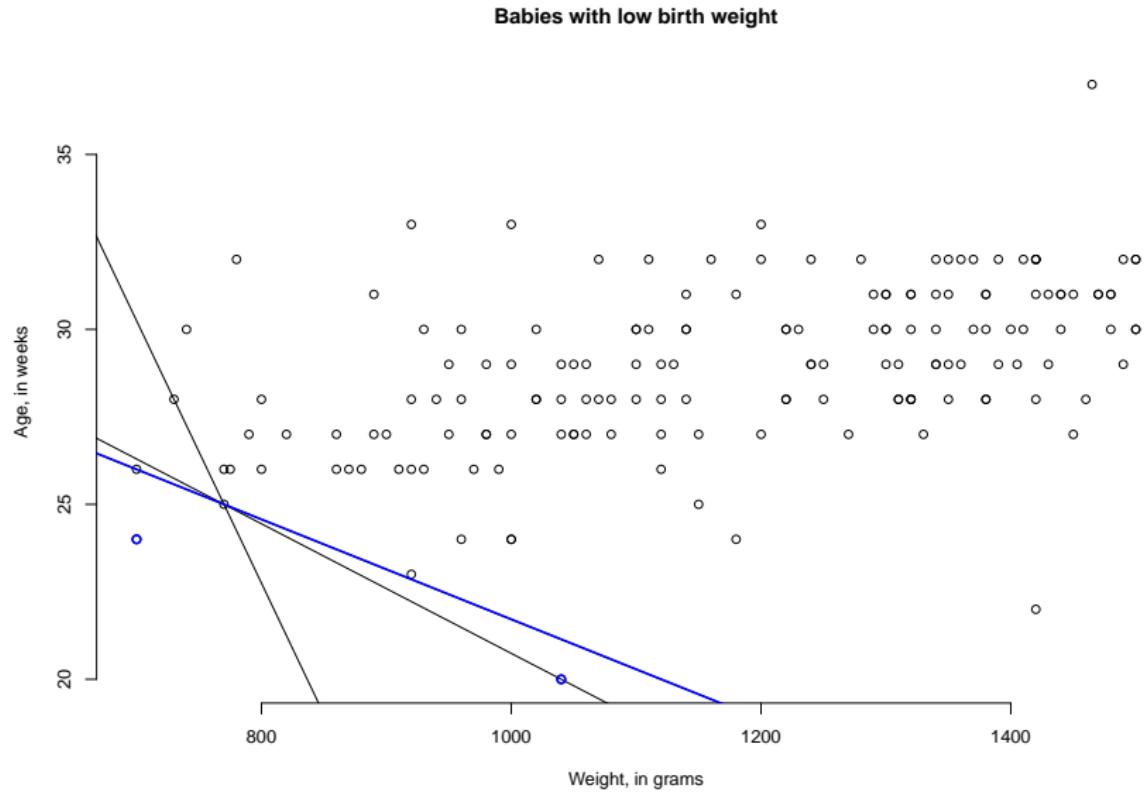
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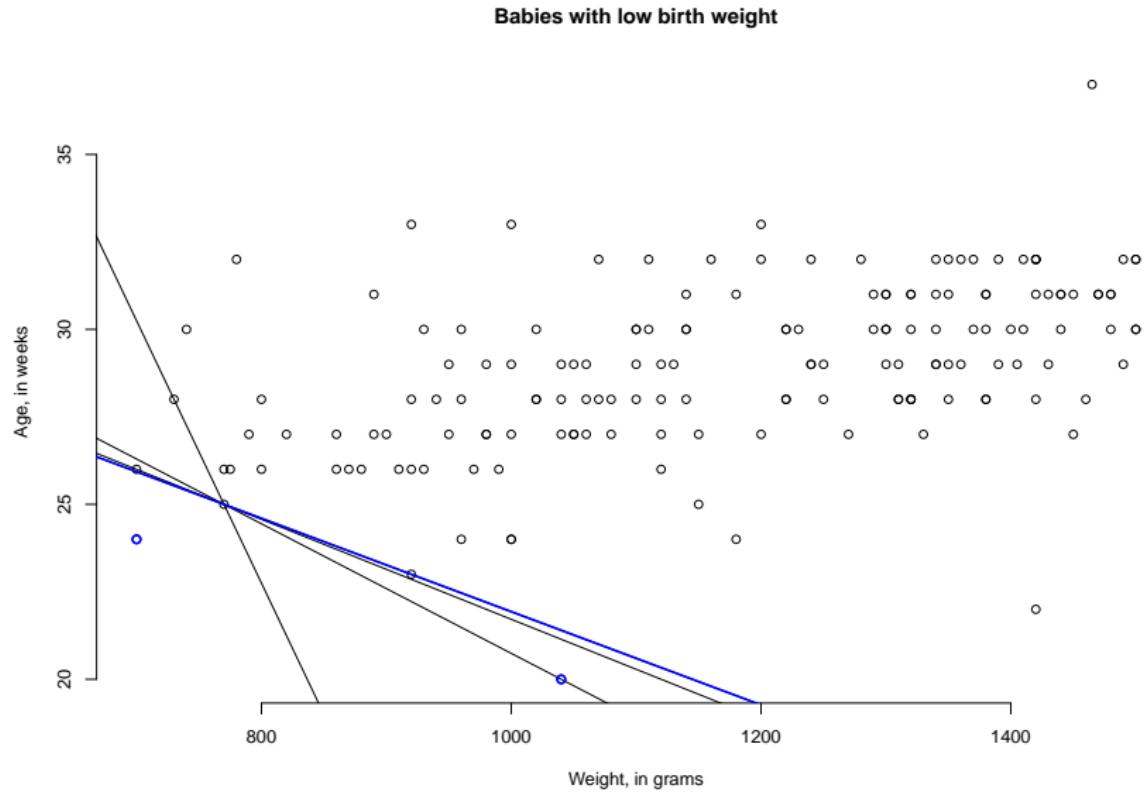
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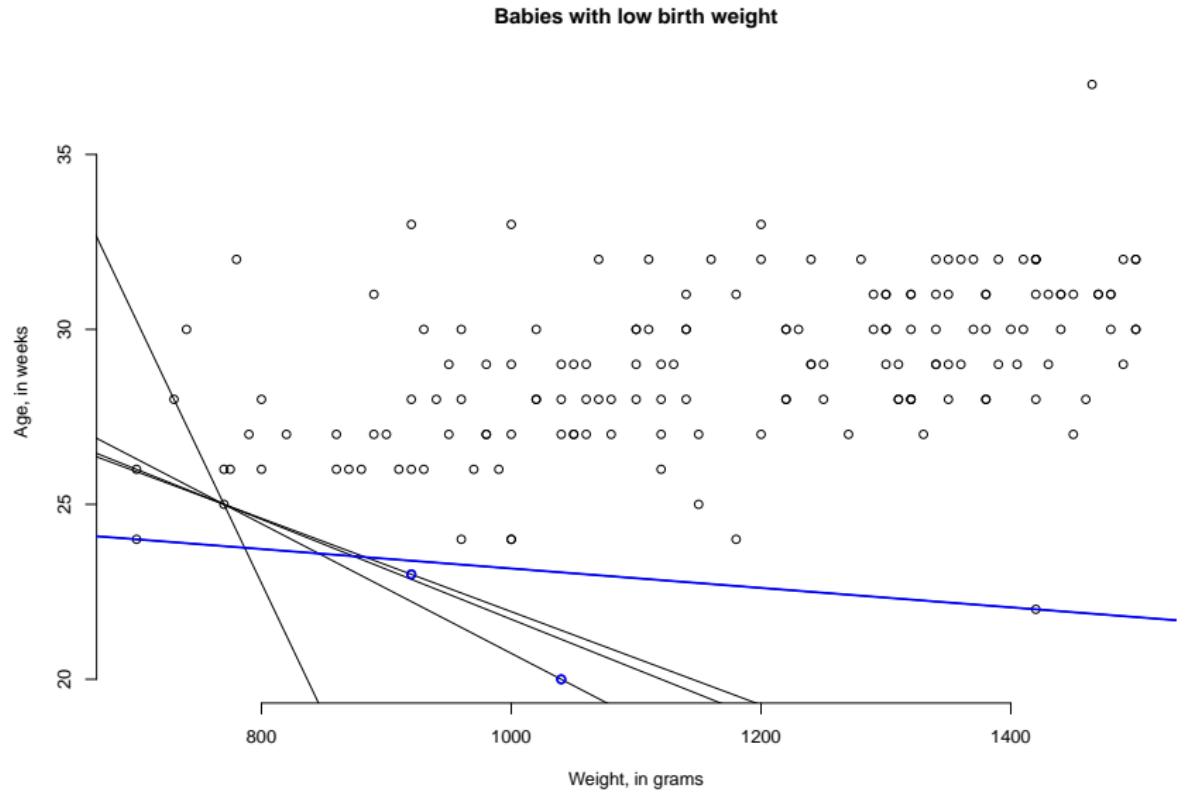
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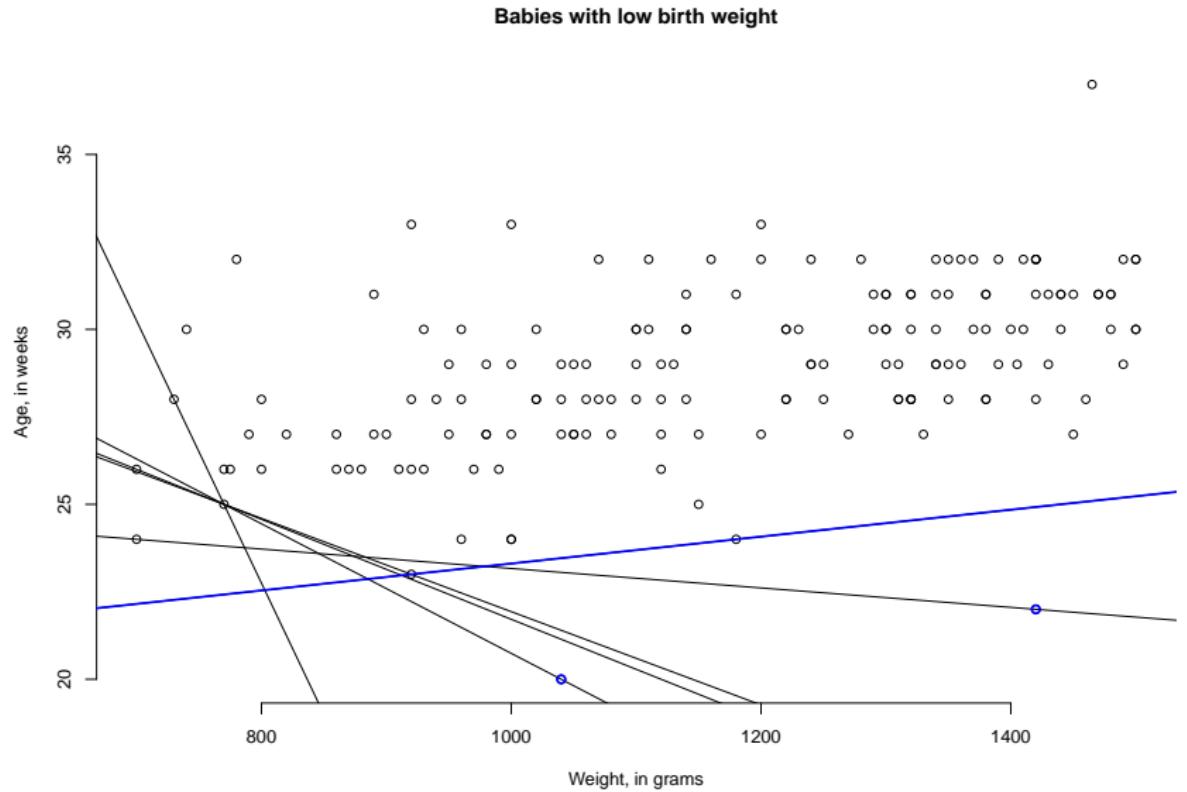
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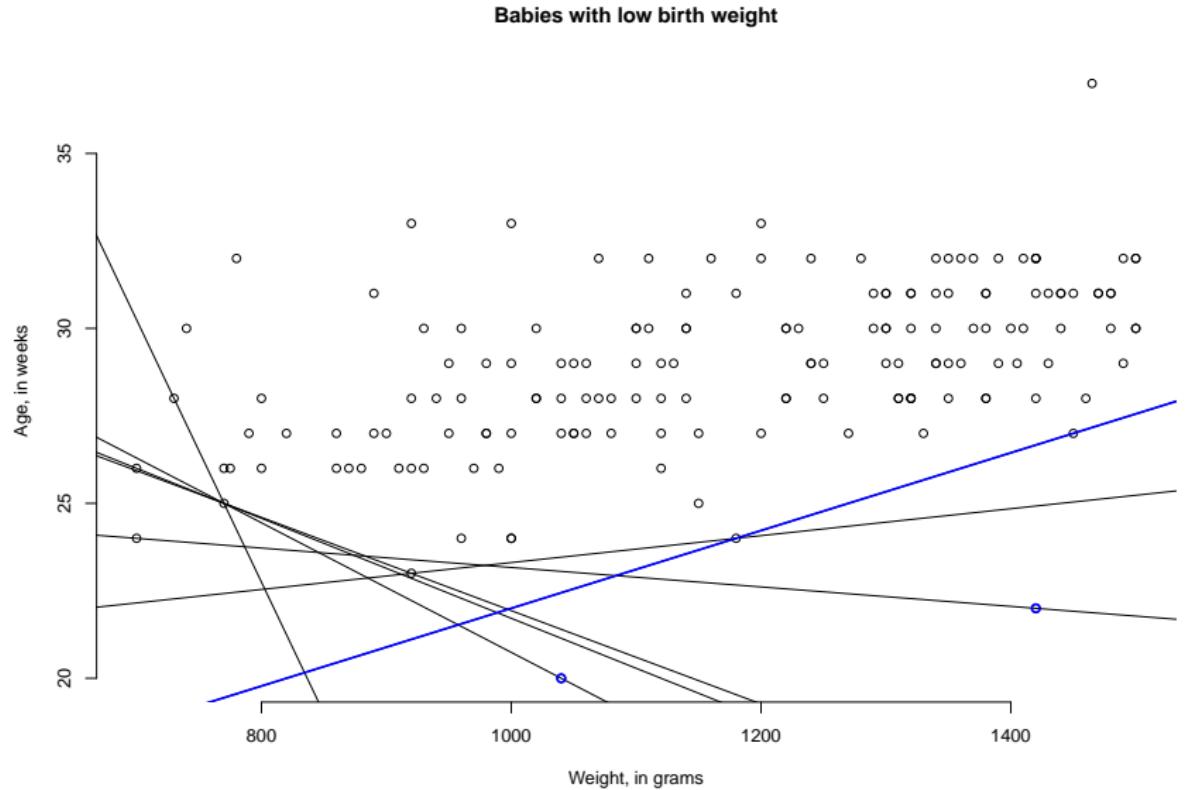
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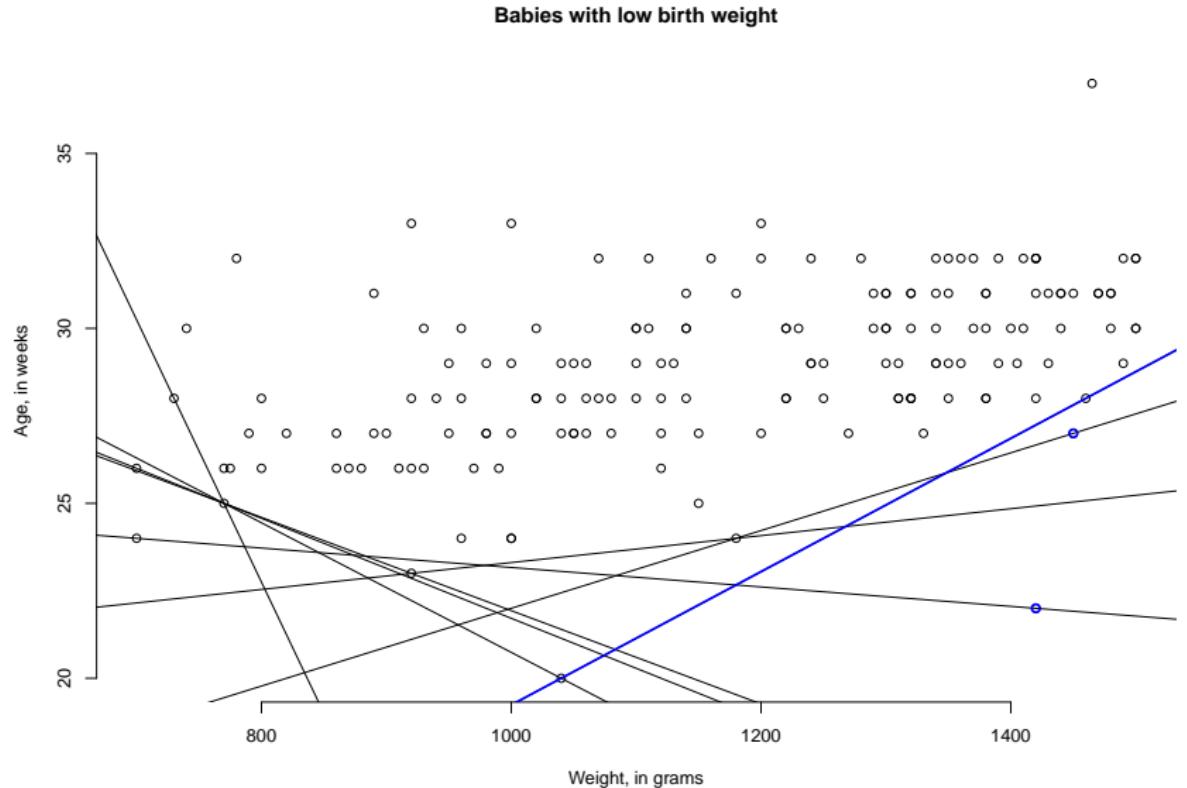
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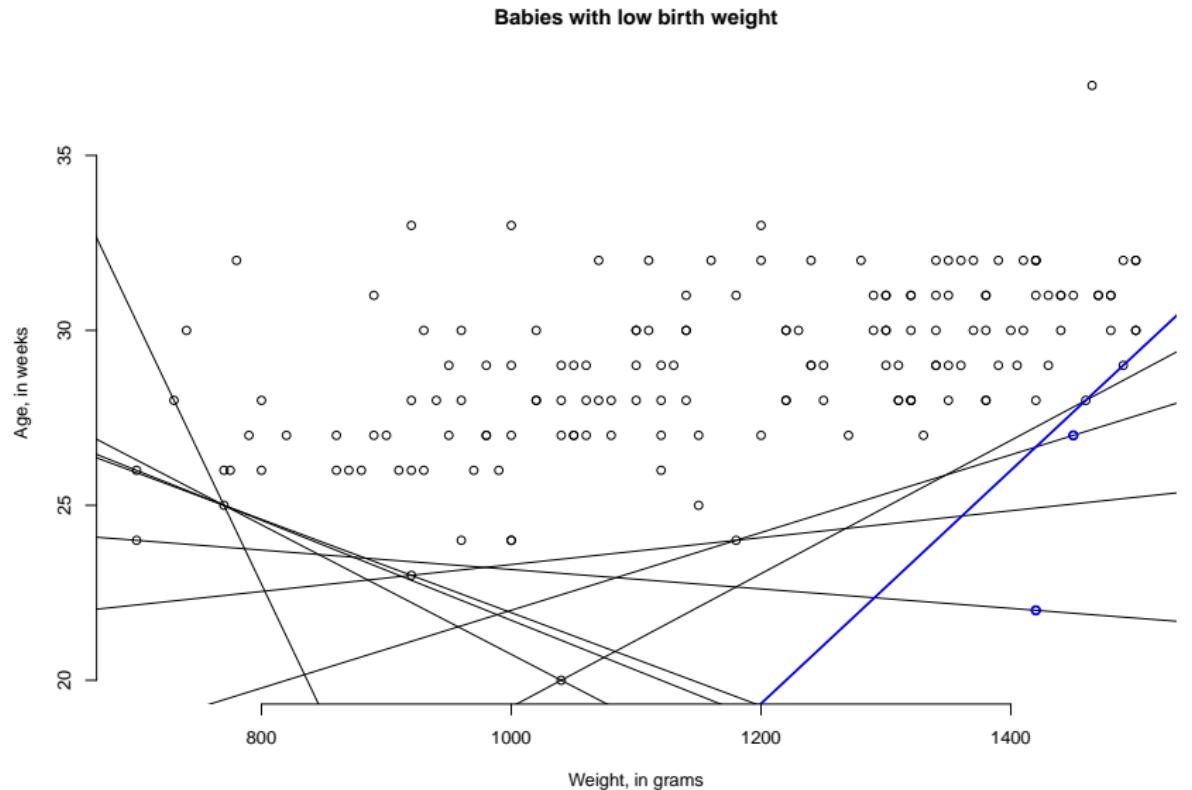
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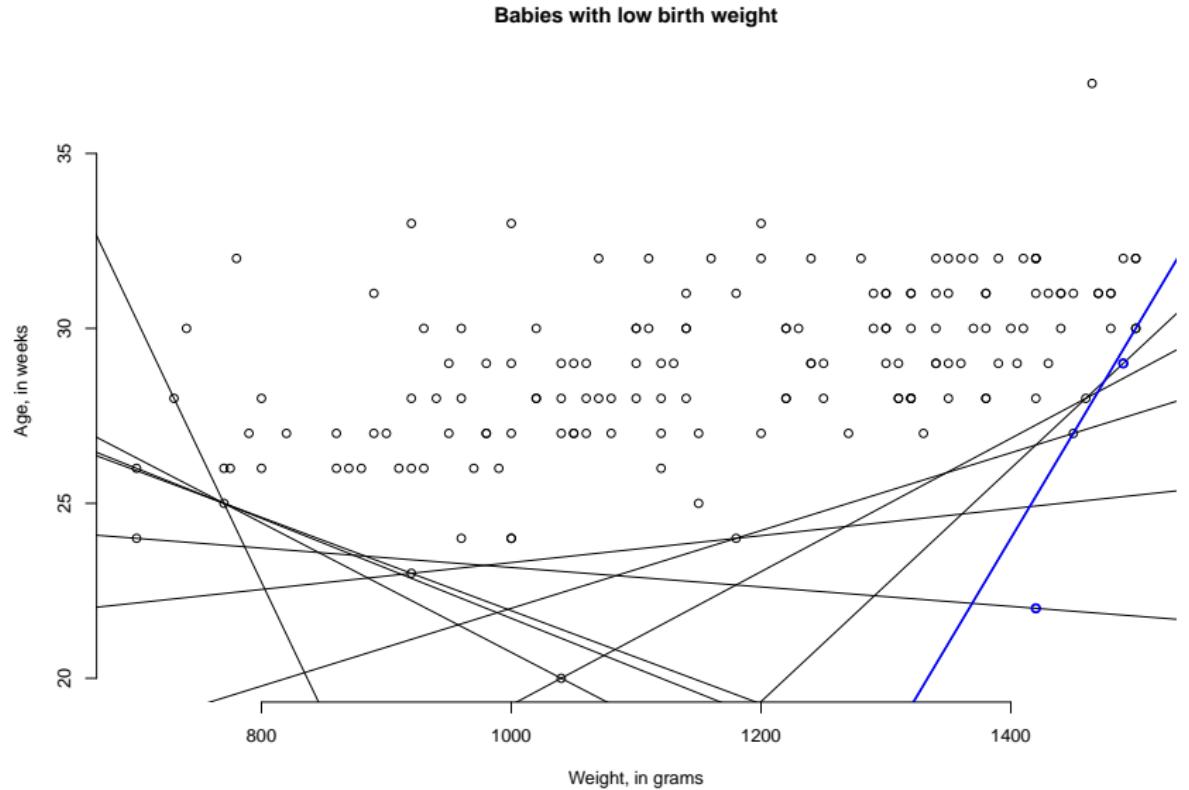
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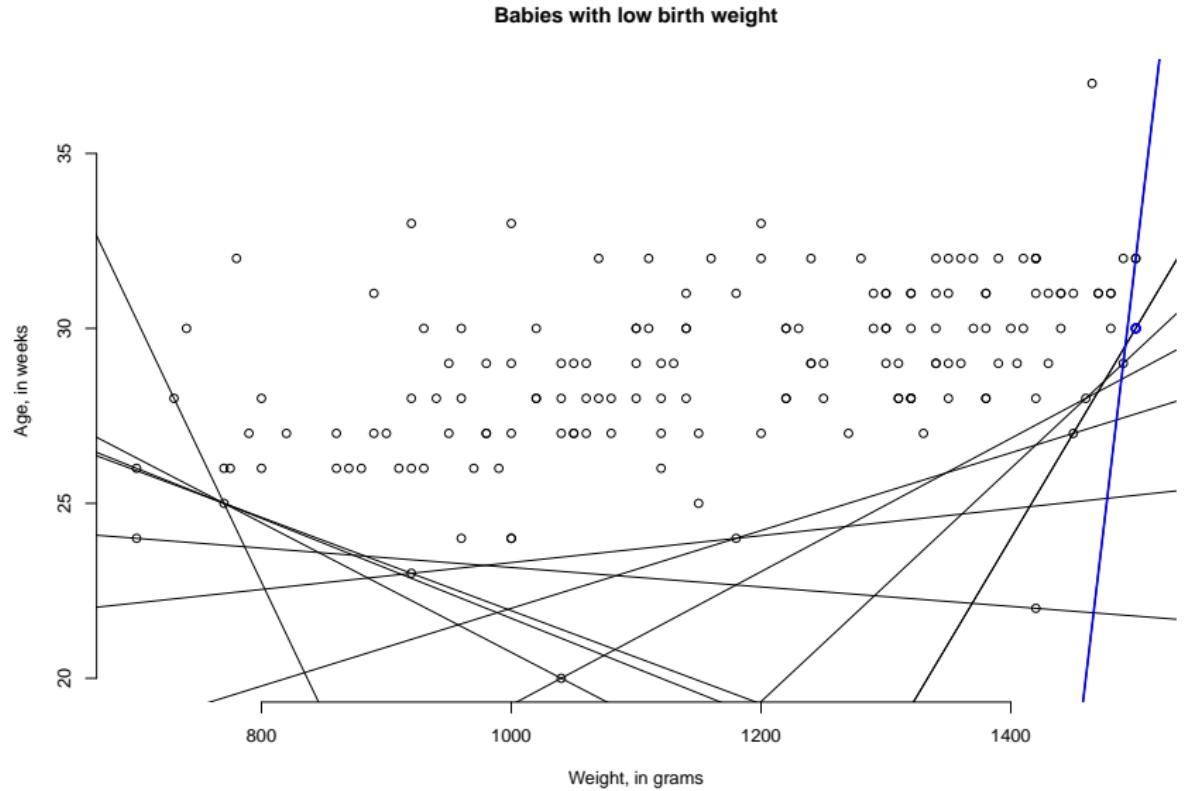
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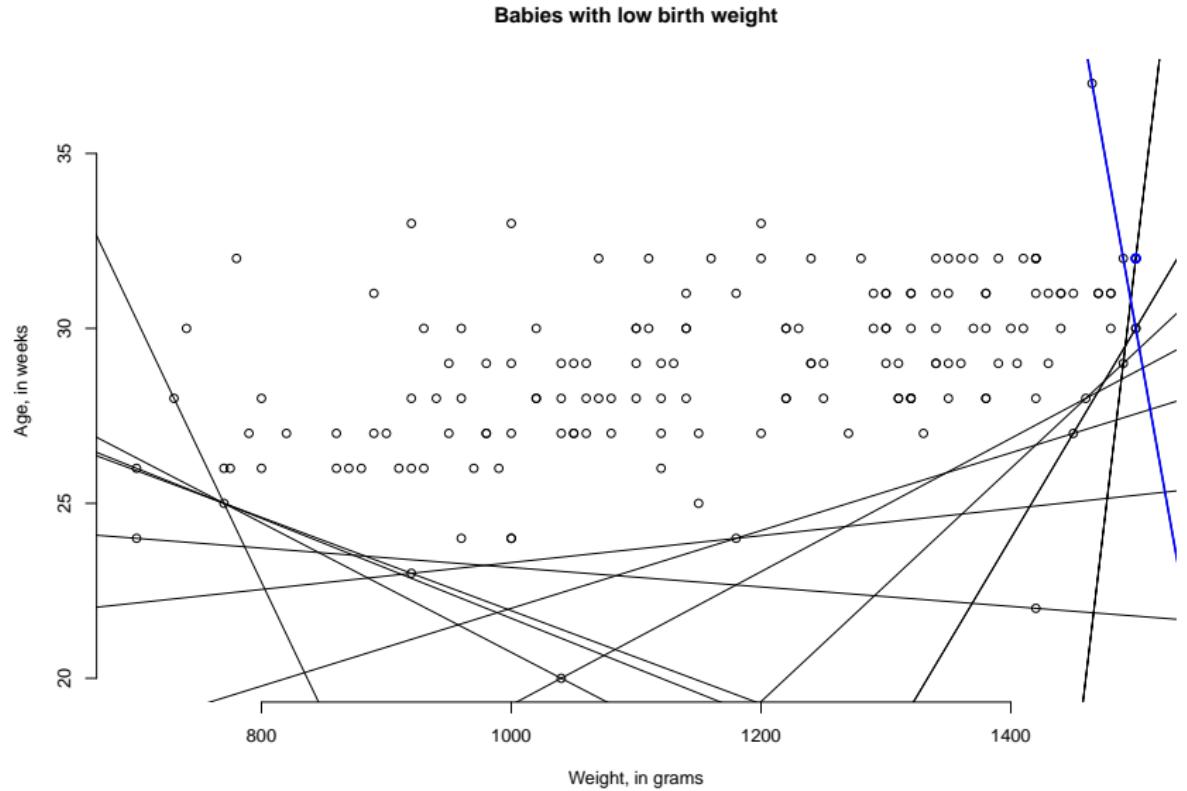
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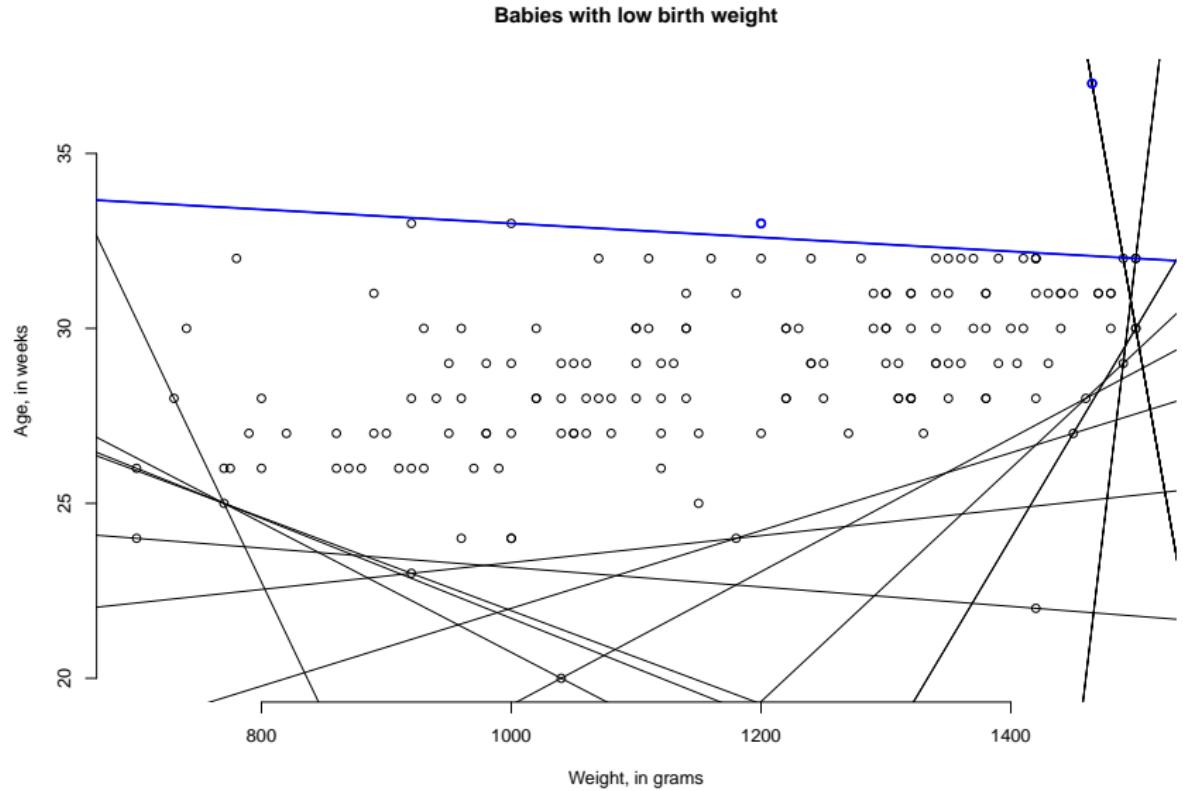
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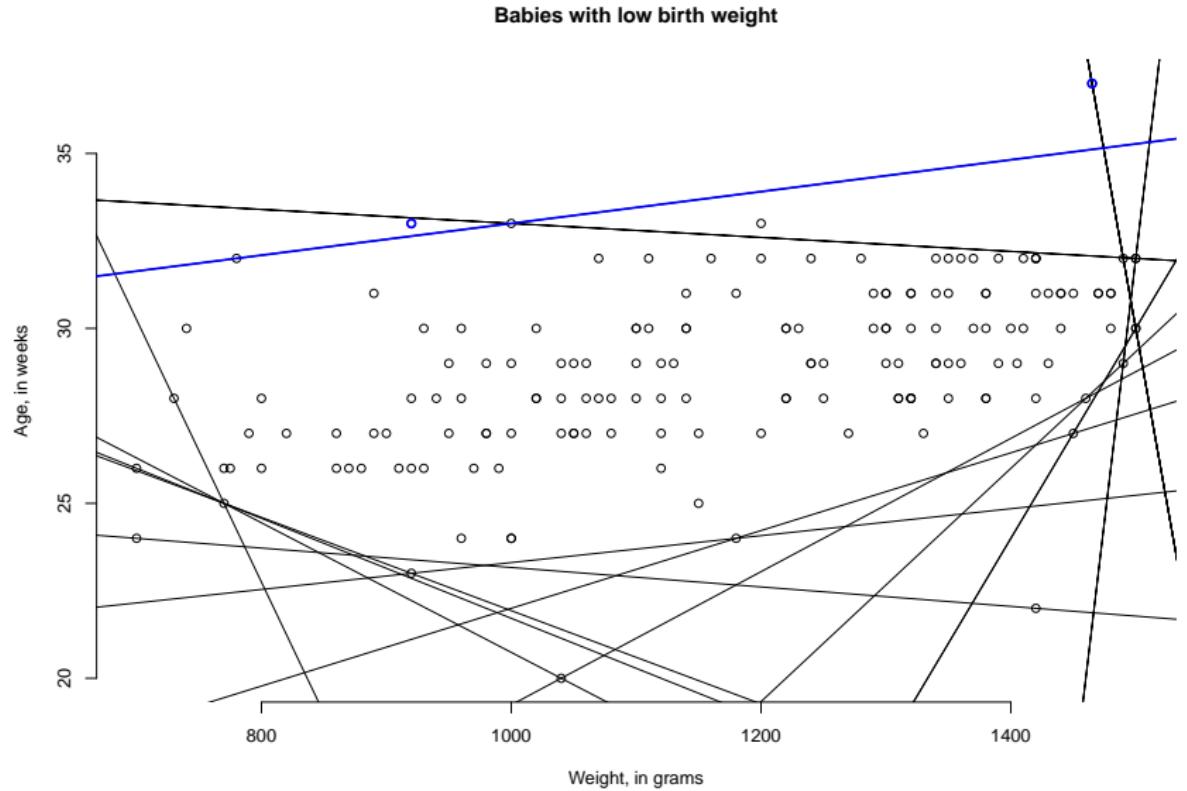
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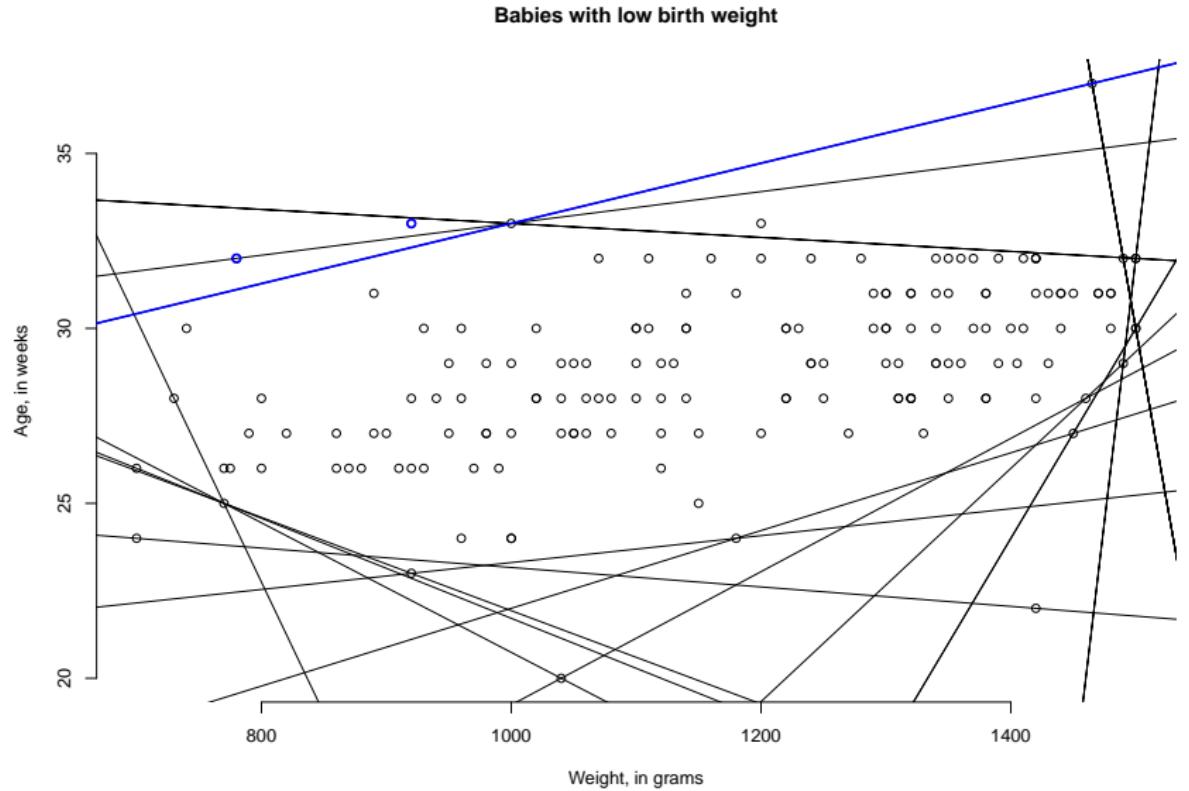
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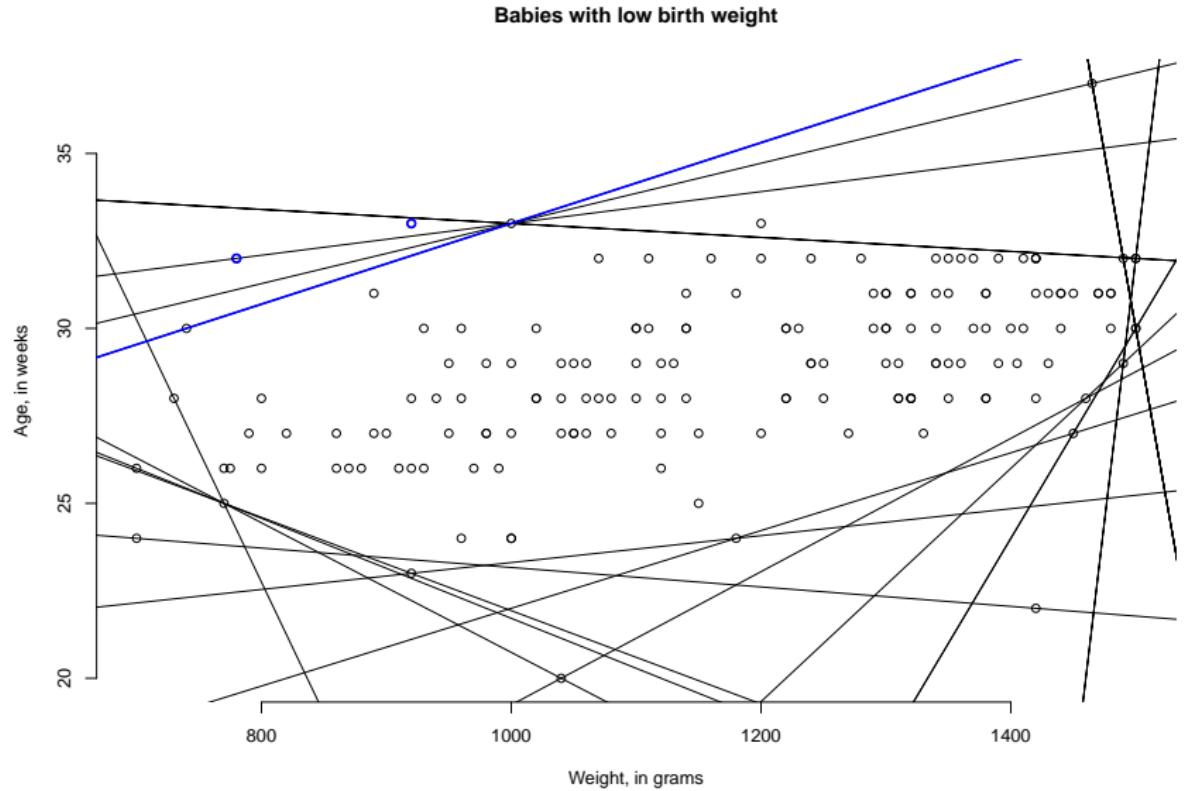
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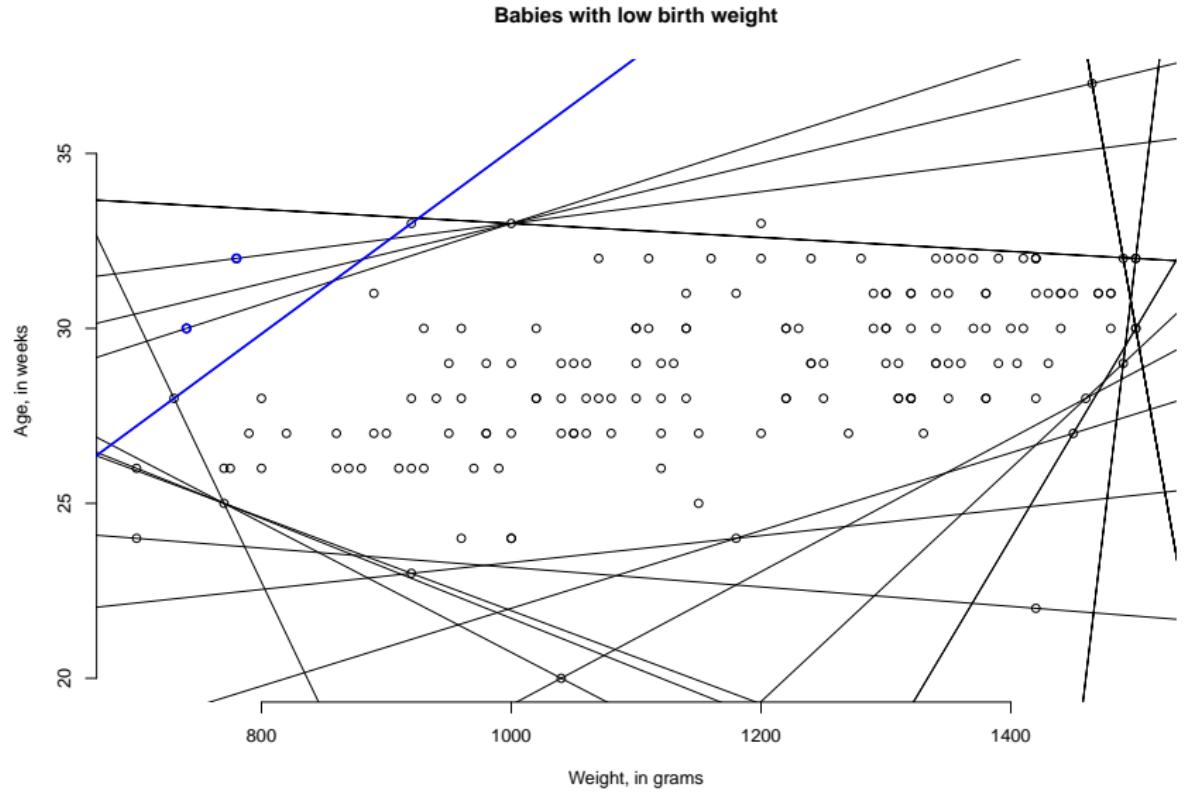
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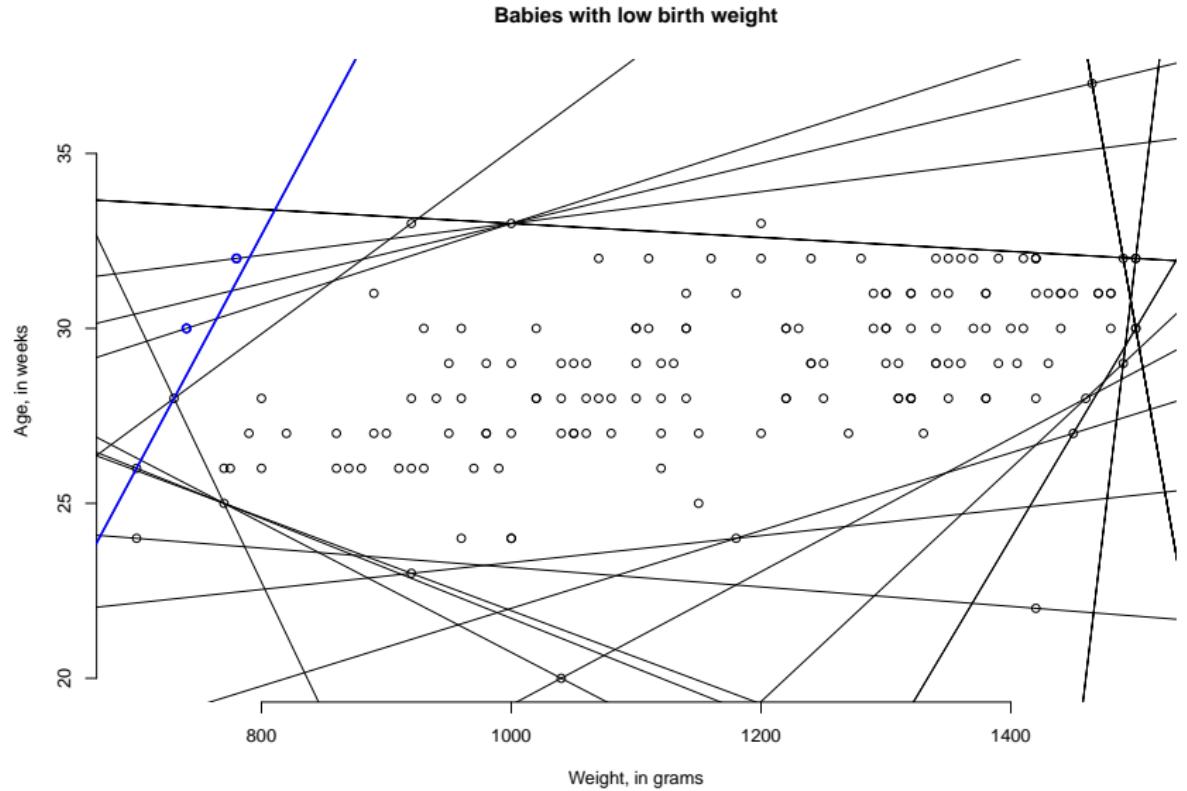
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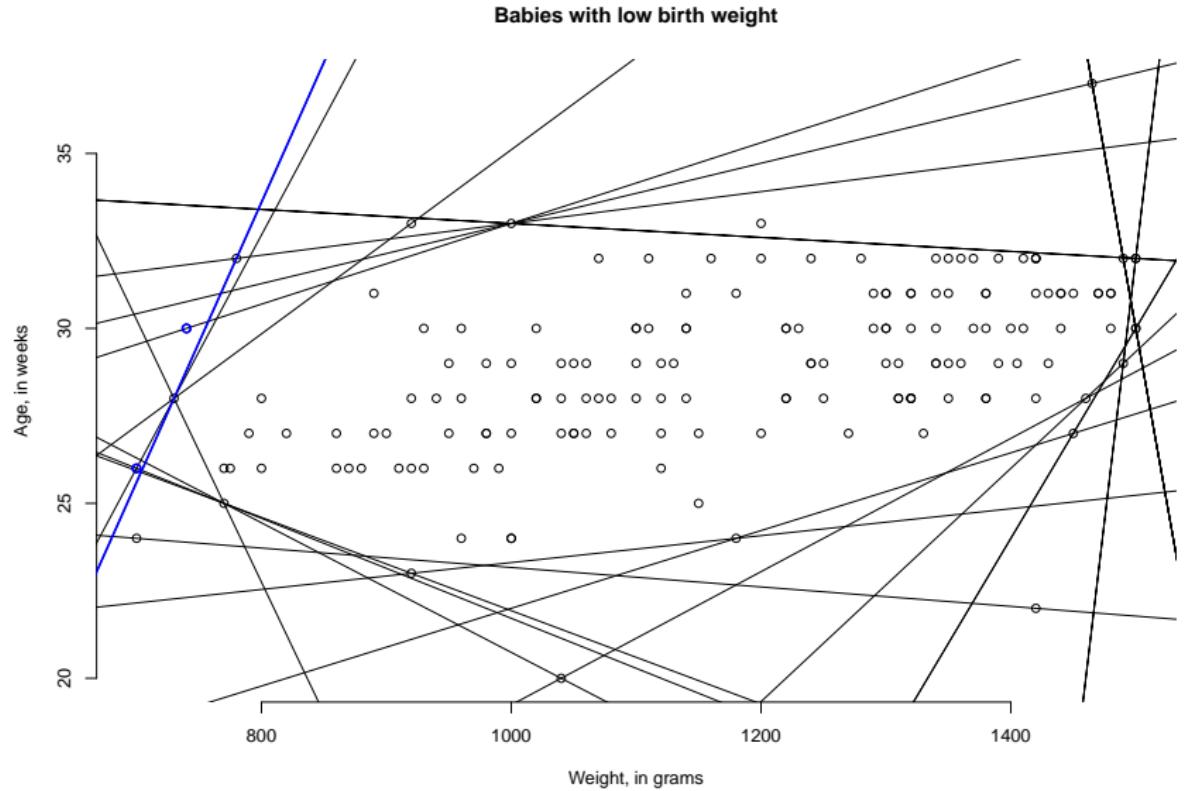
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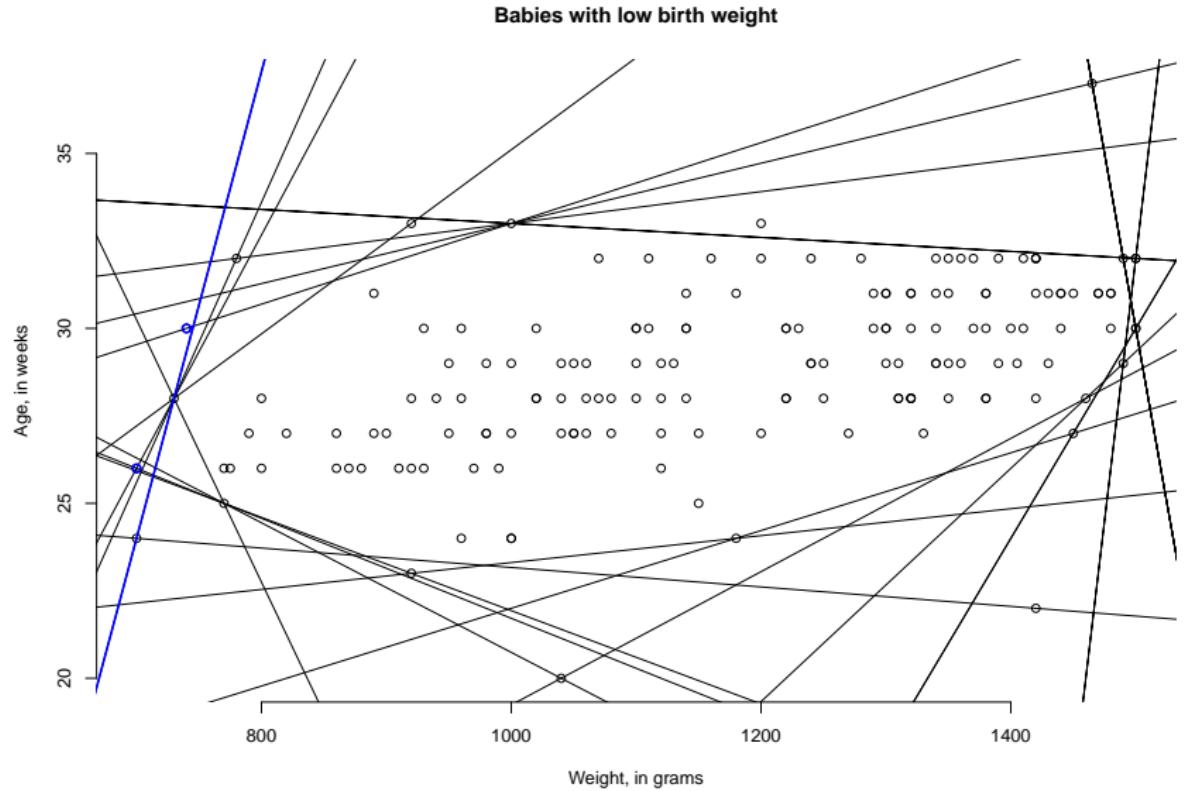
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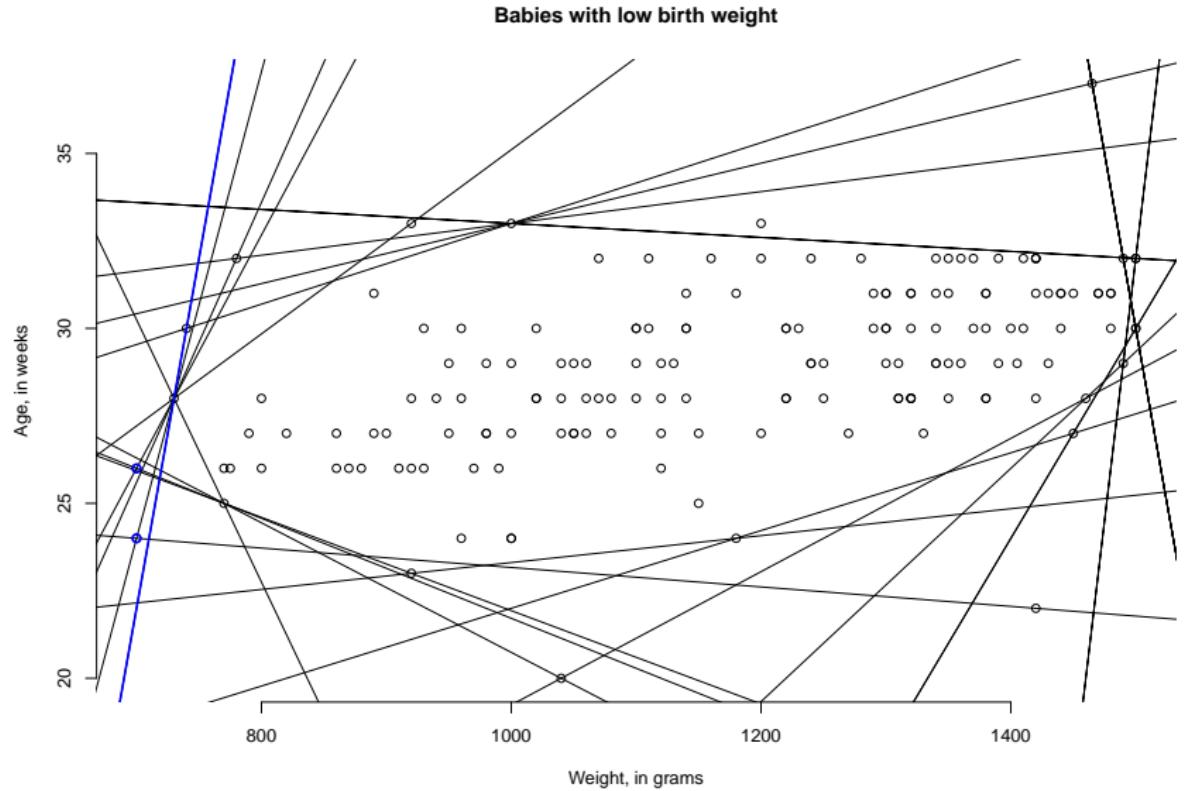
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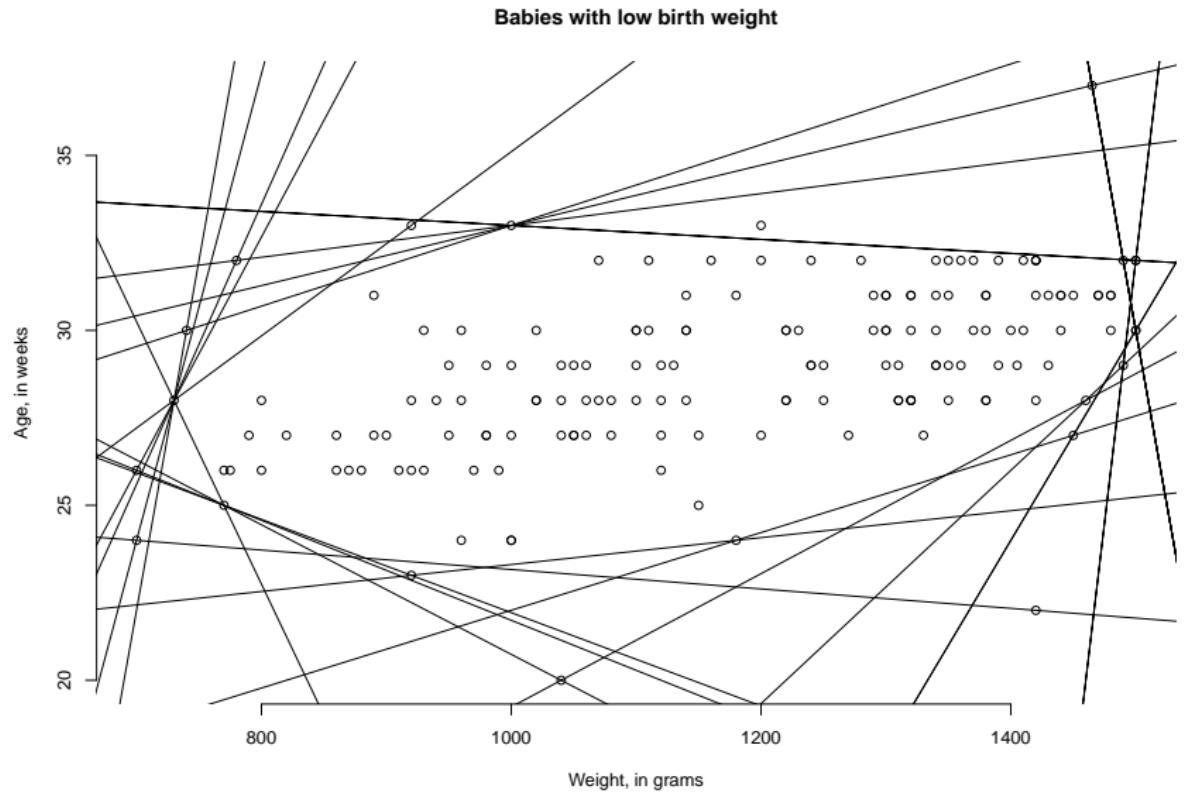
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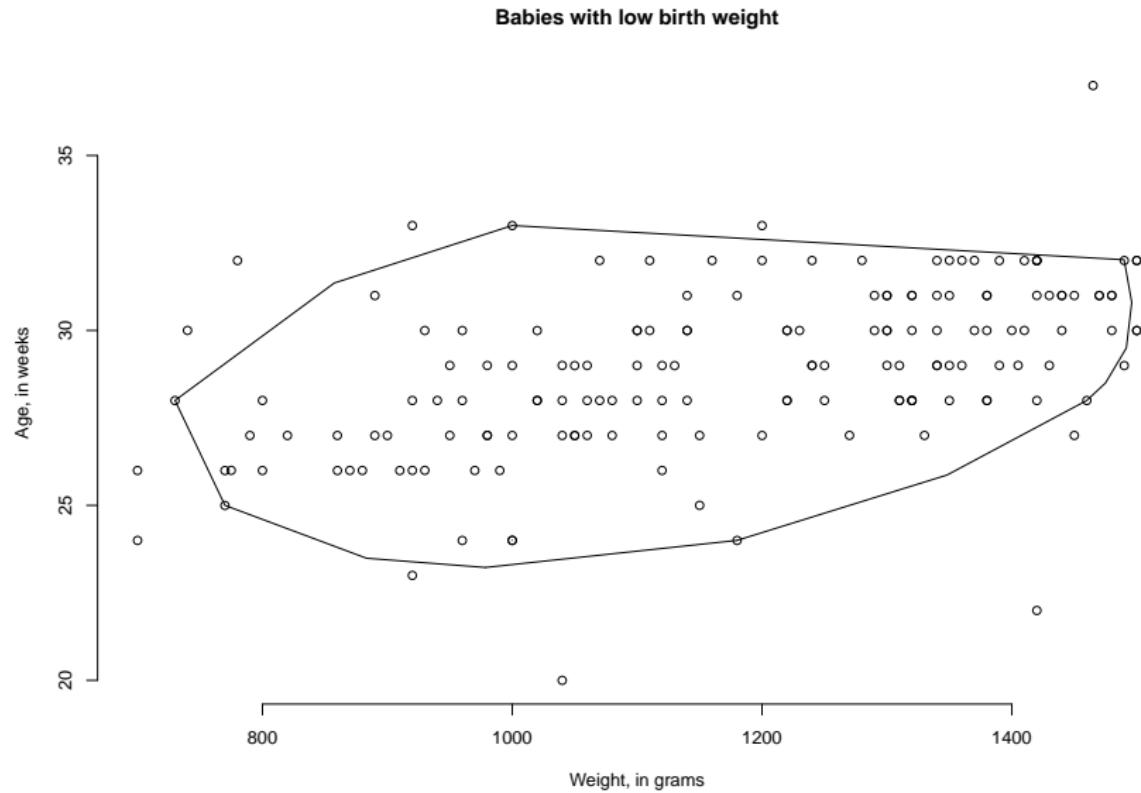
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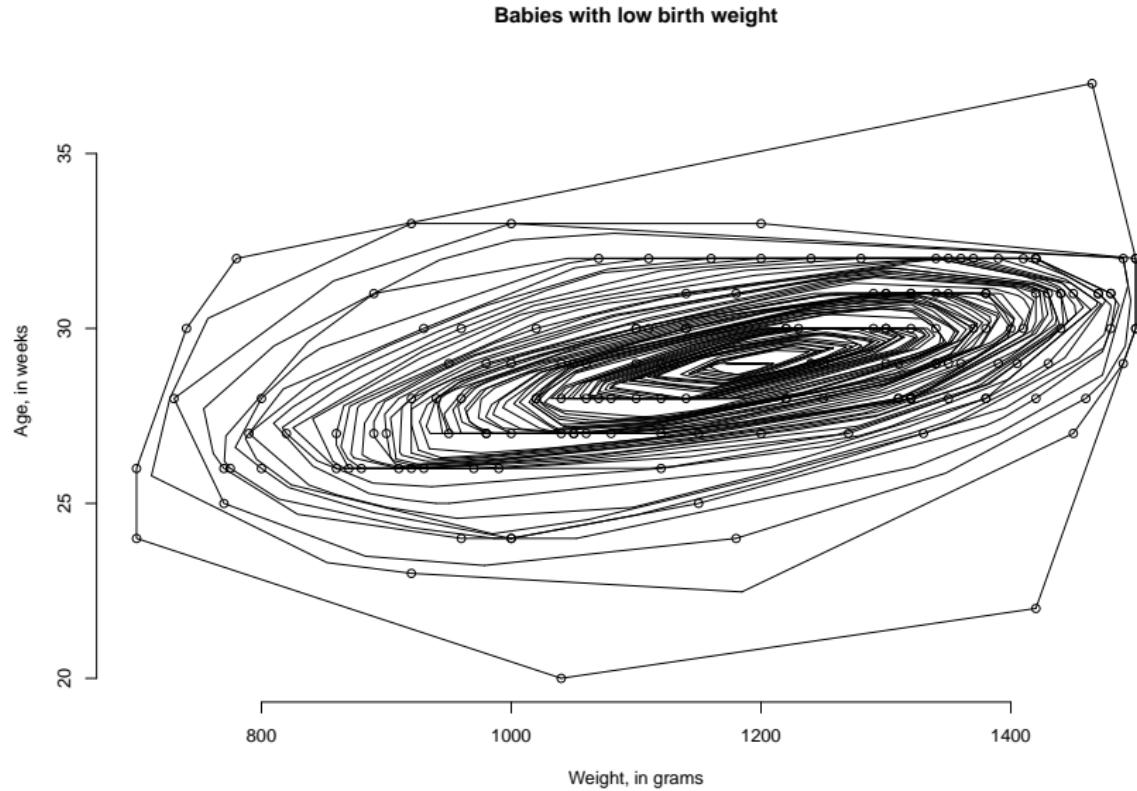
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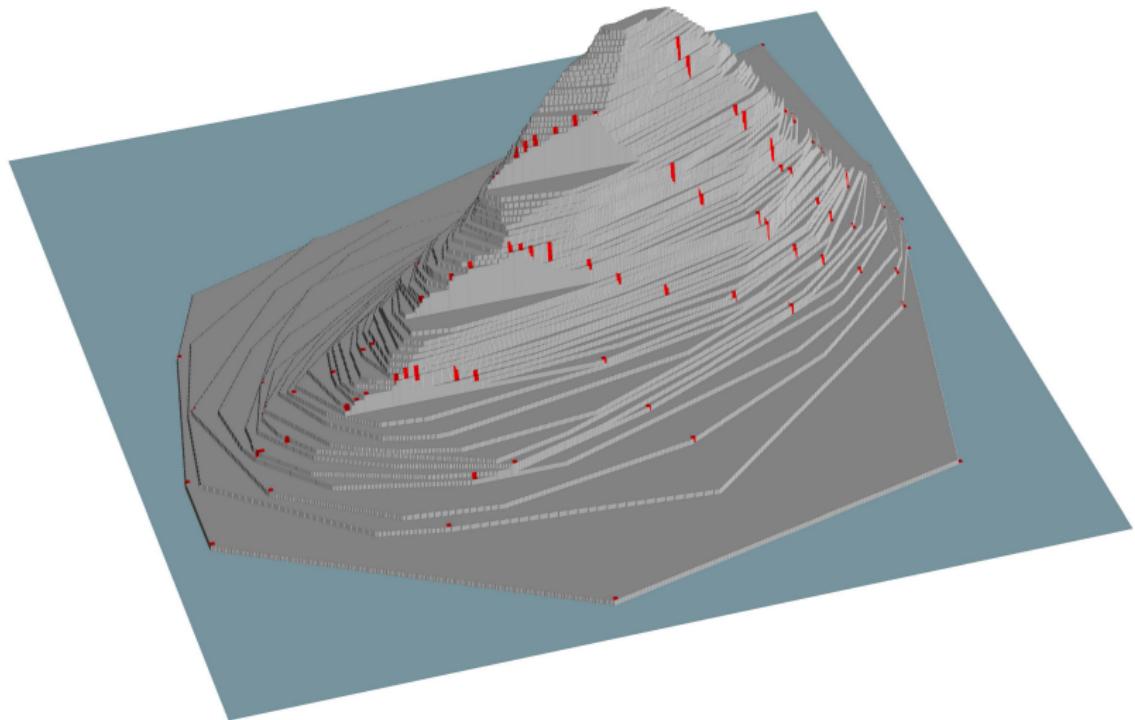
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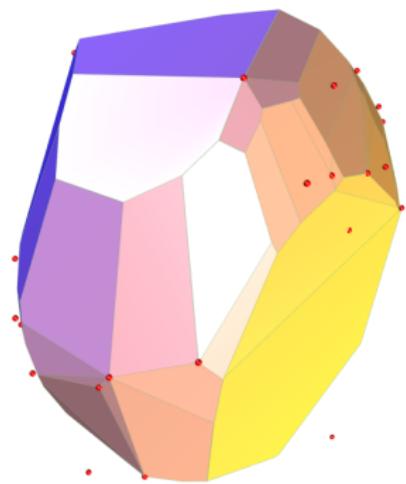
Tukey (=halfspace, location) data depth



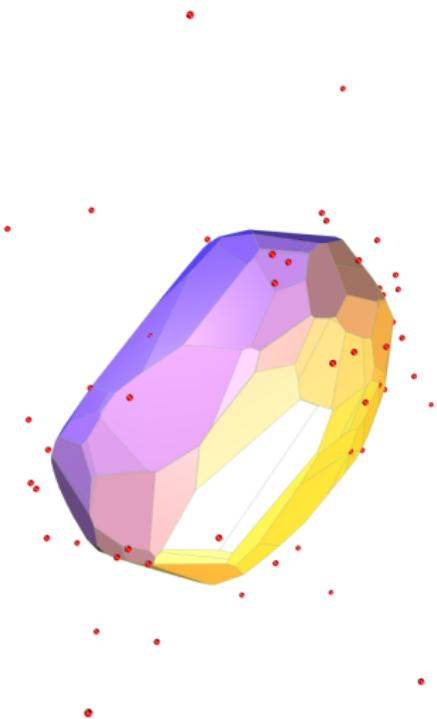
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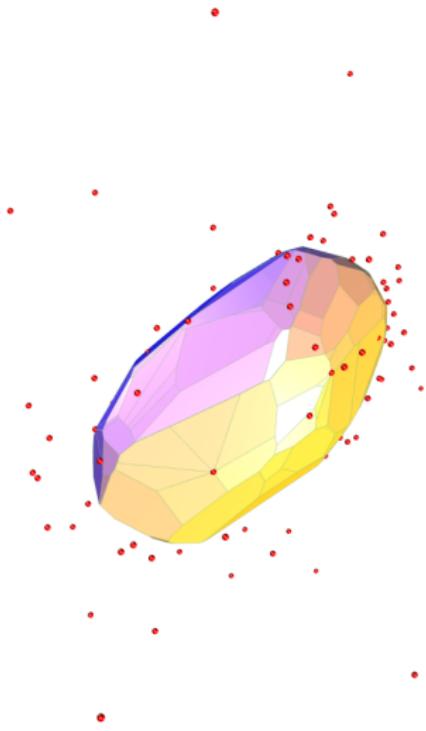
Tukey (=halfspace, location) depth region: $\tau = 2/161$



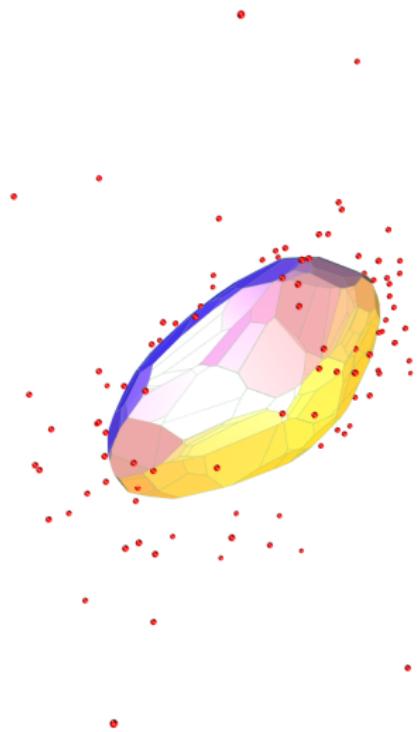
Tukey (=halfspace, location) depth region: $\tau = 5/161$



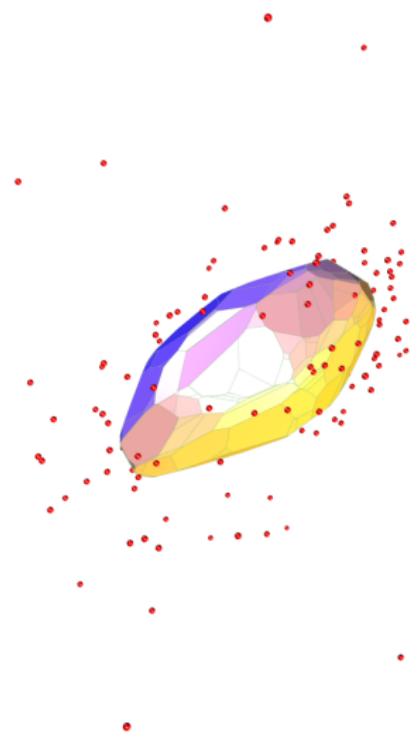
Tukey (=halfspace, location) depth region: $\tau = 9/161$



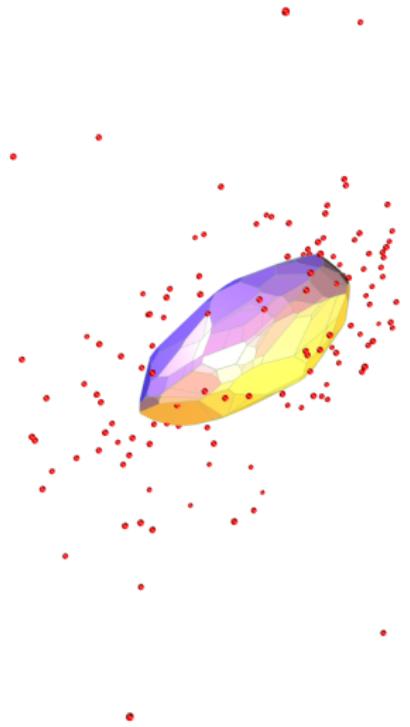
Tukey (=halfspace, location) depth region: $\tau = 13/161$



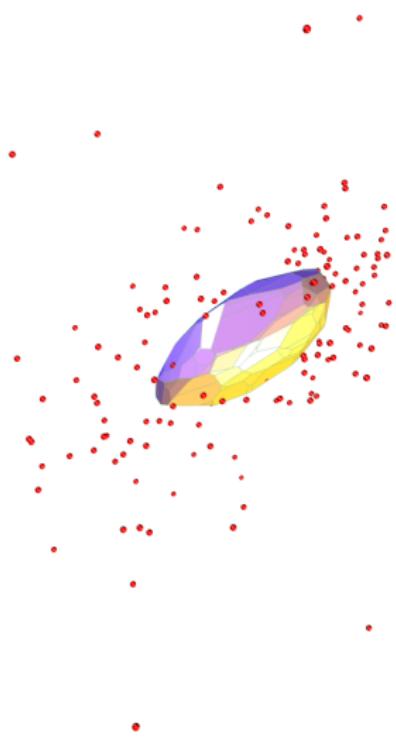
Tukey (=halfspace, location) depth region: $\tau = 17/161$



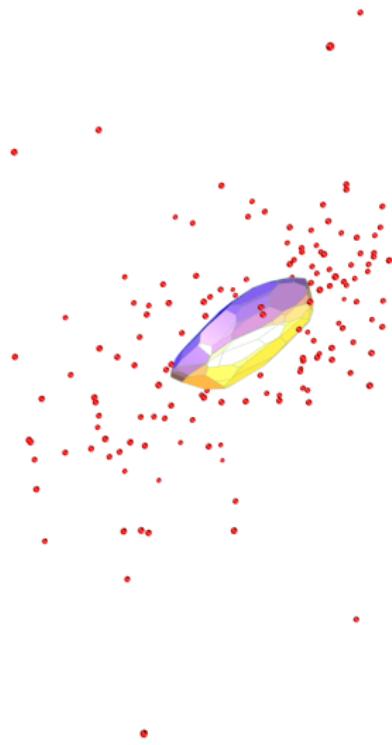
Tukey (=halfspace, location) depth region: $\tau = 25/161$



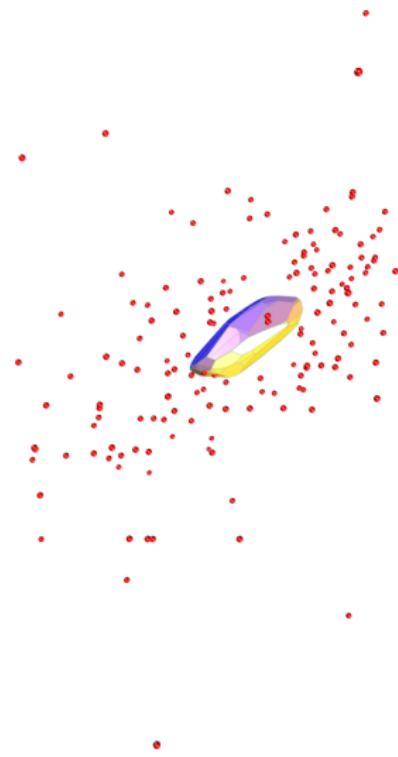
Tukey (=halfspace, location) depth region: $\tau = 33/161$



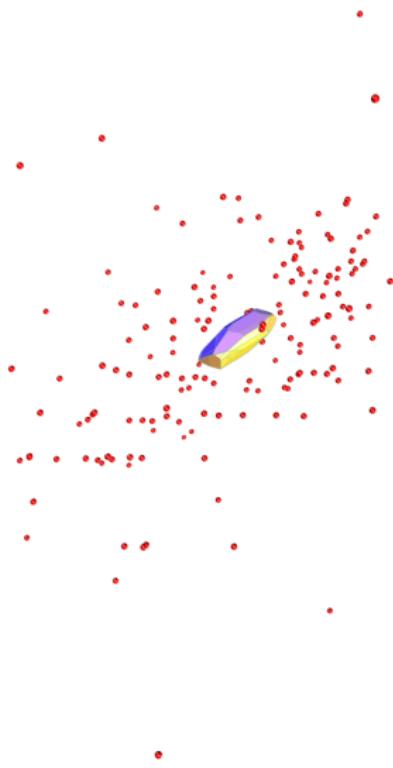
Tukey (=halfspace, location) depth region: $\tau = 41/161$



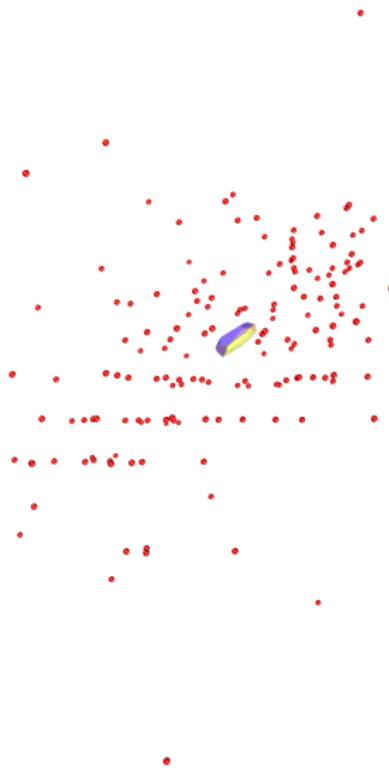
Tukey (=halfspace, location) depth region: $\tau = 49/161$



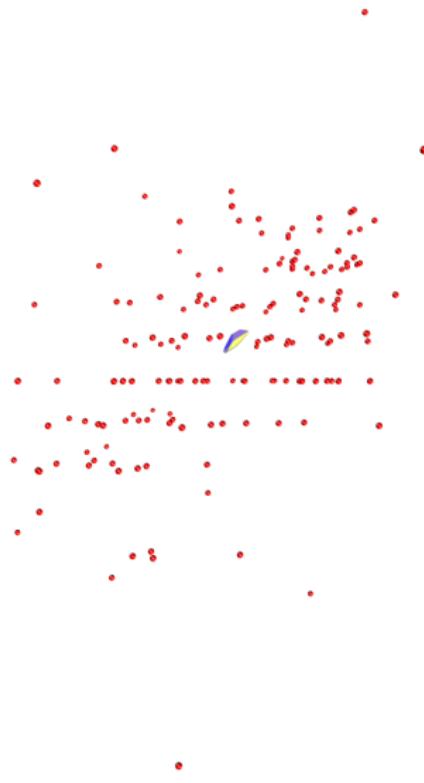
Tukey (=halfspace, location) depth region: $\tau = 57/161$



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Mahalanobis depth (Mahalanobis, 1936)

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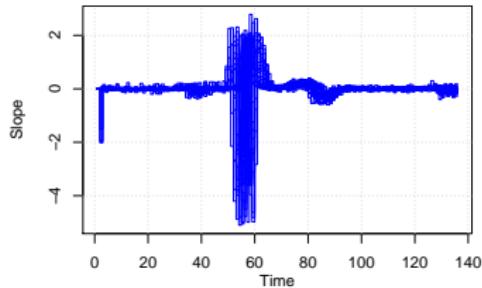
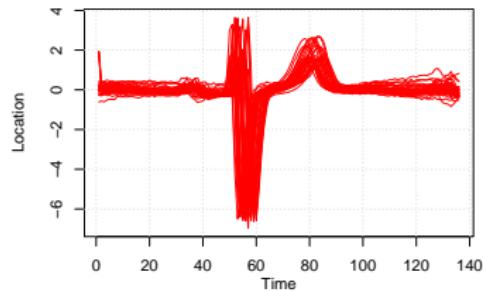
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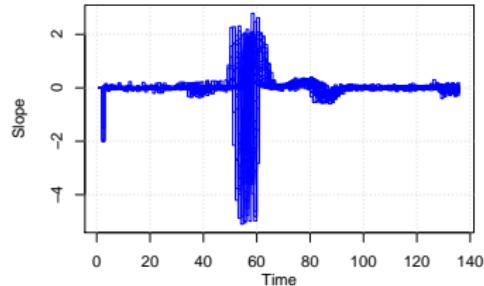
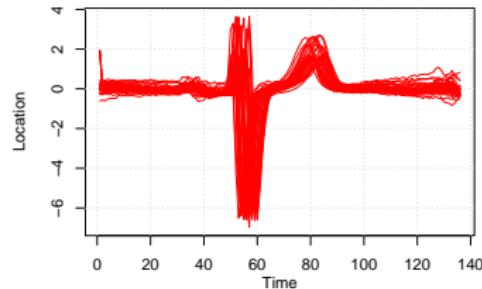
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 - ▶ by a single elliptical contour characterizes a multivariate **normal distribution** or one within an affine **family of non-degenerate elliptical distributions**.

ECG five days data



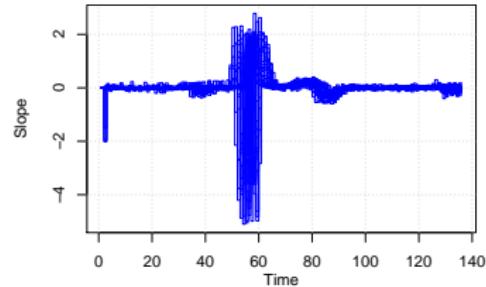
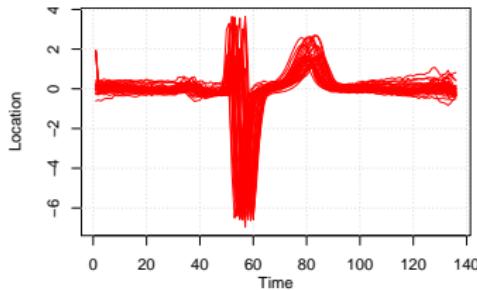
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$$\hat{f}_i \mapsto \mathbf{x}_i = \left[\int_0^T \hat{f}_i(t) dt, \int_0^T \hat{f}'_i(t) dt \right],$$

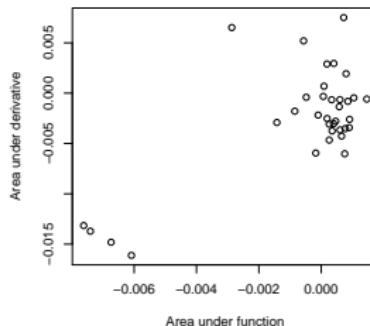
with $\hat{f}_i(t)$ being the function obtained by connecting the points $(t_{ij}, f_i(t_{ij})), j = 1, \dots, N_i$ with line segments, $\hat{f}'_i(t)$ its derivative.

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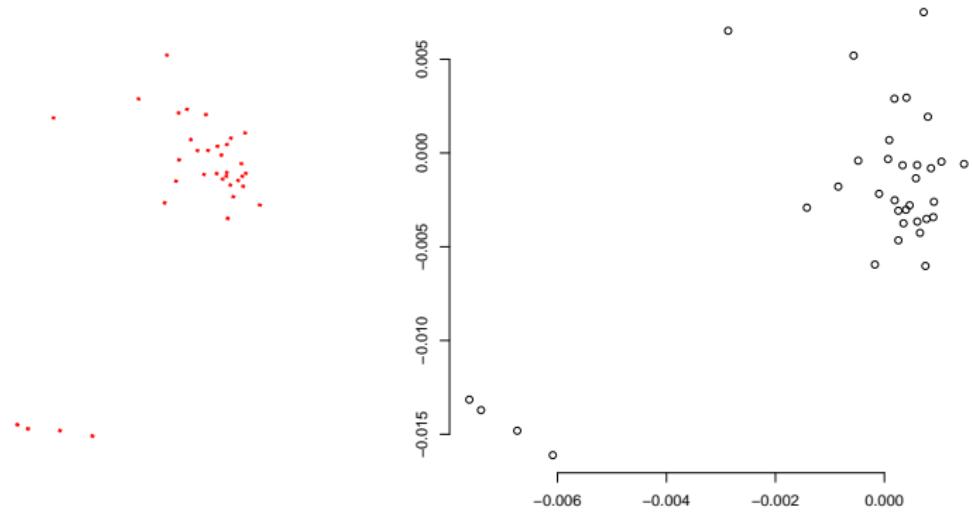


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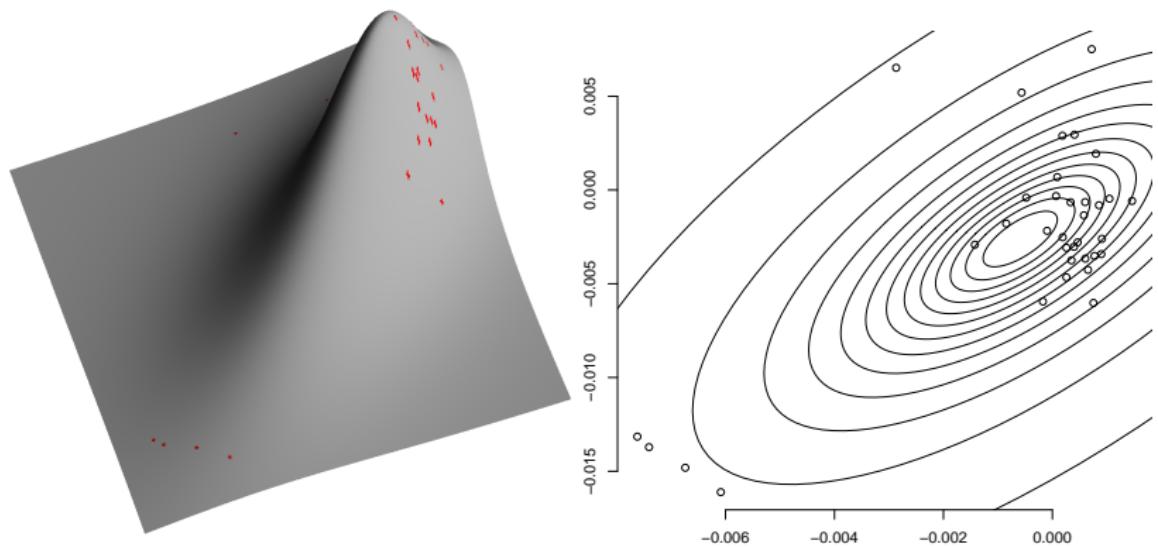
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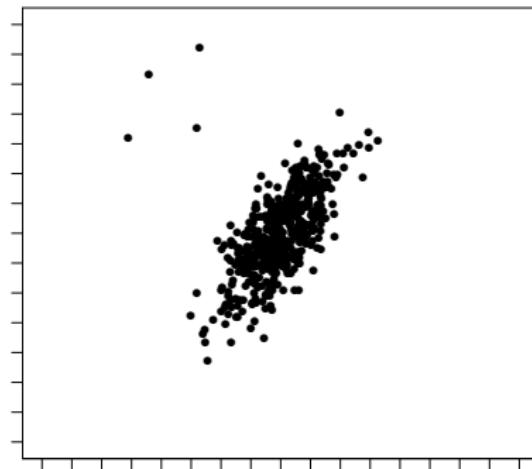
Mahalanobis depth (Mahalanobis, 1936)



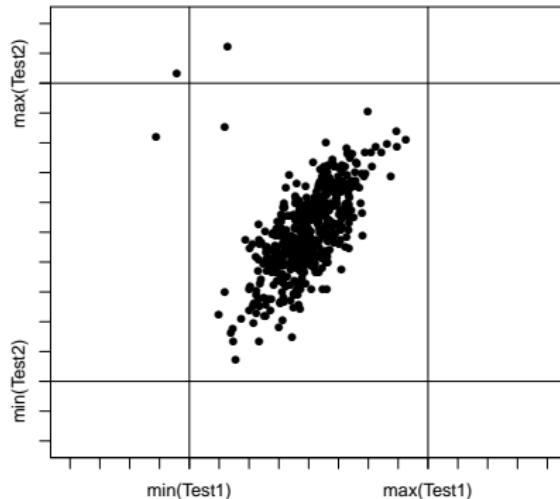
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Multivariate anomaly detection: an example

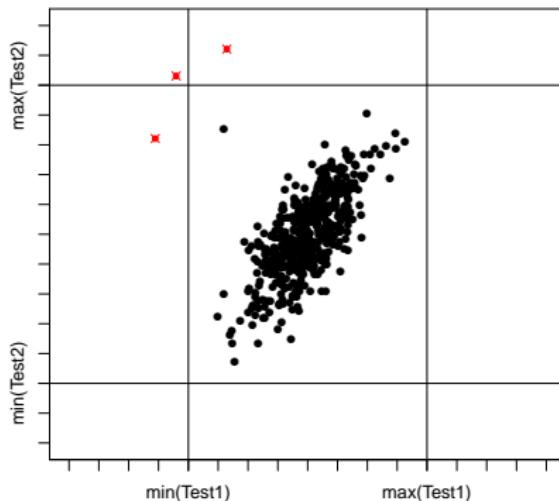


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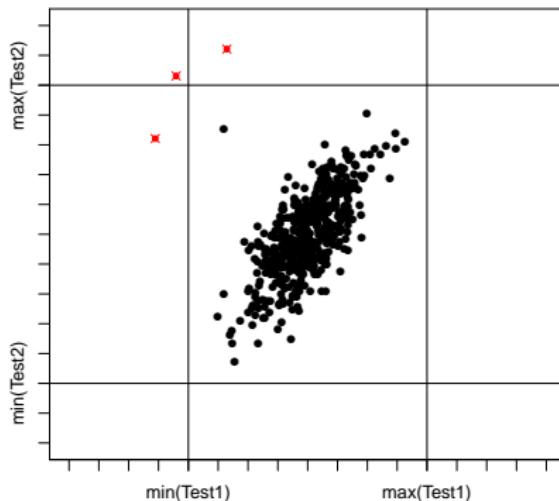
- ▶ Checking for **minimum** and **maximum** in each test result.

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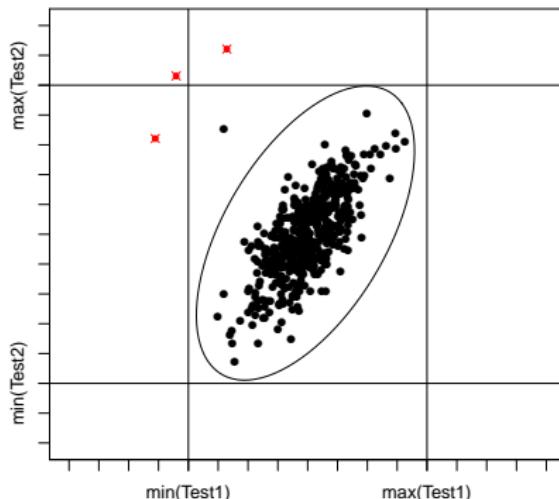
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$$x \notin [\min(\text{Test1}), \max(\text{Test1})] \times [\min(\text{Test2}), \max(\text{Test2})].$$

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

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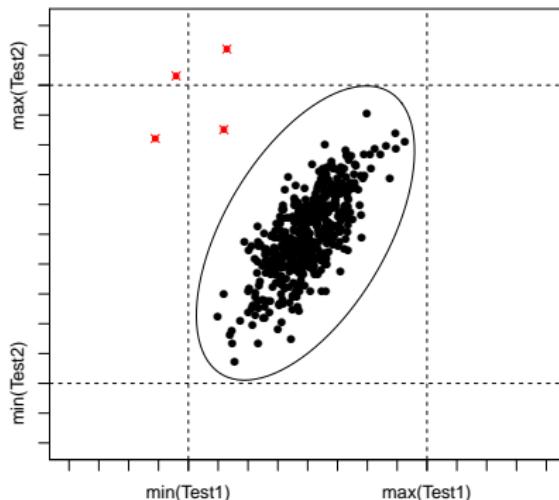


- ▶ **Mahalanobis distance** of an observation $x \in \mathbb{R}^2$ (from the mean) is defined as follows:

$$d_{Mah}(x|\boldsymbol{\Sigma}) = (x - \mu)^\top \boldsymbol{\Sigma}^{-1} (x - \mu),$$

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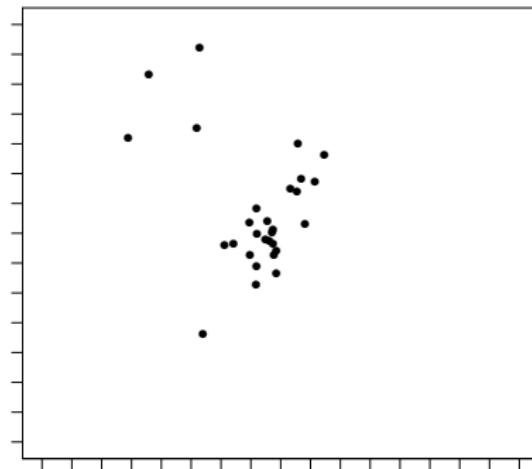
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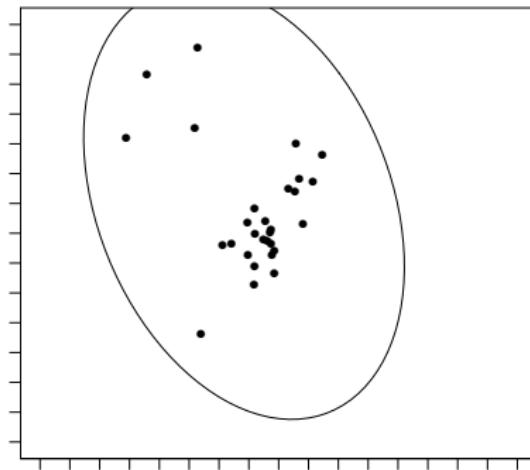
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Multivariate anomaly detection: robustness

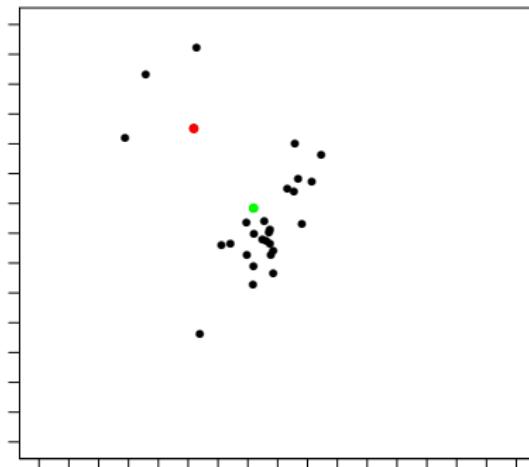


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- ▶ Mahalanobis distance (moment estimators) **not robust**.

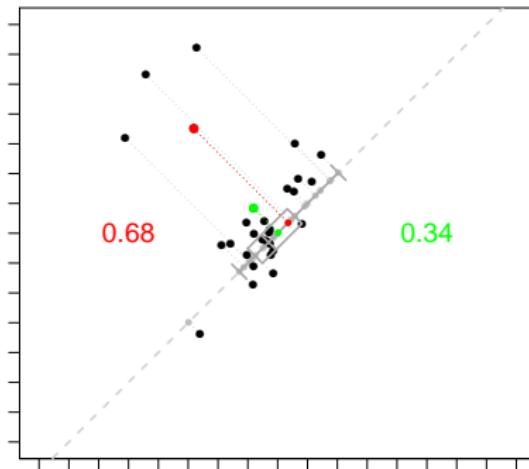
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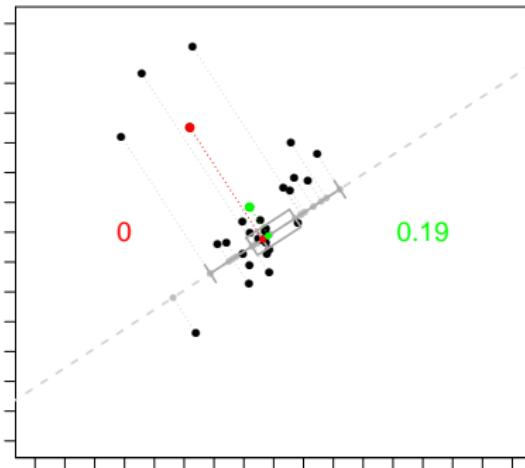
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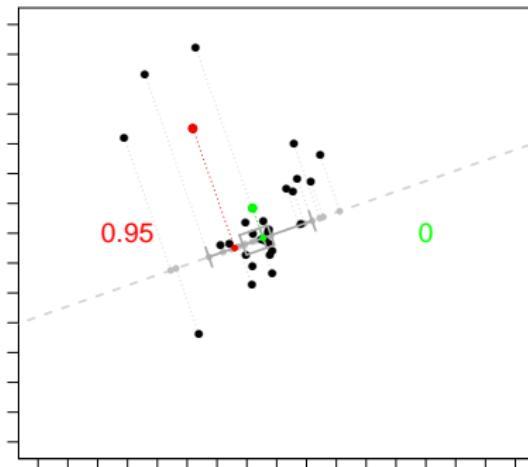
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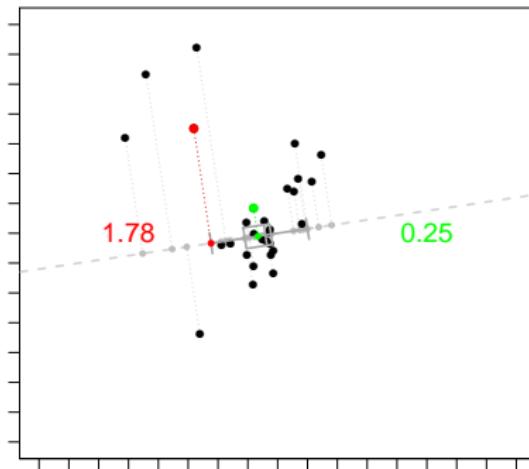
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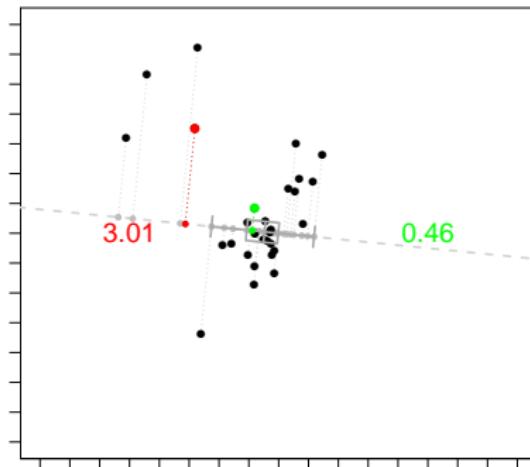
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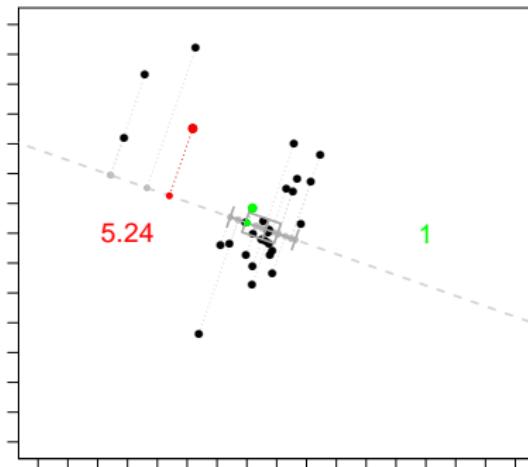
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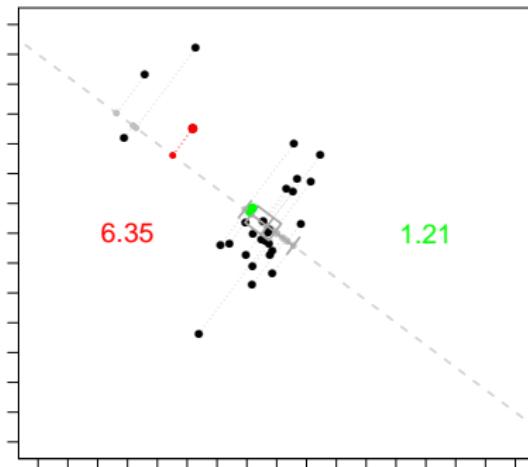
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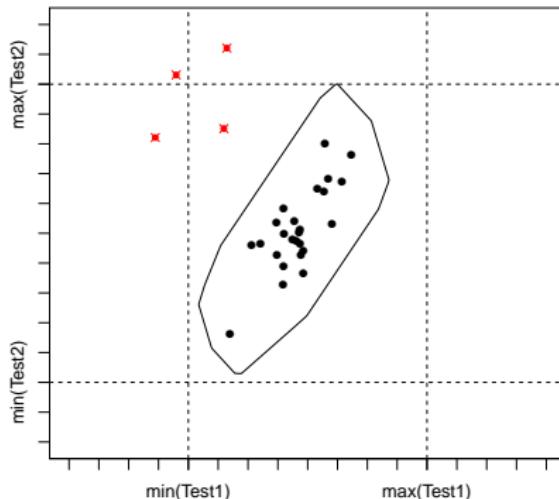
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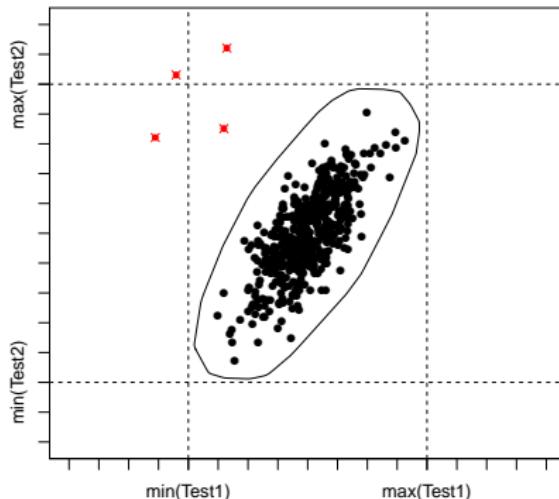


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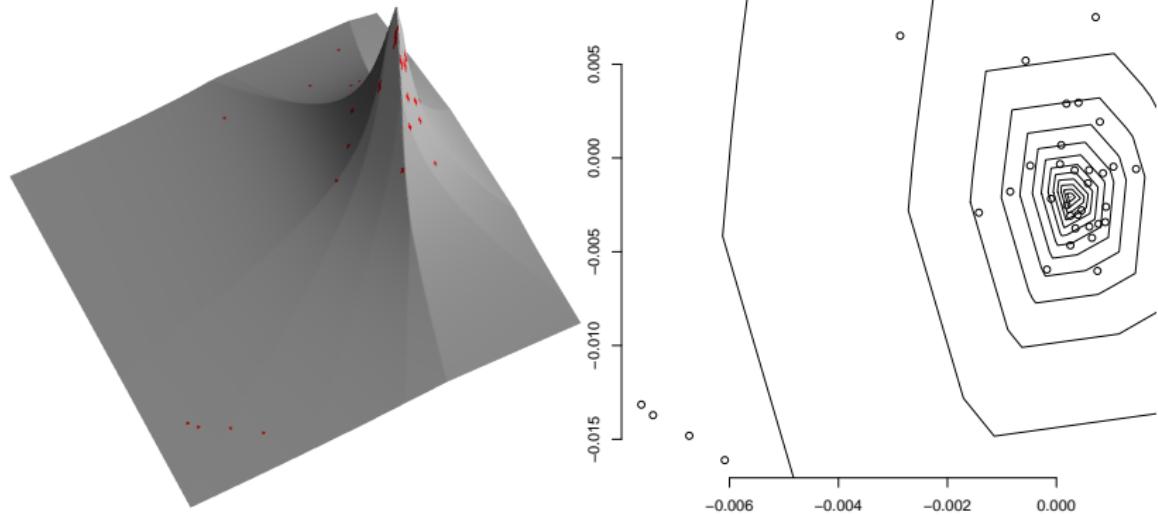
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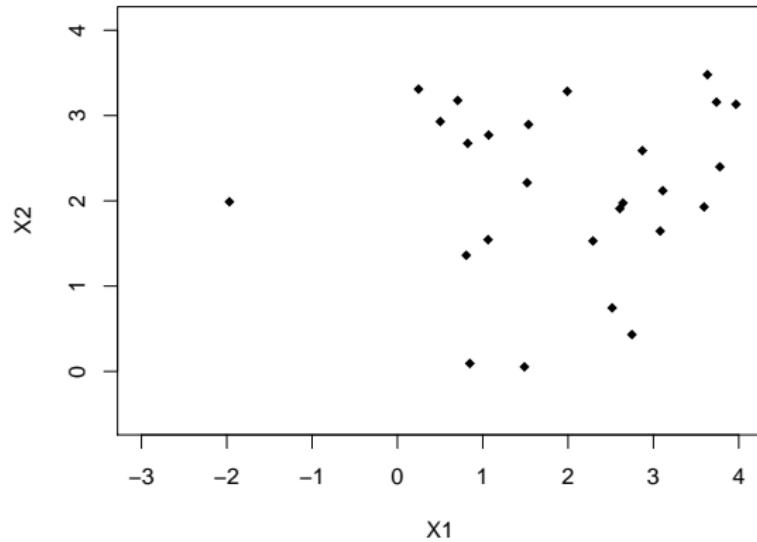
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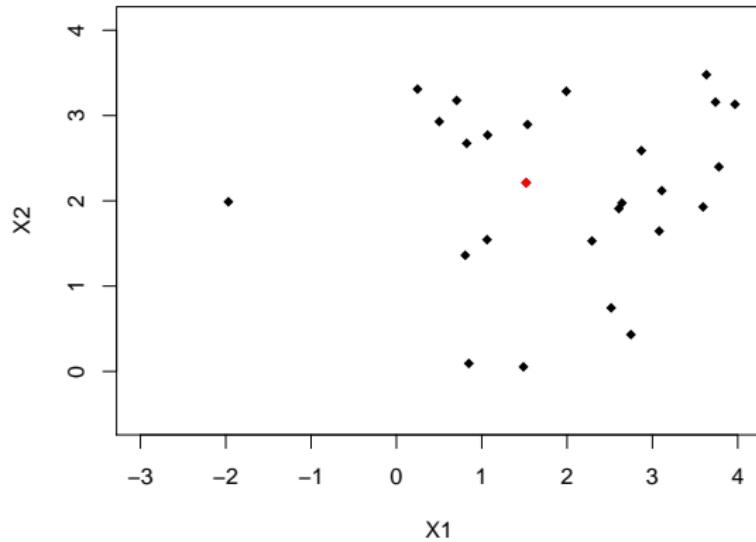
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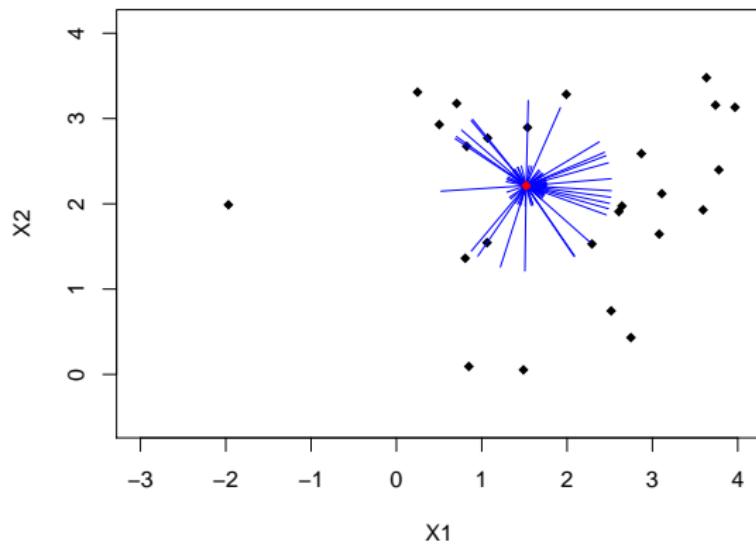
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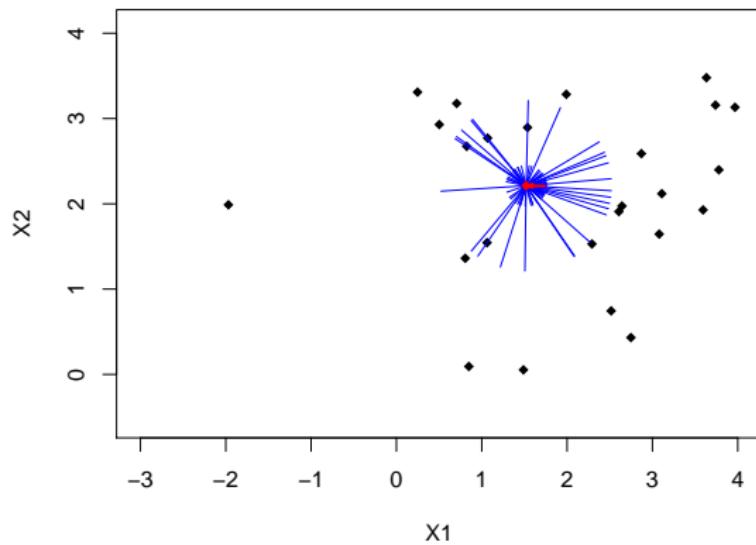
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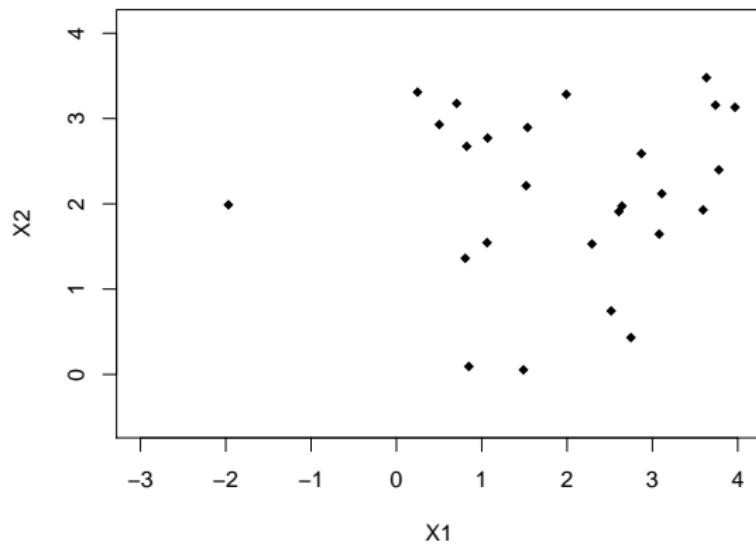
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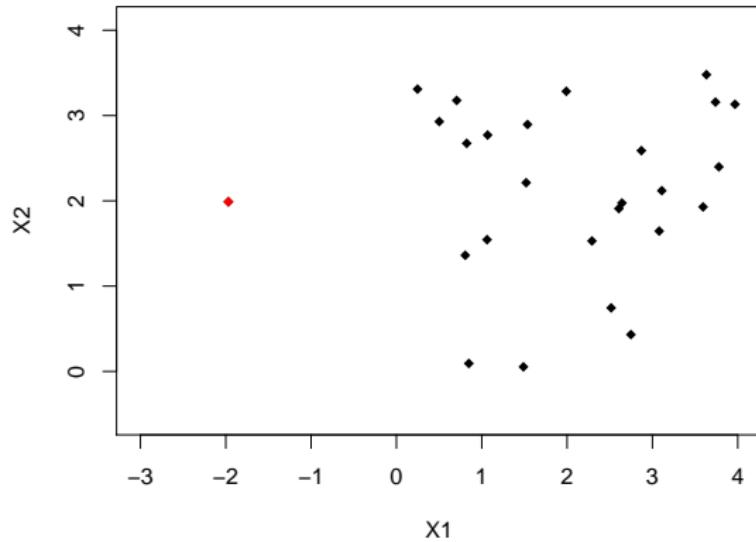
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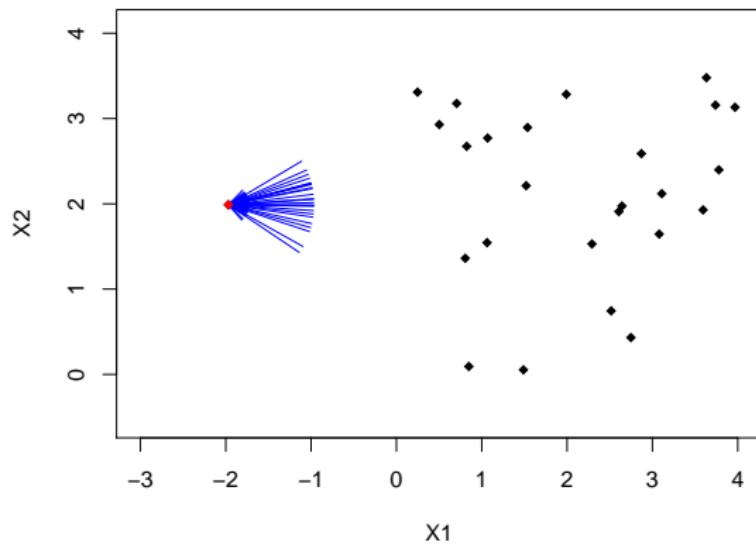
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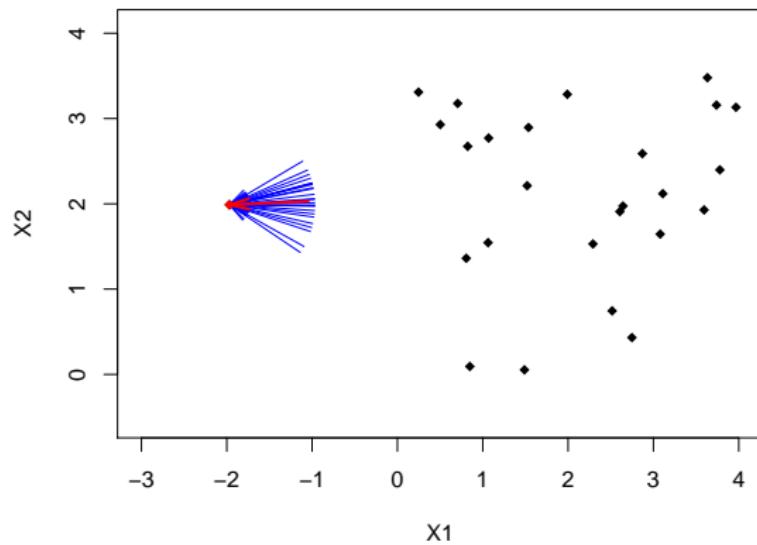
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$$D^{spt}(\mathbf{x}|X) = 1 - \left\| \mathbb{E}[\nu(\boldsymbol{\Sigma}^{-\frac{1}{2}}(\mathbf{x} - X))] \right\|,$$

with

$$\nu(\mathbf{y}) = \begin{cases} \frac{\mathbf{y}}{\|\mathbf{y}\|} & \text{if } \mathbf{y} \neq \mathbf{0}, \\ \mathbf{0} & \text{if } \mathbf{y} = \mathbf{0}. \end{cases}$$

Properties:

- ▶ satisfies **D1 – D5**, but not **D4con**, is continuous;
- ▶ if $\boldsymbol{\Sigma}$ is orthogonal, satisfies **D2iso** only;

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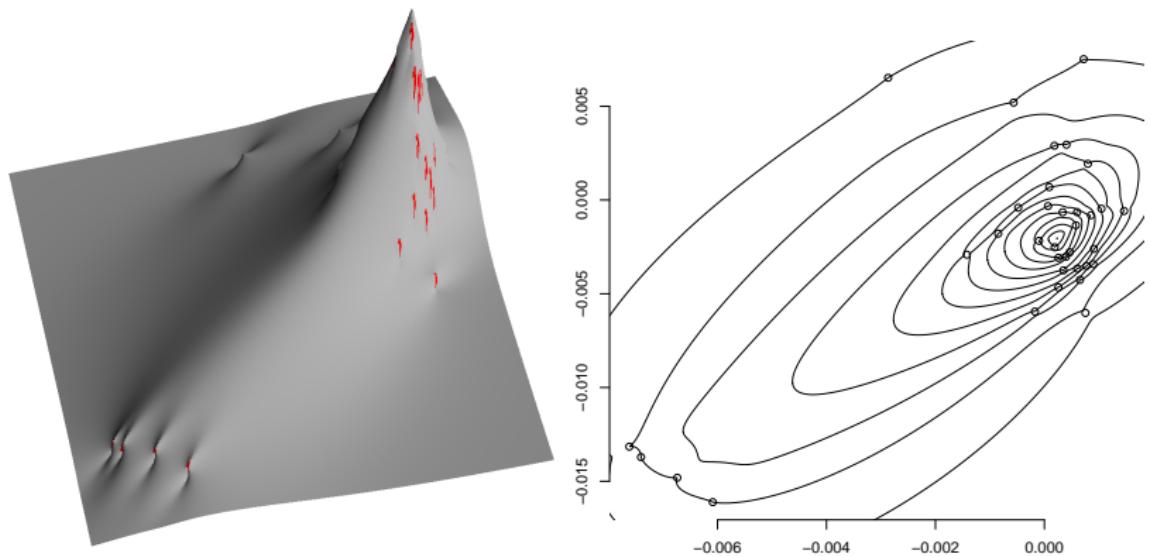
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Properties:

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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)



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Practical session

Functional data framework

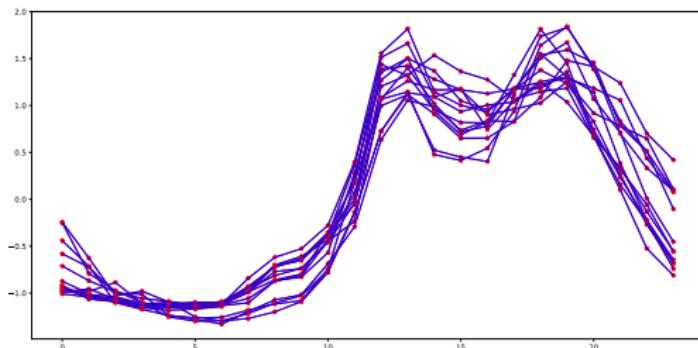
- ▶ Let $\mathbf{F} = \{\mathbf{F}(t) \in \mathbb{R}^d, t \in [0, 1]\}$ be a random variable that takes its values in a (multivariate) functional space.

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Functional data framework

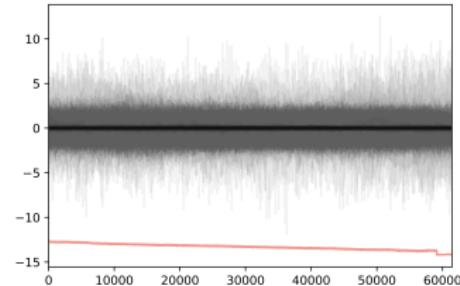
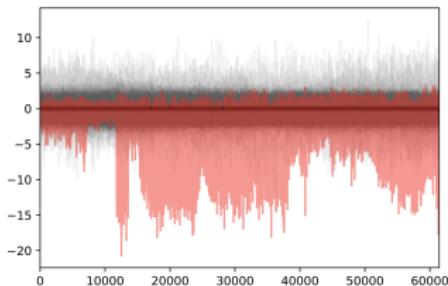
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- ▶ The first step: reconstruct **functional object** from partial observations (time-series) with interpolation or basis decomposition.



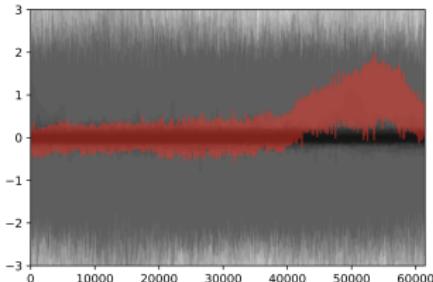
Taxonomy of functional anomalies

A non-complete taxonomy of functional abnormalities:

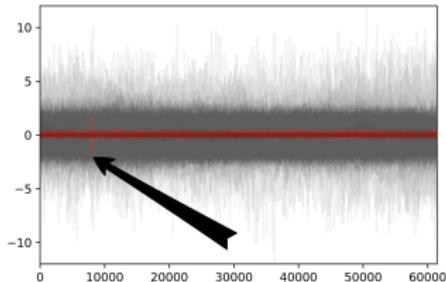
Magnitude (=location, shift) anomalies



Shape anomalies



Isolated anomalies



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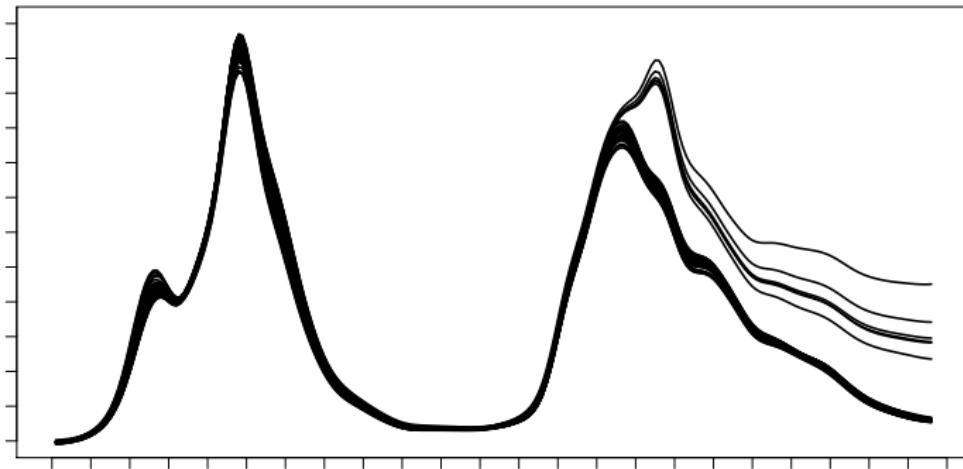
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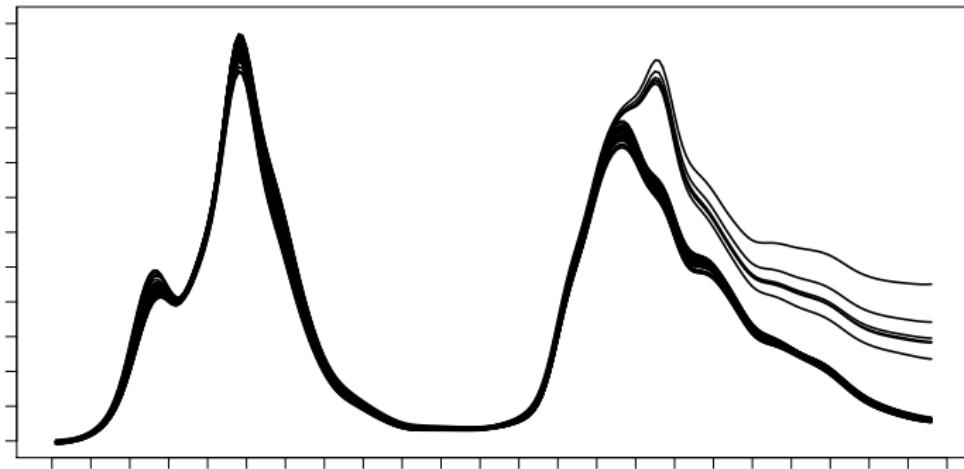
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Practical session

Detection of (multivariate) functional anomalies



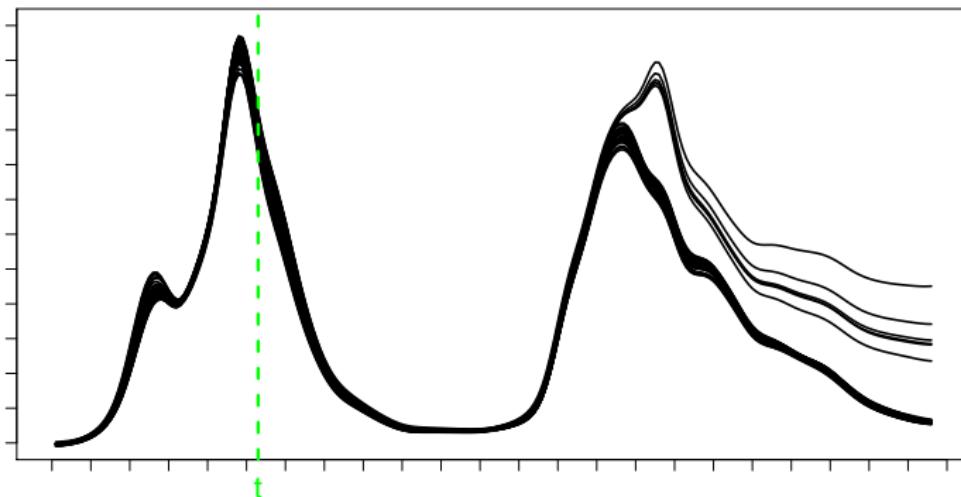
Detection of (multivariate) functional anomalies



- ▶ **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

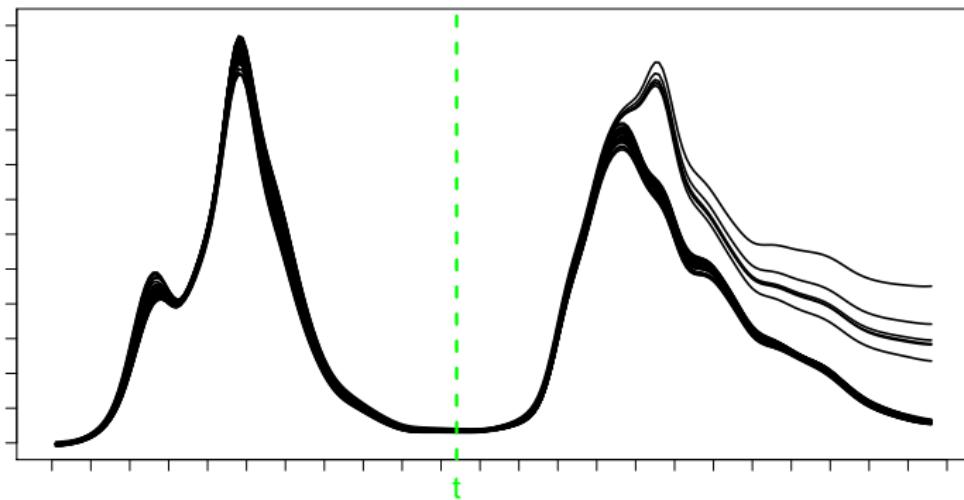


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$$D(\mathbf{f}|\mathcal{F}) = \int_{t_{\min}}^{t^{\max}} D^1(\mathbf{f}(\textcolor{blue}{t}) | \{\mathbf{f}_1(\textcolor{blue}{t}), \dots, \mathbf{f}_n(\textcolor{blue}{t})\}) dt,$$

where $D^d(\cdot|\cdot)$ is a multivariate data depth, as defined above.

Detection of (multivariate) functional anomalies

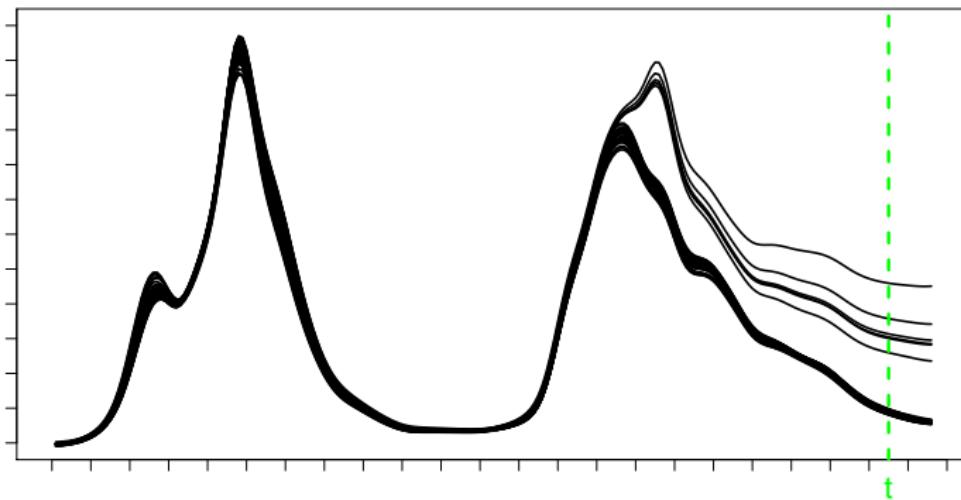


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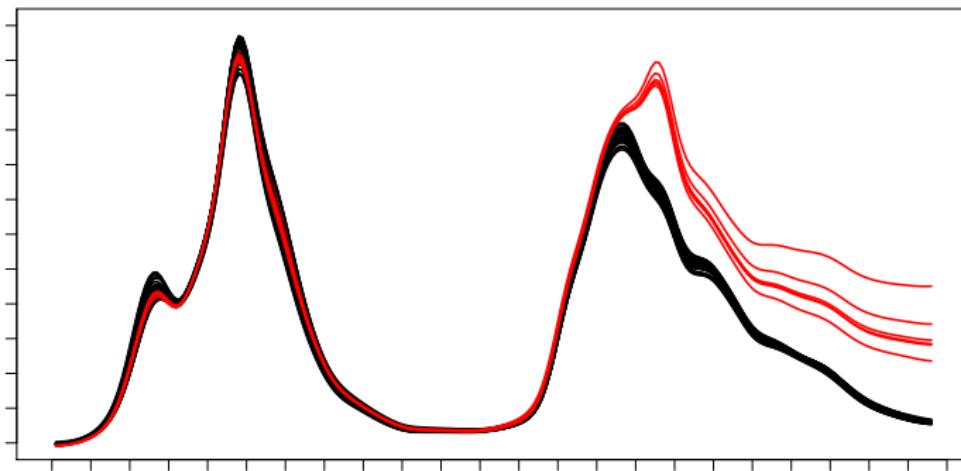


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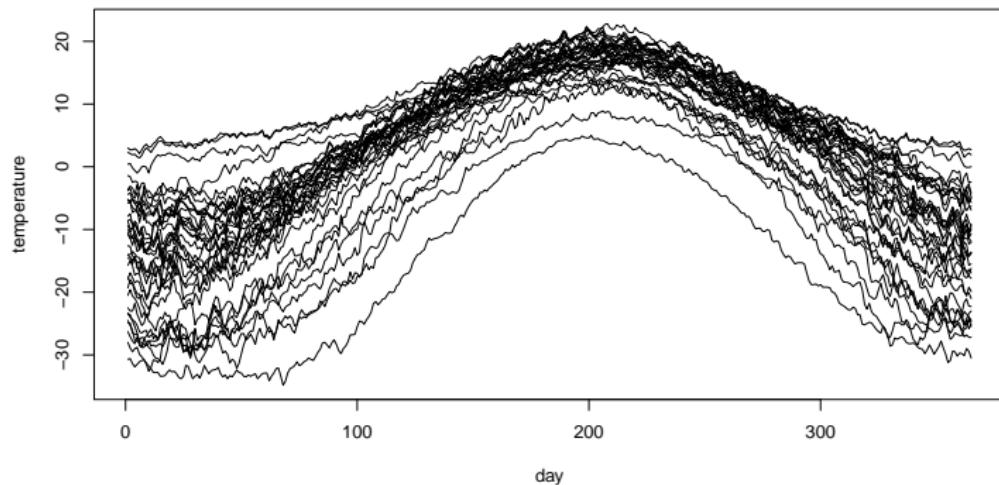
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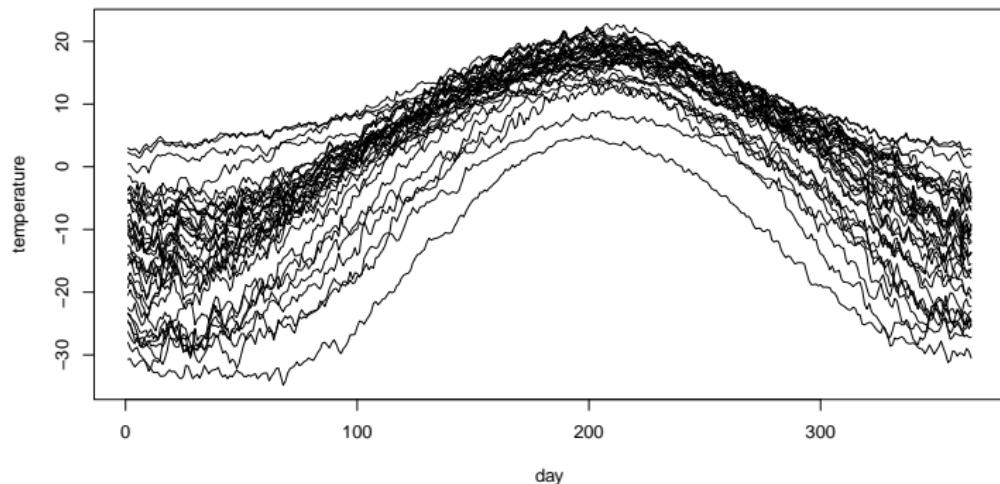
- ▶ Label \mathbf{f} as **anomaly** if $D(\mathbf{f}|\mathcal{F}) < \min(D)$.

Integrated depth for functional data



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

Integrated depth for functional data

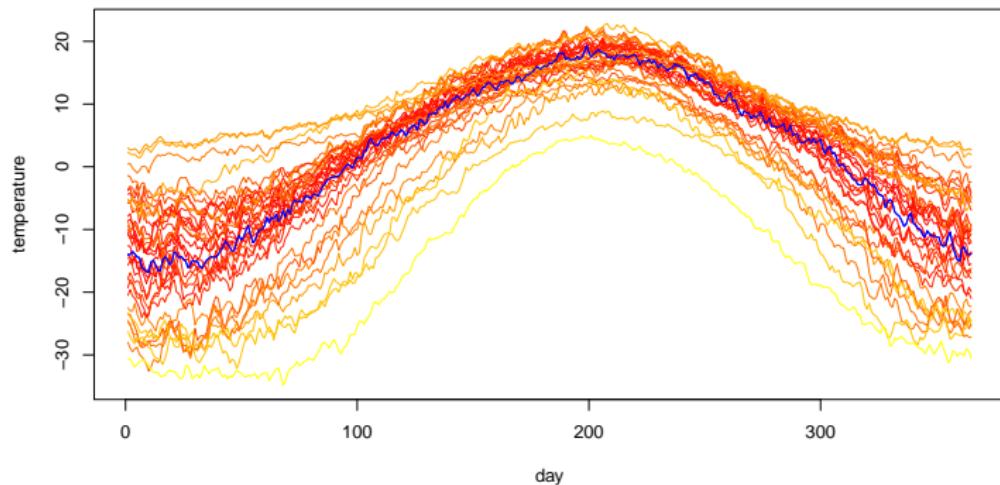


Let \mathbf{F} be a stochastic process with continuous paths defined on $[0, 1]$, and \mathbf{f} its realization. Then:

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

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

Integrated depth for functional data

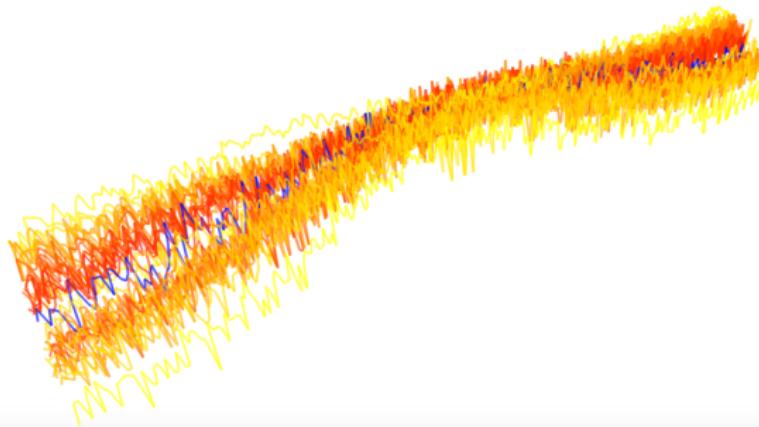


Let \mathbf{F} be a stochastic process with continuous paths defined on $[0, 1]$, and \mathbf{f} its realization. Then:

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

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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Functional isolation forest

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

- ▶ **Functional isolation forest** is an adaptation of the multivariate **isolation forest** algorithm
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- ▶ Project the observations f on (**random**) **elements d of a dictionary $\mathcal{D} \in \mathcal{H}$** chosen to be rich enough to explore different properties of data and well appropriate to be sampled in a representative manner.

Functional isolation forest

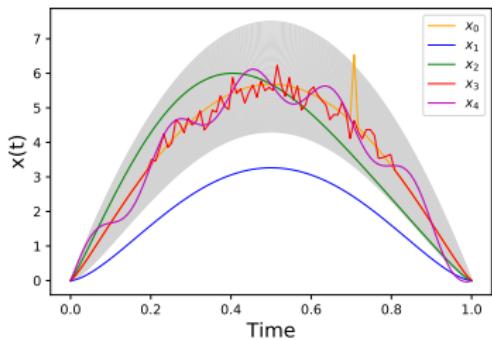
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- ▶ Project the observations \mathbf{f} on (**random**) **elements d of a dictionary $\mathcal{D} \in \mathcal{H}$** chosen to be rich enough to explore different properties of data and well appropriate to be sampled in a representative manner.
- ▶ 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):

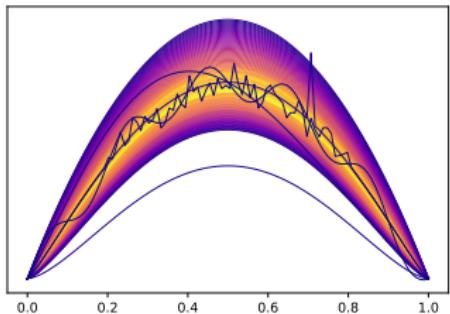
$$\langle \mathbf{f}, \mathbf{d} \rangle := \lambda \times \frac{\langle \mathbf{f}, \mathbf{d} \rangle_{L_2}}{\|\mathbf{f}\| \|\mathbf{d}\|} + (1 - \lambda) \times \frac{\langle \mathbf{f}', \mathbf{d}' \rangle_{L_2}}{\|\mathbf{f}'\| \|\mathbf{d}'\|}, \quad \lambda \in [0, 1].$$

Functional isolation forest: an example

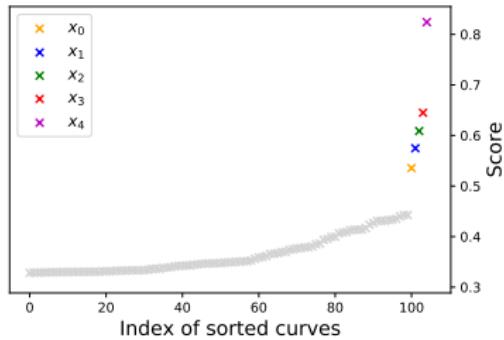
Functional data set with anomalies



Color-indicated anomaly score



Anomaly score



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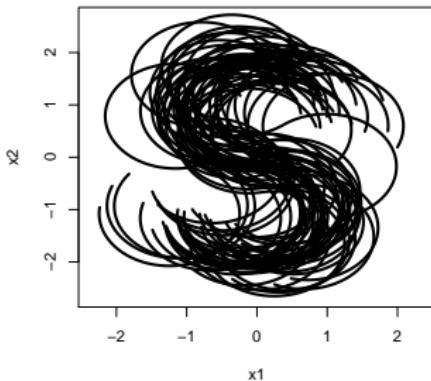
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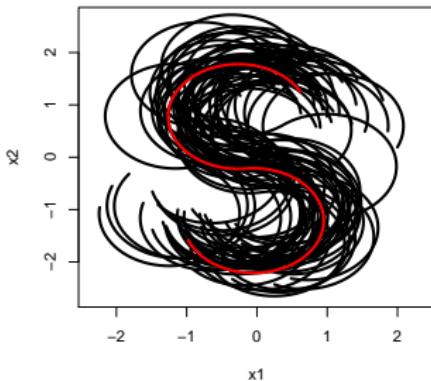
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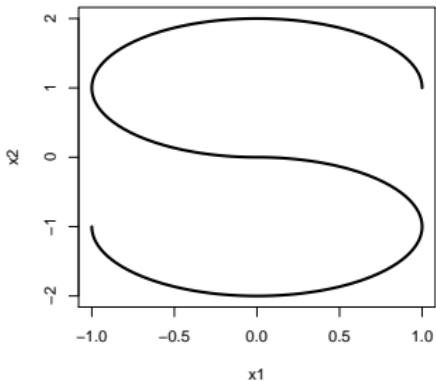
Functional depth: Motivation 1



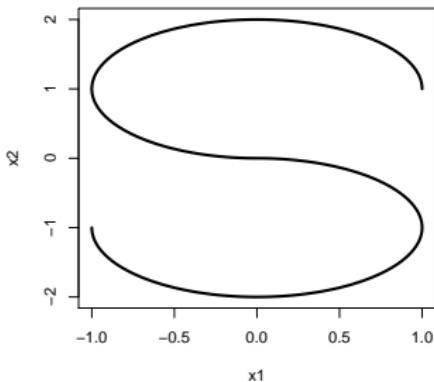
Functional depth: Motivation 1



Functional depth: Motivation 1



Functional depth: Motivation 1



Regard the following different parametrizations of a curve:

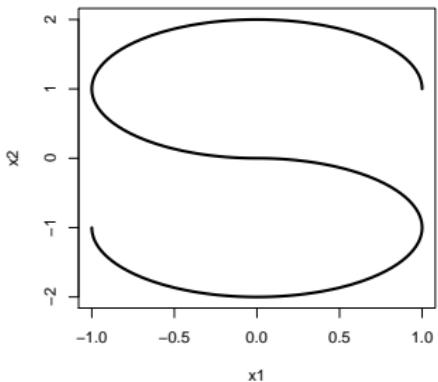
Parametrization A:

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

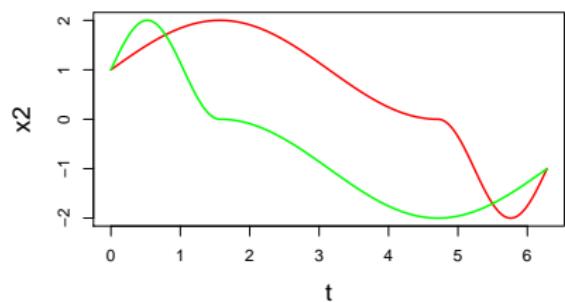
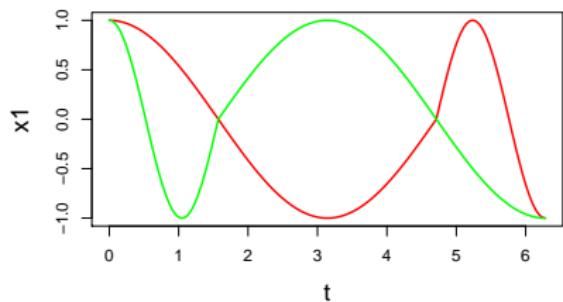
Parametrization B:

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

Functional depth: Motivation 1

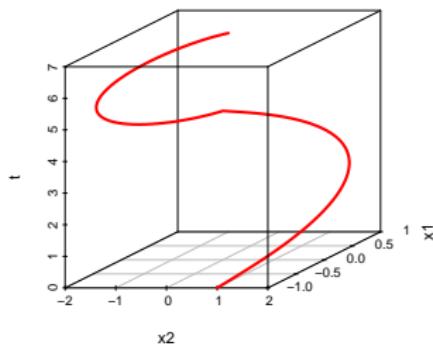


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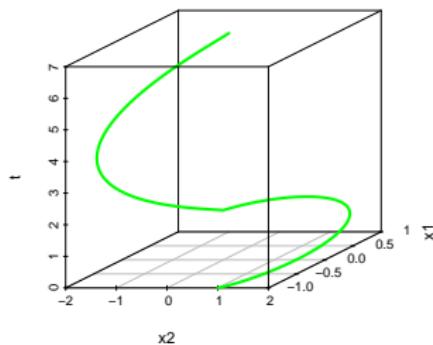


Functional depth: Motivation 1

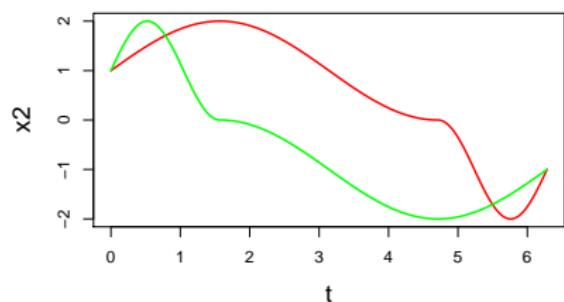
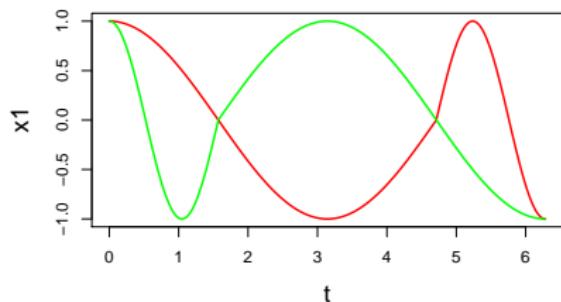
Parametrization A



Parametrization B

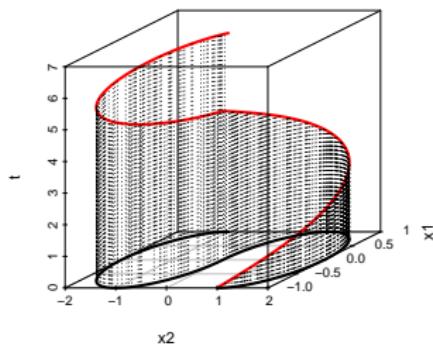


Parametrization:

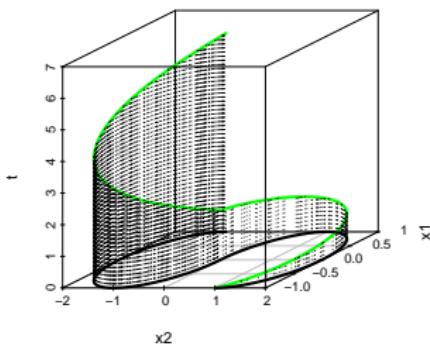


Functional depth: Motivation 1

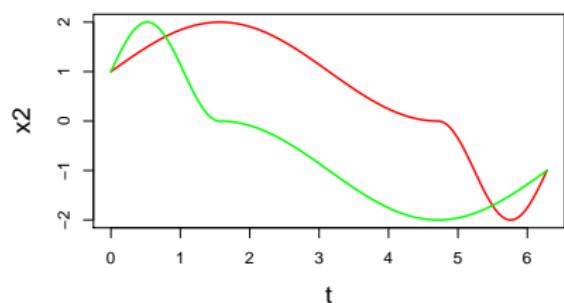
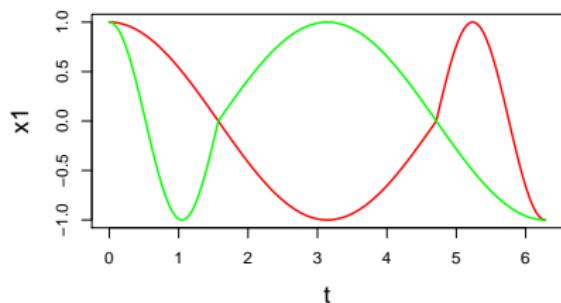
Parametrization A



Parametrization B

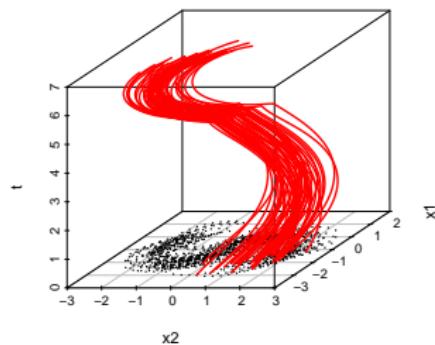


Parametrization:

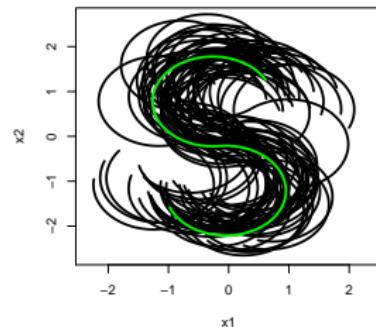
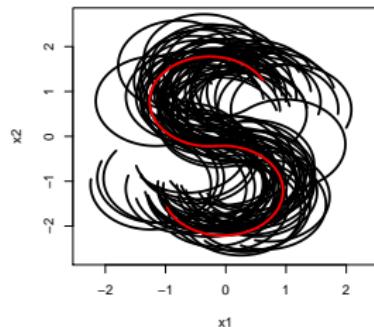
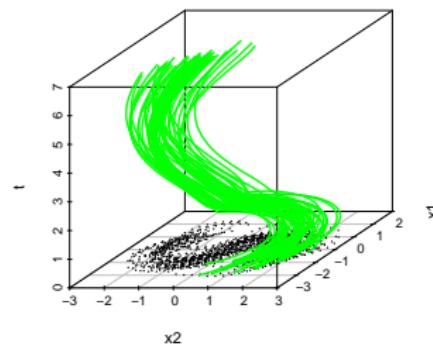


Functional depth: Motivation 1

Parametrization A

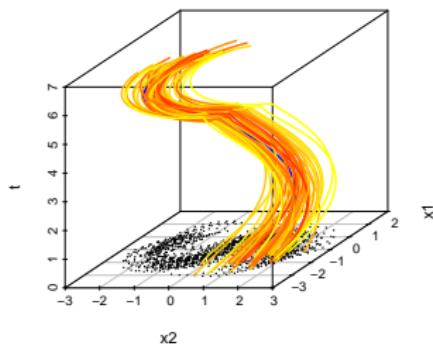


Parametrization B

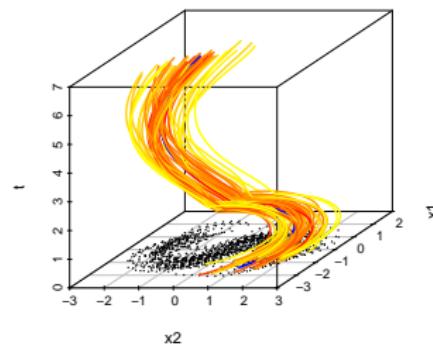


Functional depth: Motivation 1

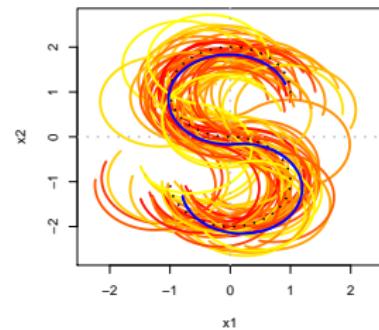
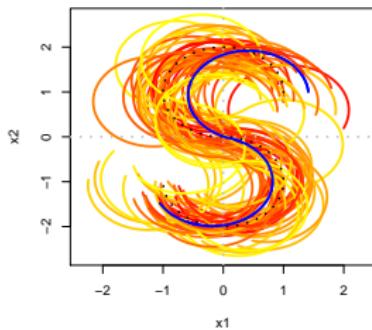
Parametrization A



Parametrization B



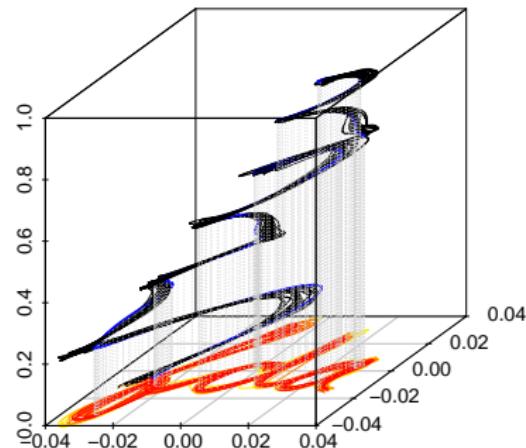
The depth-induced orders differ!



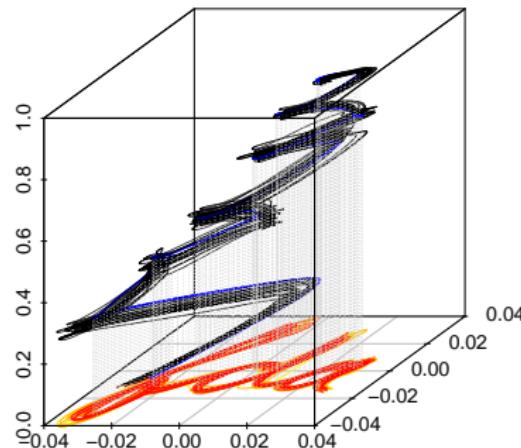
Functional depth: Motivation 2

Functional halfspace depth for the FDA-data

Parametrization by time



Parametrization by length



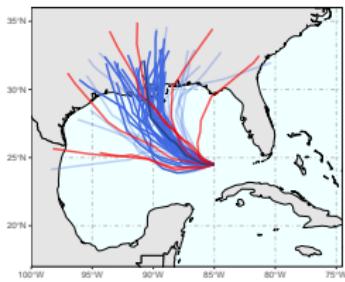
Depth-induced ranking for parametrizations by time and by length:

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

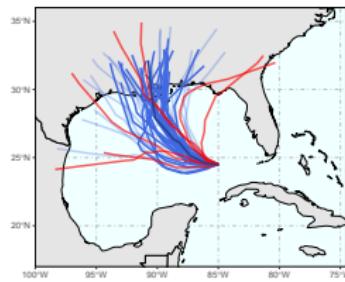
Functional depth: Motivation 3

Simulated hurricane tracks: **curve boxplot**

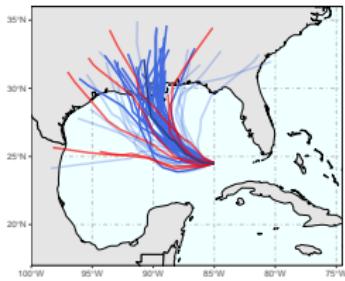
MFH depth – par. time



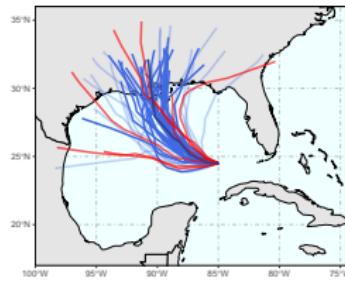
MFH depth - par. length



mSB depth – par. time



mSB depth – par. length



The space of curves

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

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A reparametrization $\gamma : [0, 1] \rightarrow [0, 1]$ is increasing continuous function: $\gamma(0) = 0$ and $\gamma(1) = 1$.

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

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- We derive the probability distribution Q_P on \mathbb{R}^d as follows: if $X \sim Q_P$, then distribution of $X | \mathcal{X} = \mathcal{C}$ is the (uniform on \mathcal{C}) probability distribution $\mu_{\mathcal{C}}$:

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

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**:

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

Data depth for an unparametrized curve

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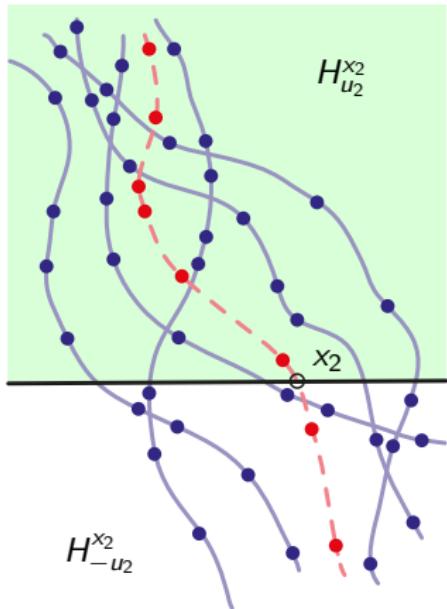
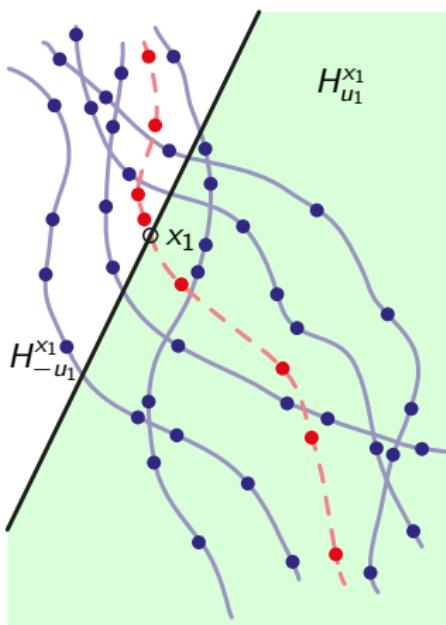
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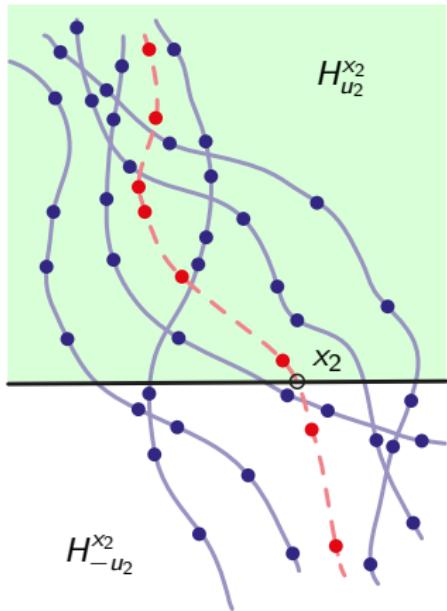
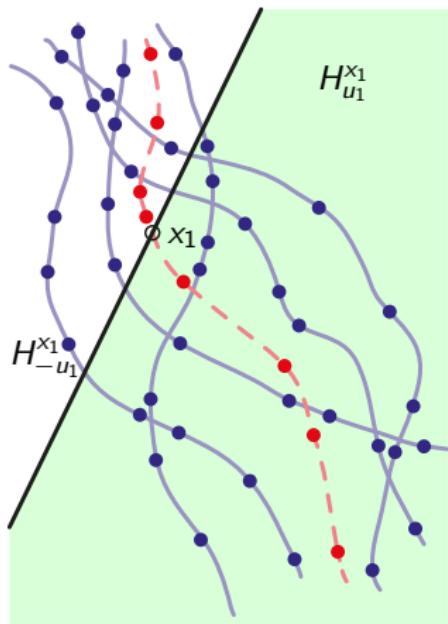
$$D(\mathcal{C}|\mathcal{X}_1, \dots, \mathcal{X}_n) = \int_{\mathcal{C}} D(\mathbf{x}|Q_n, \mu_{\mathcal{C}}) d\mu_{\mathcal{C}}(\mathbf{x}),$$

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

Data depth for an unparametrized curve: intuition



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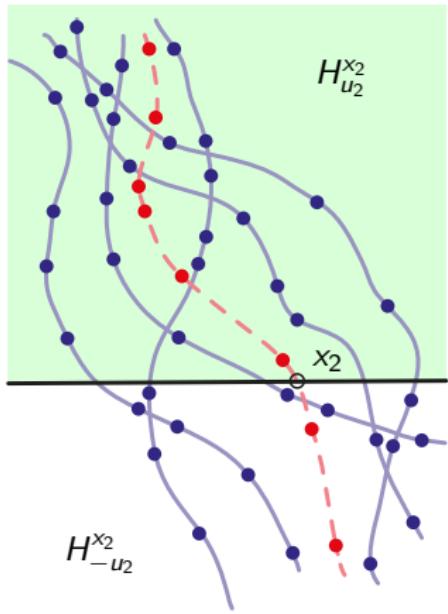
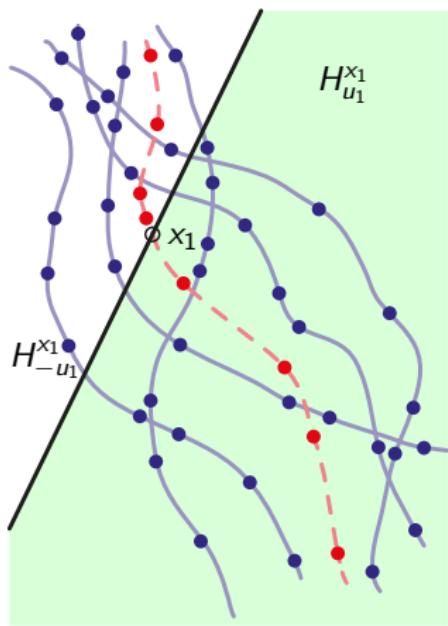
Traditional reasoning:

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

Curve-based reasoning:

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Data depth for an unparametrized curve: empirical version

- ▶ 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 δ_x is the Dirac measure in $x \in \mathbb{R}^d$.

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 $\mathbb{X}_{n,m} = \{X_{i,j}, i = 1, \dots, n, j = 1, \dots, m\}$

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

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- ▶ 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 $\widehat{Q}_{n,m}(H) = 0$ or $\widehat{\mu}_m(H) > \Delta$, 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:

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

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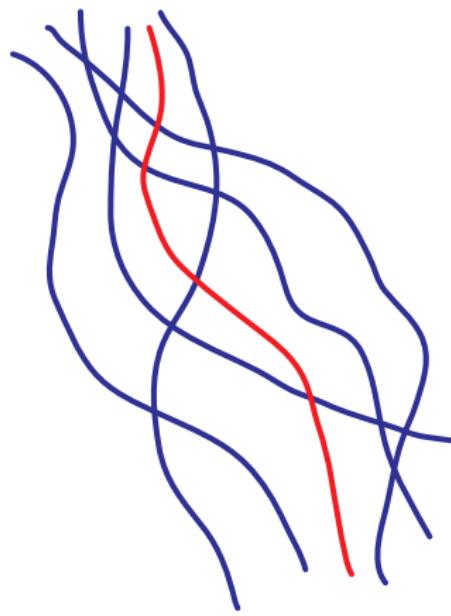
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with the depth of an arbitrary point $x \in \mathbb{R}^d$ w.r.t. $\widehat{Q}_{n,m}$ being:

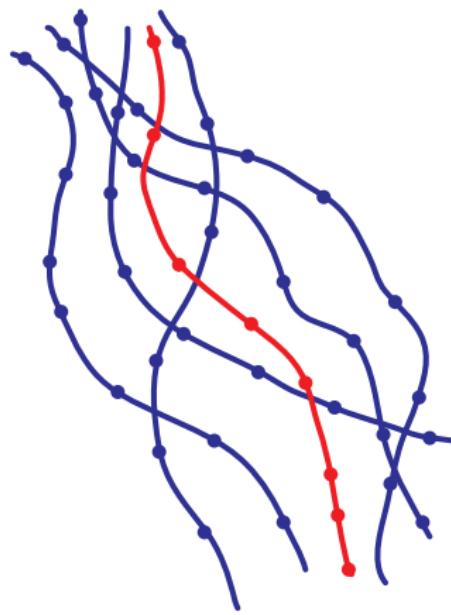
$$\widehat{D}(x | \widehat{Q}_{n,m}, \widehat{\mu}_m, \mathcal{H}_\Delta^{n,m}) = \inf \left\{ \frac{\widehat{Q}_{n,m}(H)}{\widehat{\mu}_m(H)} : H \in \mathcal{H}_\Delta^{n,m}, x \in \partial H \right\}$$

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

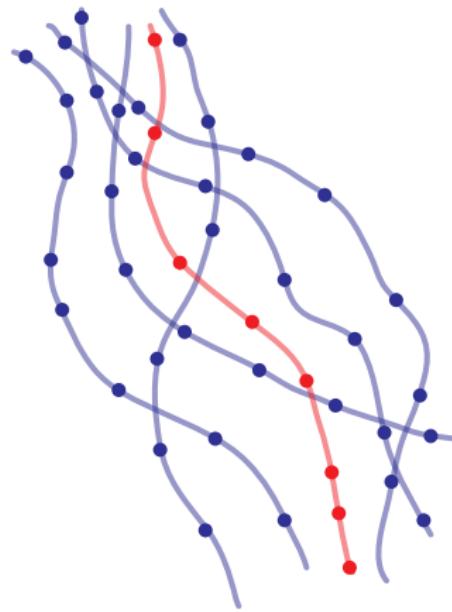
Calculation of the Tukey curve depth



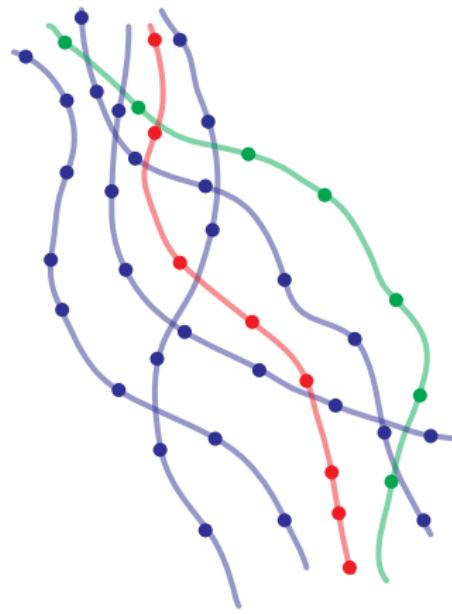
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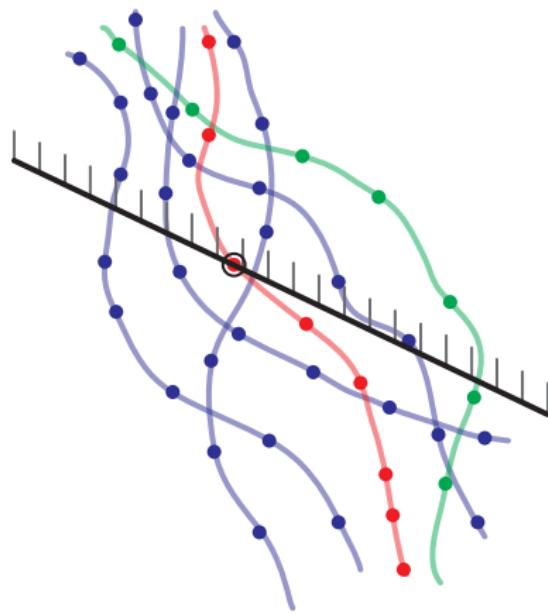
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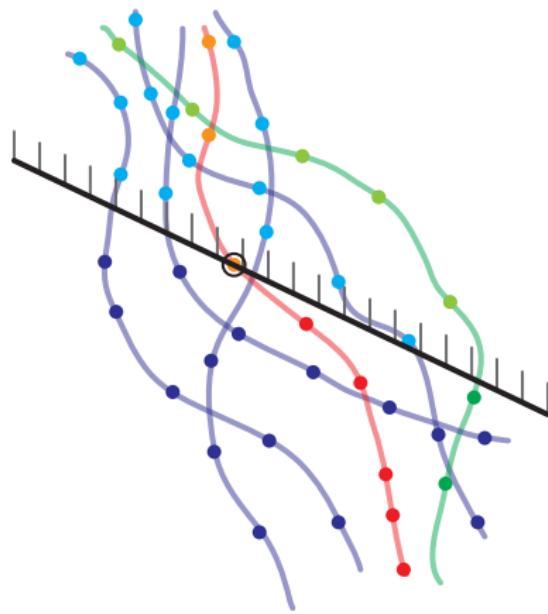
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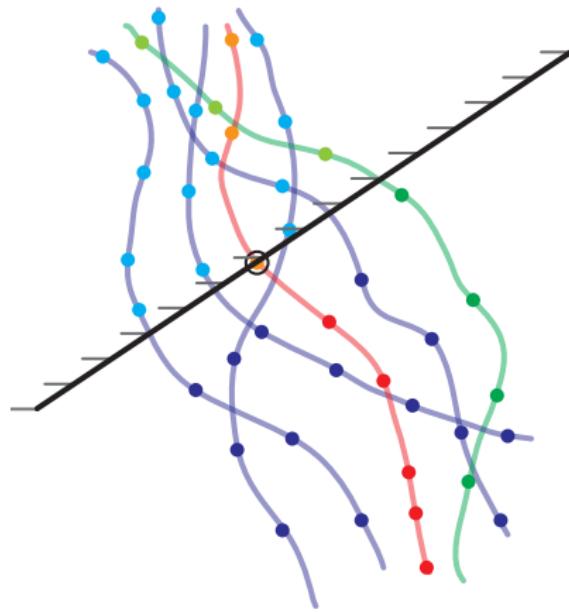


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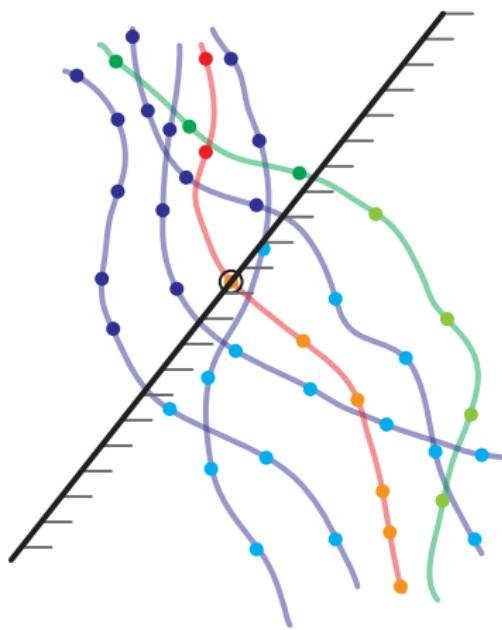
$$D(\mathbb{Y}_{2,c} | Q_m, \mathcal{H}_{m,b}) = \frac{\frac{1}{5} \left(\frac{5}{7} + \frac{3}{8} + \frac{6}{8} + \frac{2}{7} + \frac{3}{6} \right)}{\frac{2}{8}} = 2.1$$

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Calculation of the Tukey curve depth



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

Data depth for an unparametrized curve: properties

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

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

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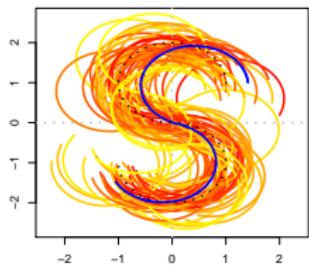
- ▶ **Vanishing at infinity:**

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

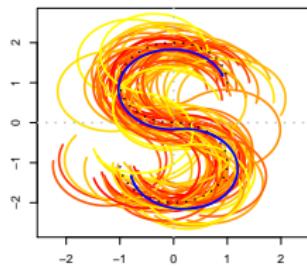
Comparison with functional depth: Example 1

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

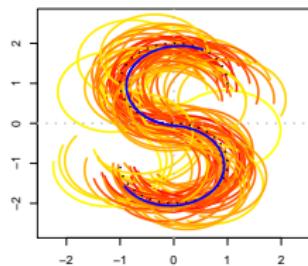
MFHD – time



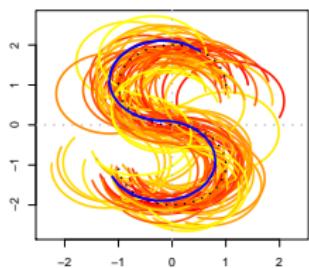
MFHD - length



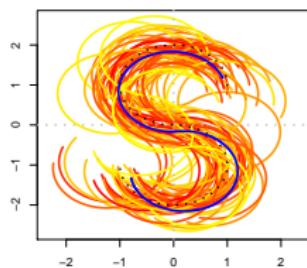
Curve depth



mSBD – time



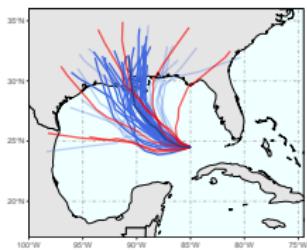
mSBD – length



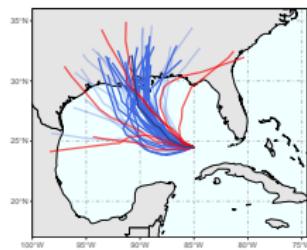
Comparison with functional depth: Example 2

Simulated hurricane tracks: **curve boxplot**

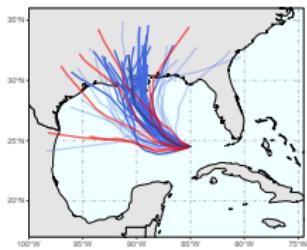
MFHD – time



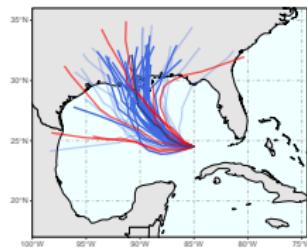
MFHD - length



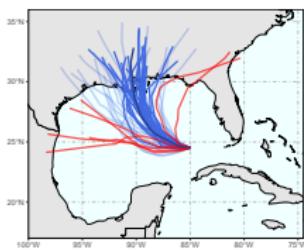
mSBD – time



mSBD – length

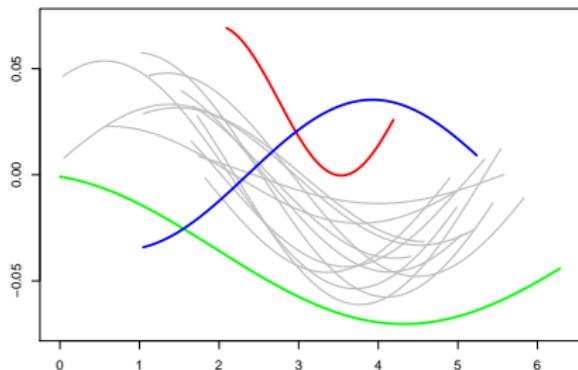


Curve depth



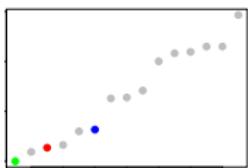
Comparison with functional depth: Anomaly detection 1

Data set 1 with introduced anomalies:

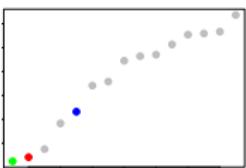


Ordered depth values:

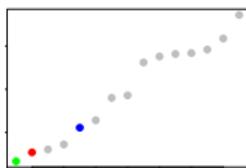
mSBD



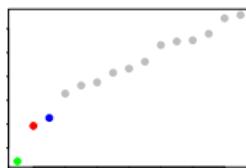
saPRJ



MFHD

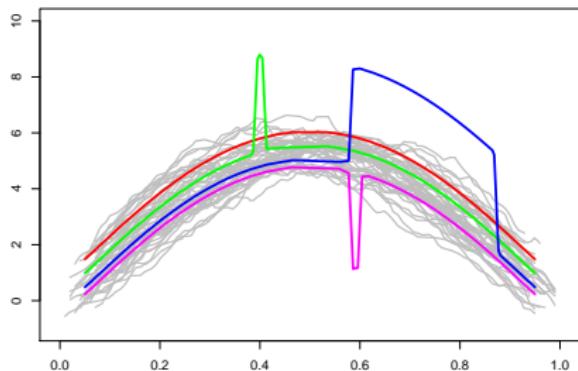


Curve depth



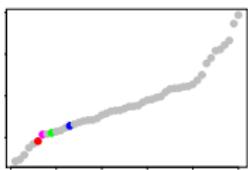
Comparison with functional depth: Anomaly detection 2

Data set 2 with introduced anomalies:

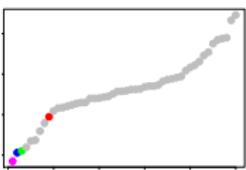


Ordered depth values:

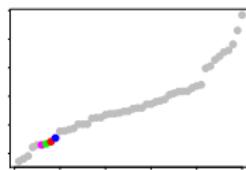
mSBD



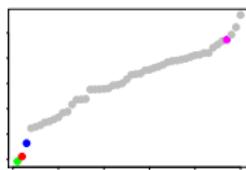
saPRJ



MFHD



Curve depth



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- Depth for curve data

Practical session

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

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- ▶ 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.
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- ▶ 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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