Unsupervised learning: Anomaly detection
Part I: Multivariate data

Pavlo Mozharovskyi

LTCI, Telecom Paris, Institut Polytechnique de Paris

Parcours Data Science BPCE

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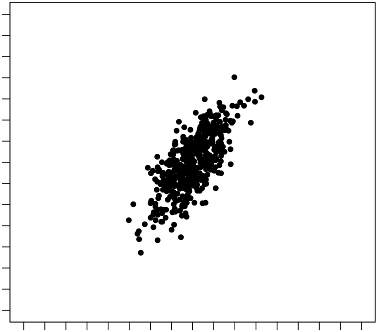
A real task

Regard two measurements during a test in a production process:



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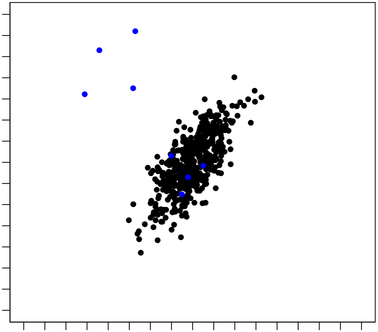

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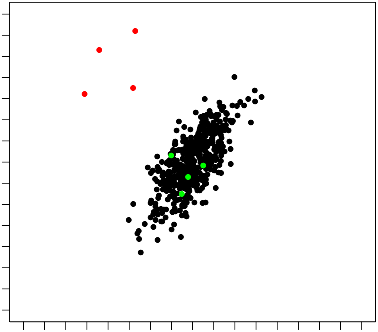

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Multivariate framework

- A training data set:

$$\boldsymbol{X} = \{\boldsymbol{x}_1, ..., \boldsymbol{x}_n\} \subset \mathbb{R}^d$$

of observations in the d-dimensional Euclidean space.

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- Construct a decision function:

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

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

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  which attributes to any (possible) $\boldsymbol{x} \in \mathbb{R}^d$ a label whether it is an anomaly (*e.g.*, $+1$) or a normal observation (*e.g.*, -1).
- It is more useful to provide an ordering on $\mathbb{R}^d$:

$$\mathbb{R}^d \to \mathbb{R} : \boldsymbol{x} \mapsto g(\boldsymbol{x}),$$

  such that abnormal observations obtain higher anomaly score.

Practical session (parts I and II)

Notebooks:

- anomdet_simulation1.Rmd,
- anomdet_hurricanes.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.

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.

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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).

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Generalized portrait:

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

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

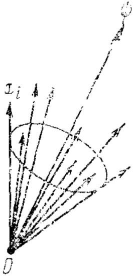

Рис. 24.

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

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

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

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

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

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Soft margin (Cortes, Vapnik; 1995):

- Allow for a portion of points from $\boldsymbol{X}$ 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

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

with $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_n)^\top$.

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

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

$$g_{OCSVM}(\boldsymbol{x}) = \operatorname{sgn}(\langle\boldsymbol{\psi}^*, \Phi(\boldsymbol{x})\rangle - \rho^*)\,.$$

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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:

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

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

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

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

The decision function is then:

$$g_{OCSVM}(\boldsymbol{x}) = \mathrm{sgn}\left(\sum_{i=1}^{n}\alpha_i K(\boldsymbol{x}_i,\boldsymbol{x}) - \rho\right),$$

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

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

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

Idea 2: Put points into a small ball.

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

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This leads to the dual:

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

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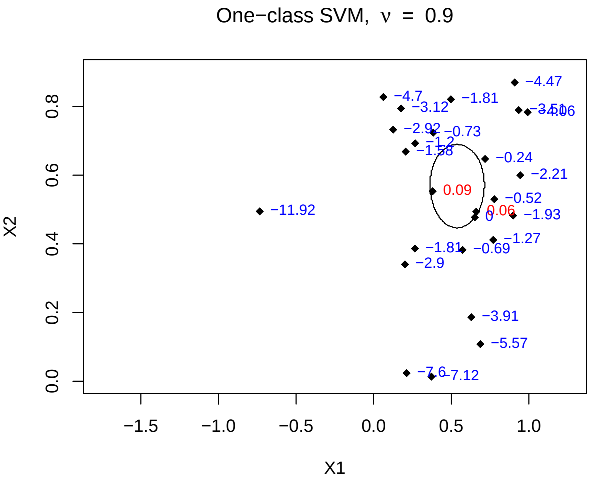
which leads to the decision function:

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

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

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

Illustration: Case 1



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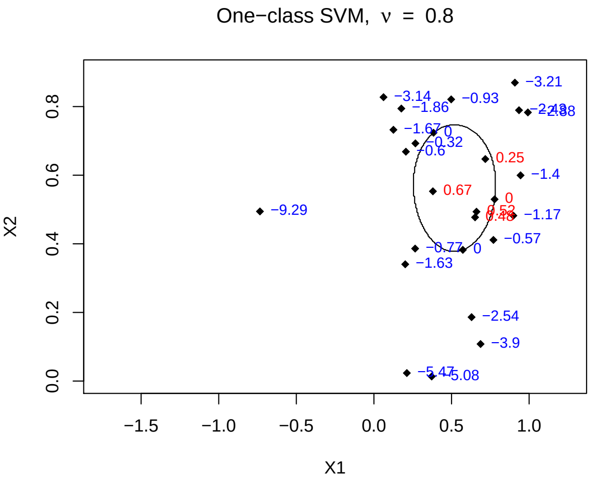

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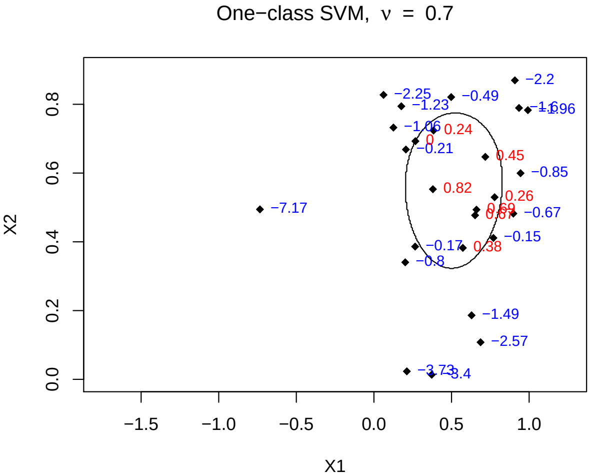

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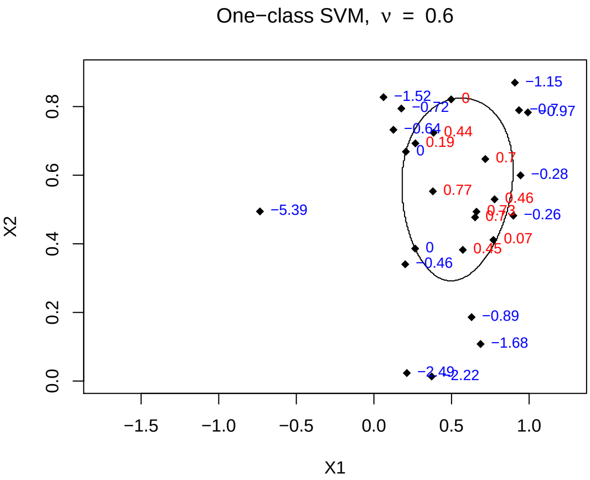

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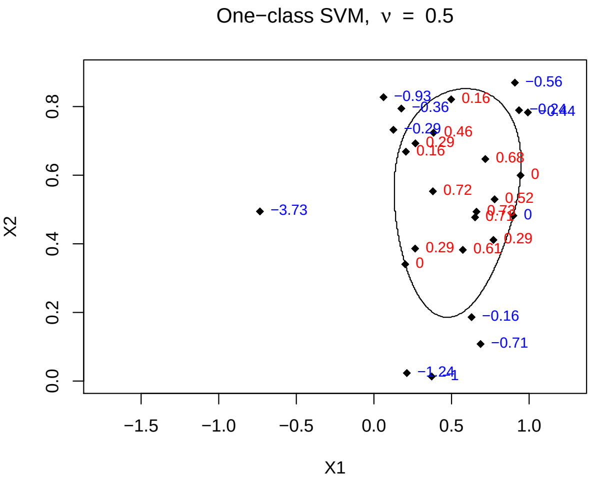

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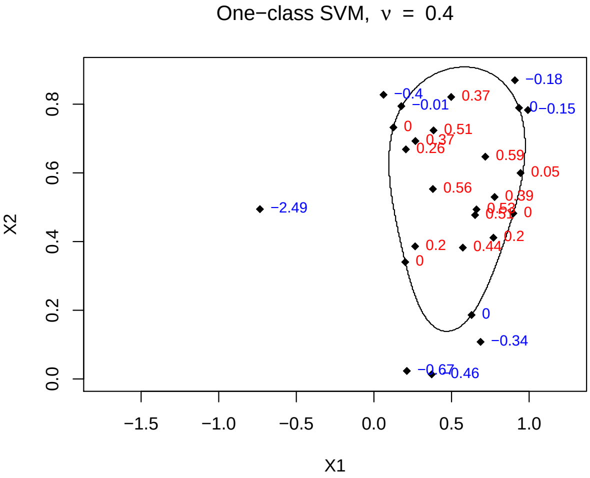

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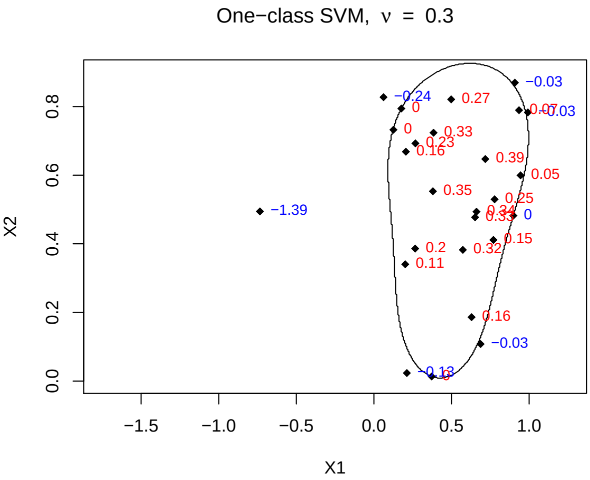

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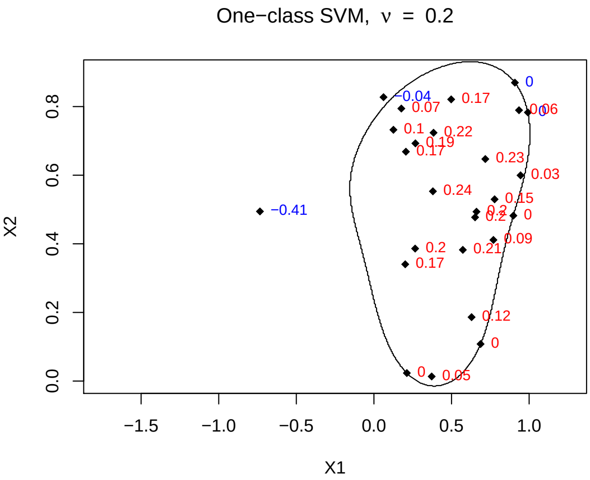

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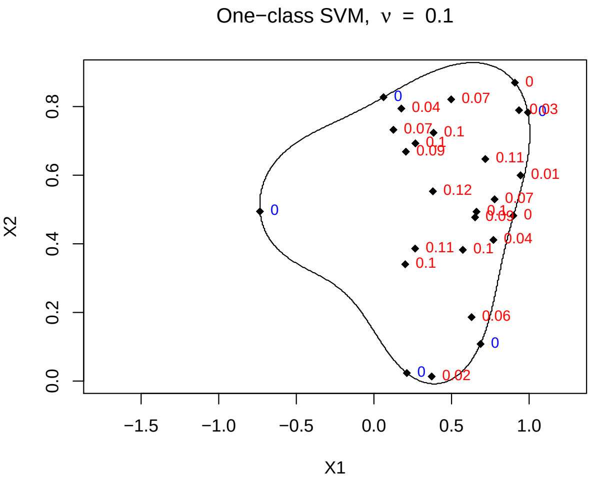

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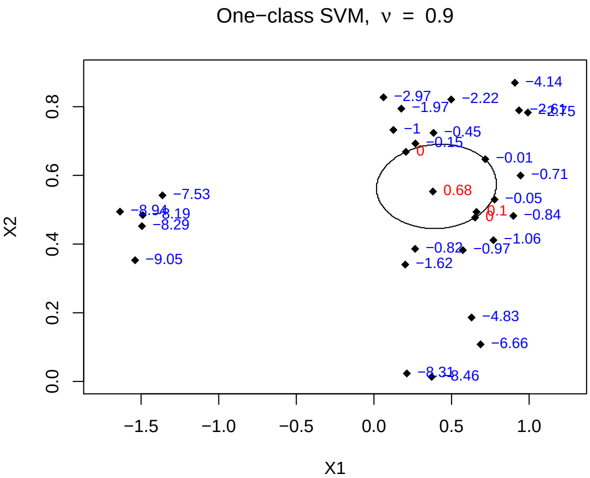

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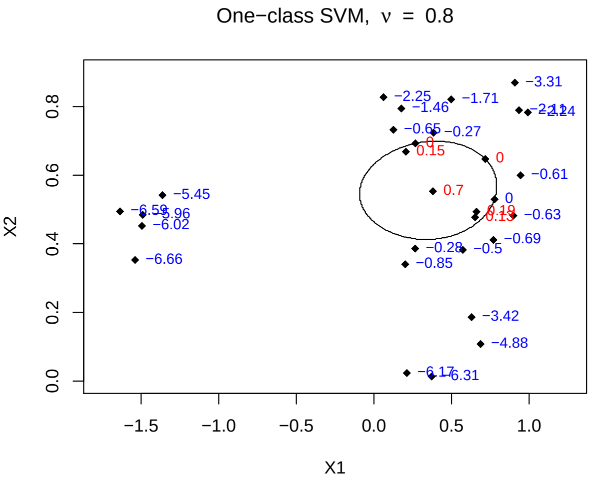

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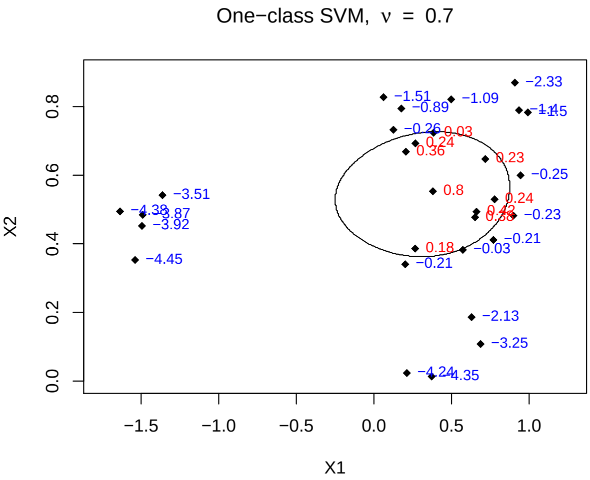

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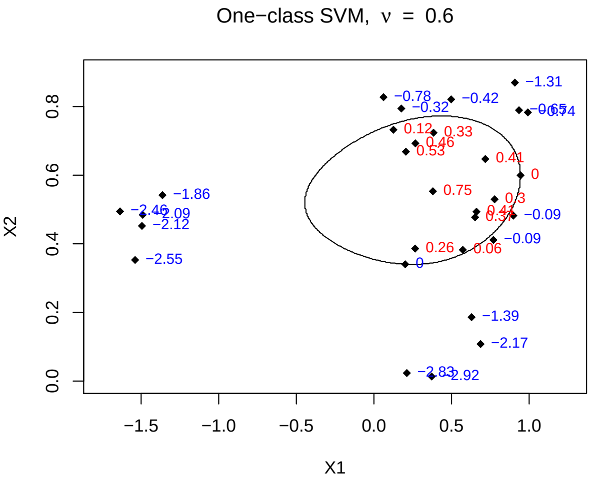

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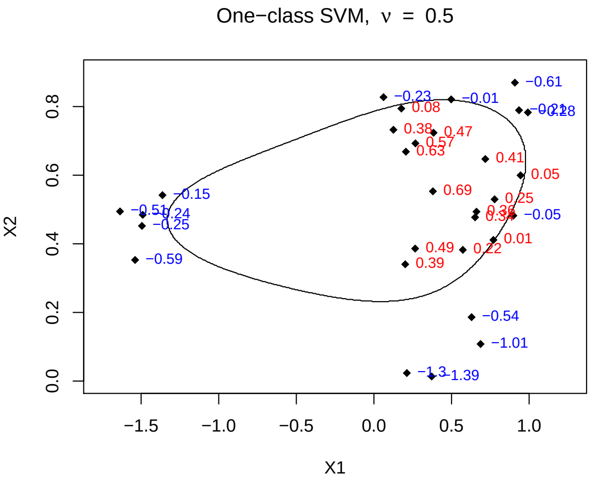

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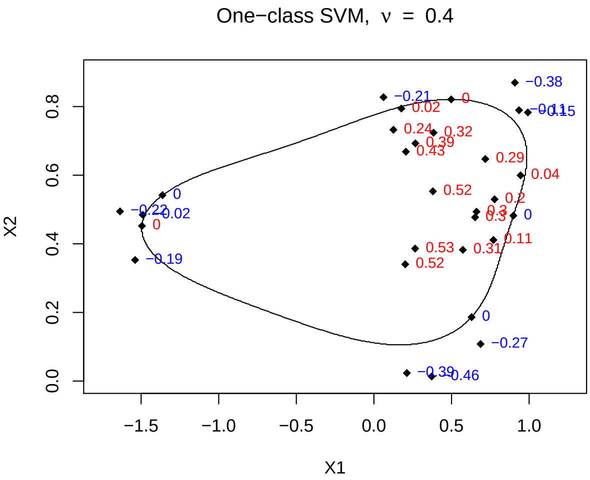

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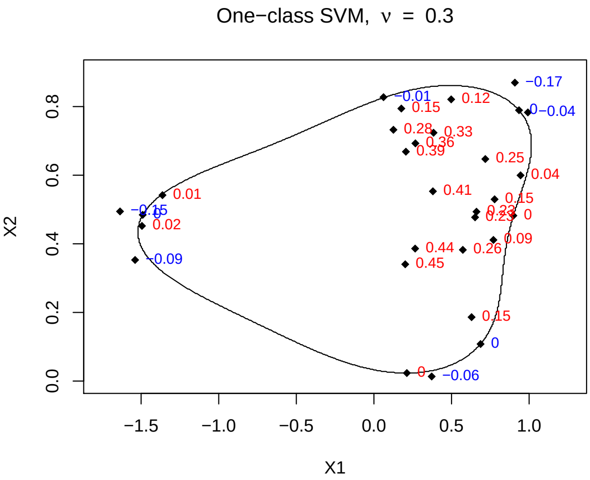

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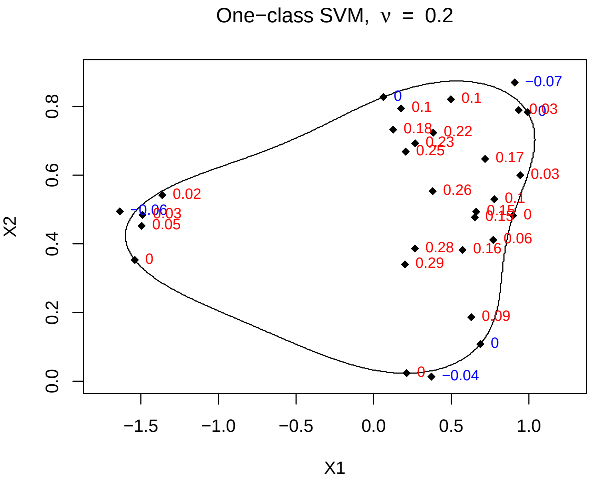

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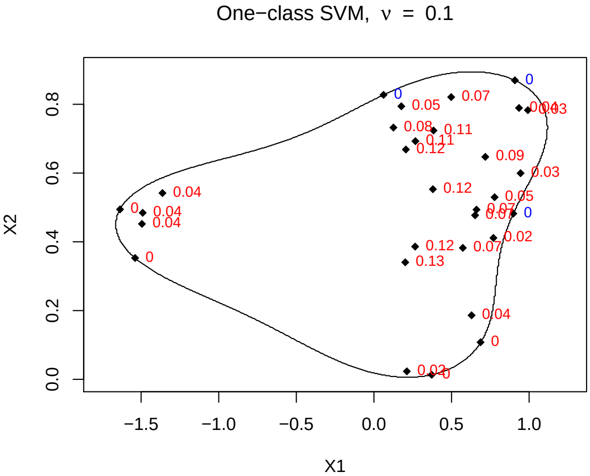

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Local outlier factor (Breunig, Kriegel, Ng, Sander; 2000)

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

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

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

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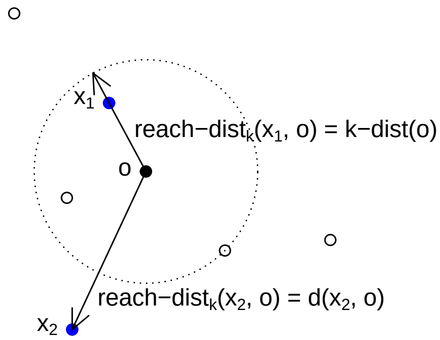
k-**neighborhood** of a point $\boldsymbol{x}$:
Given the $k\text{-}dist(\boldsymbol{x})$, the k-neighborhood of $\boldsymbol{x}$, denoted $N_k(\boldsymbol{x})$, contains every point whose distance from $\boldsymbol{x}$ is not greater than the $k\text{-}dist(\boldsymbol{x})$, *i.e.*:

$$N_k(\boldsymbol{x}) = \left\{ \boldsymbol{q} \in \boldsymbol{X} \setminus \{\boldsymbol{x}\} \,\middle|\, d(\boldsymbol{x}, \boldsymbol{q}) \leq k\text{-}dist(\boldsymbol{x}) \right\}.$$

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

Reachability distance of order k of point $\boldsymbol{x}$ w.r.t. point $\boldsymbol{o}$:
For $k \in \mathbb{N}$, the reachability distance of order k of point $\boldsymbol{x}$ with respect to point $\boldsymbol{o}$ is defined as:

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



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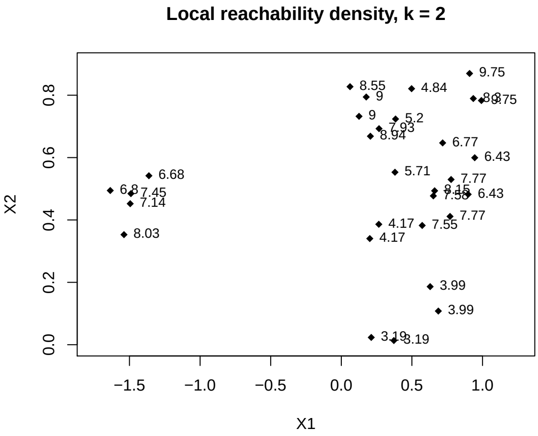

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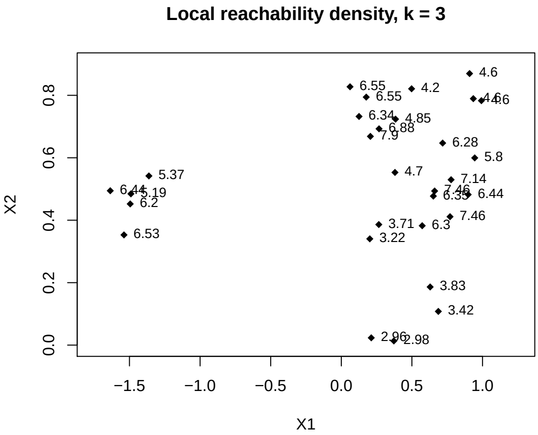

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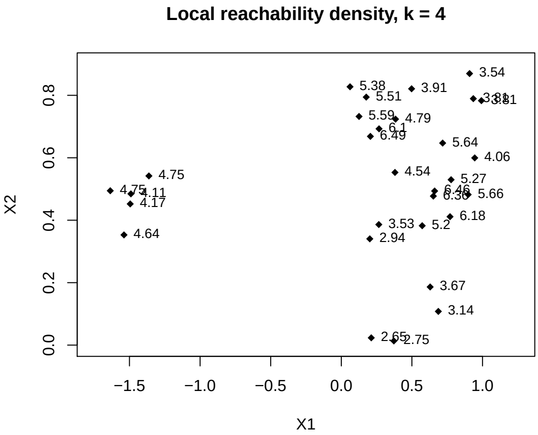

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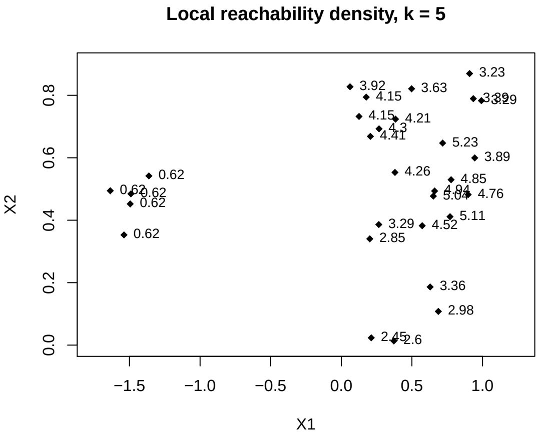

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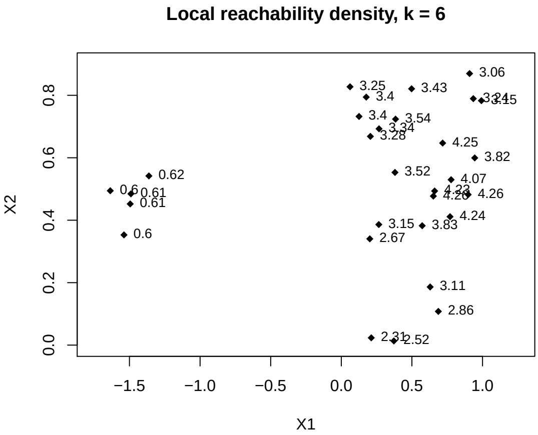

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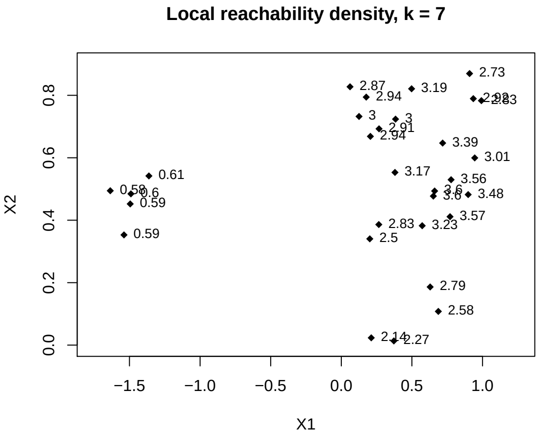

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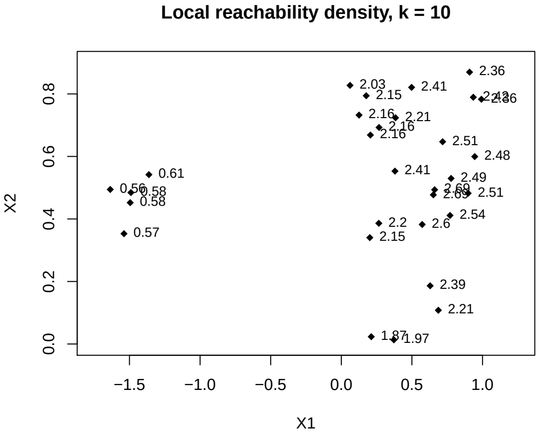

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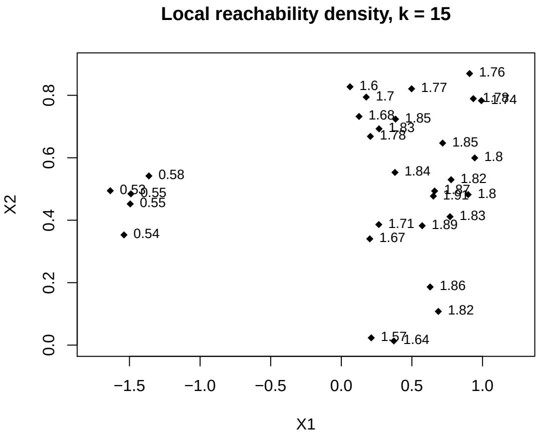

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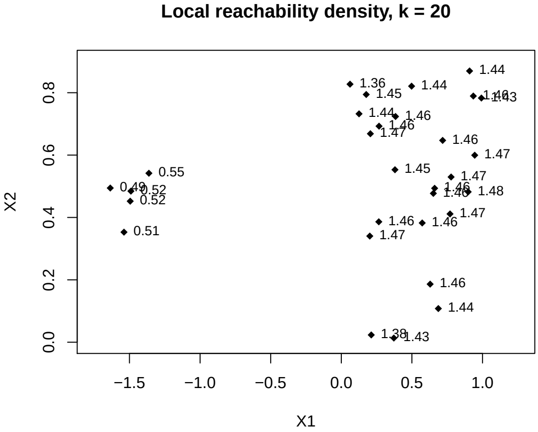

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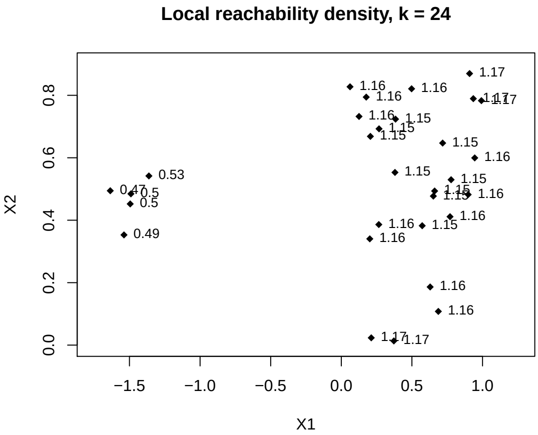

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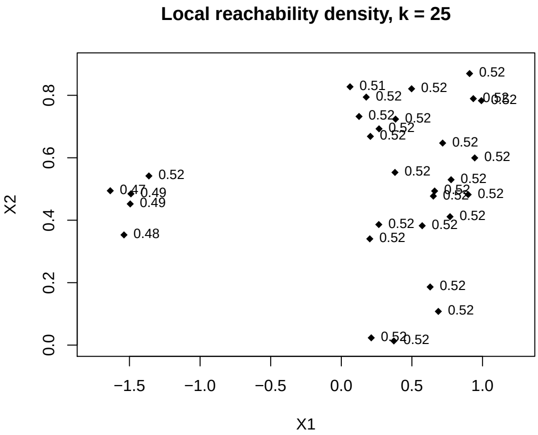

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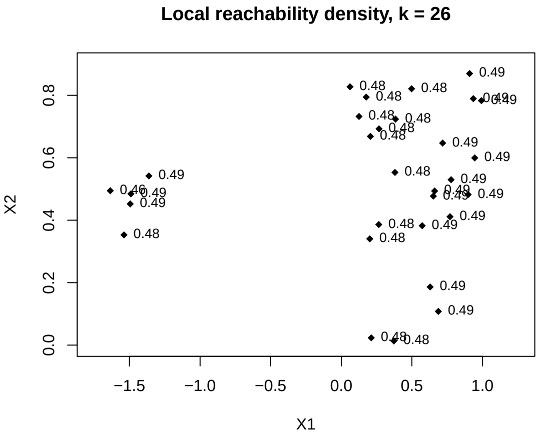

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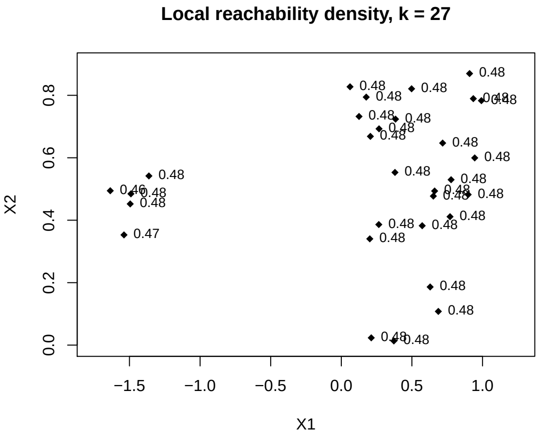

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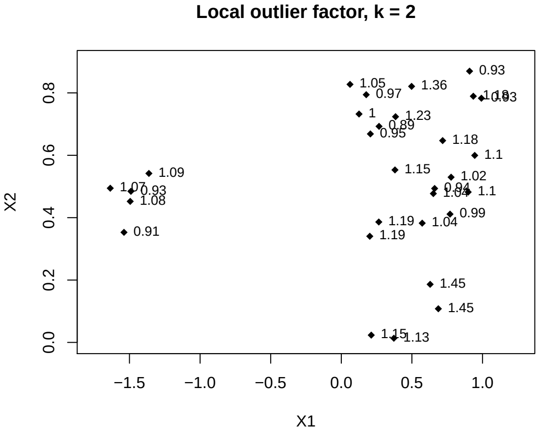

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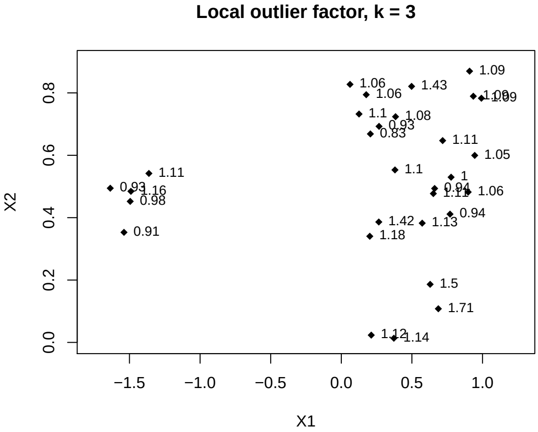

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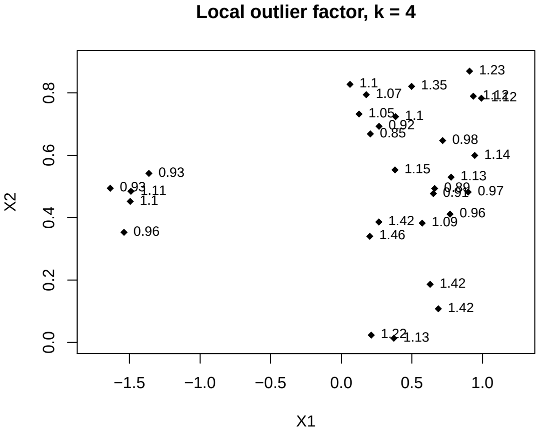

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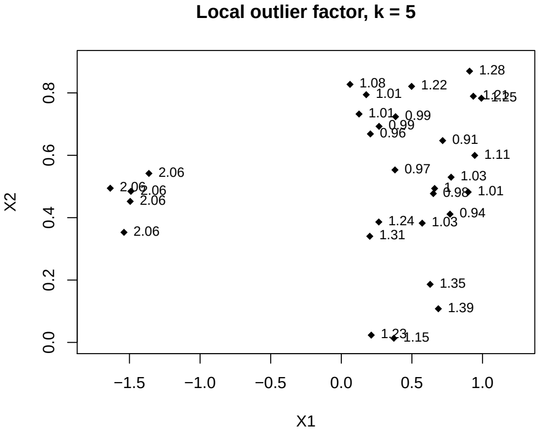

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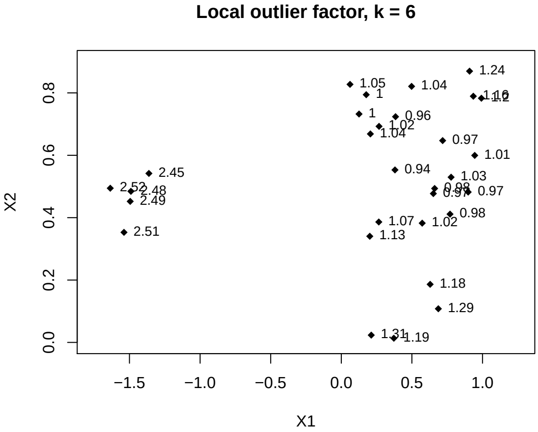

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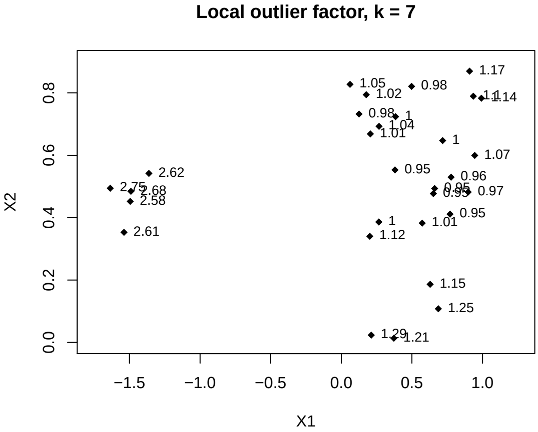

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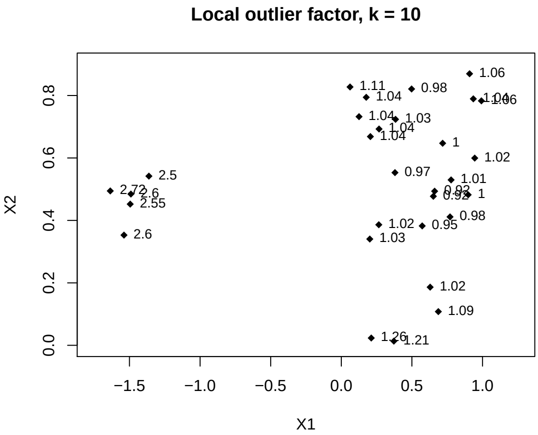

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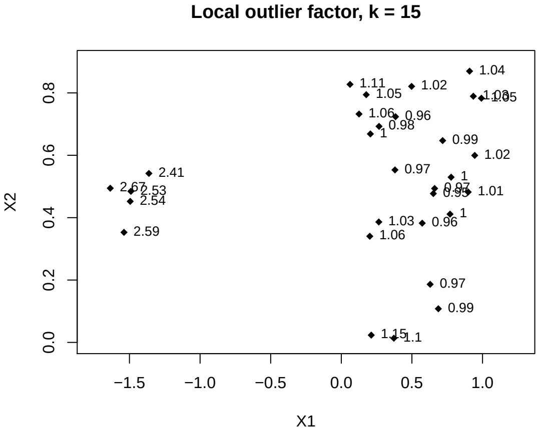

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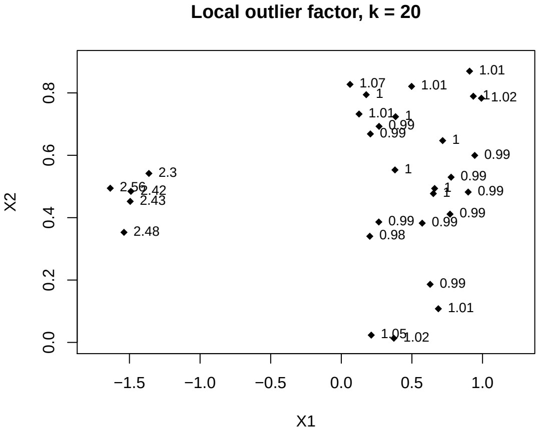

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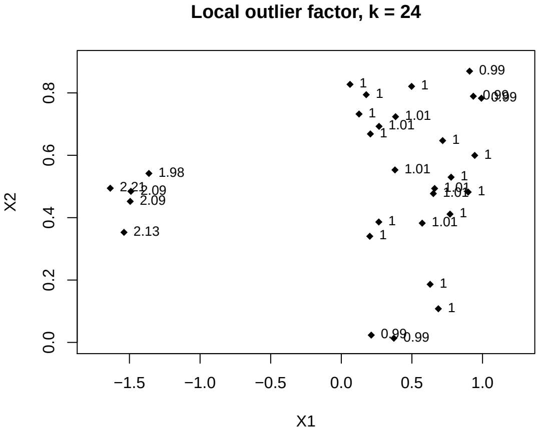

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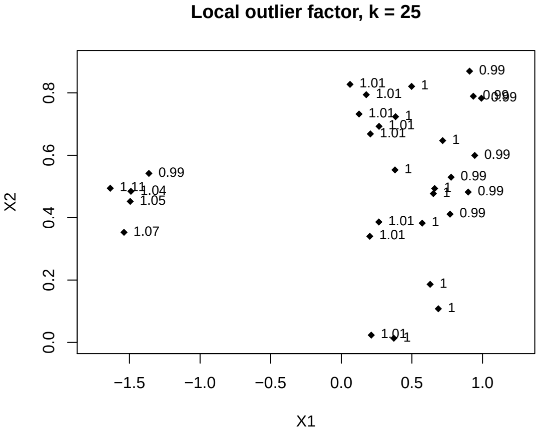

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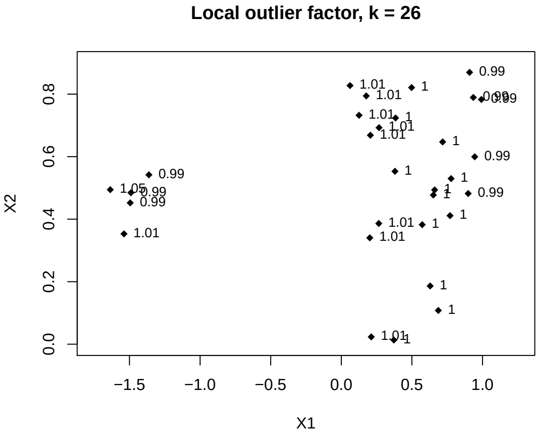

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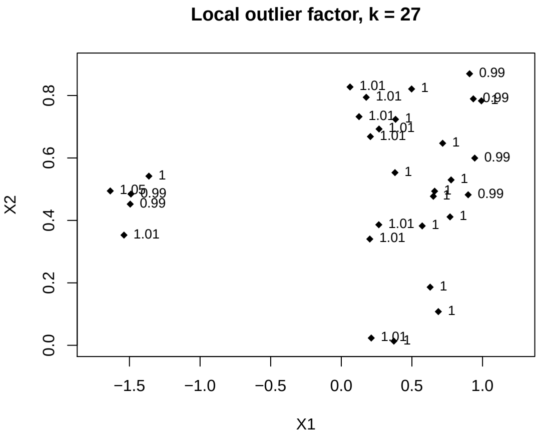

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- Since no supervised feedback is given, isolation forest is based on purely random (uniform) variable-based partitioning.
- **Main idea:** Outlying observations are isolated faster.
- Tree-kind partitioning is done until "full isolation": outlying 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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Stop when only one observation is in each node: isolation.

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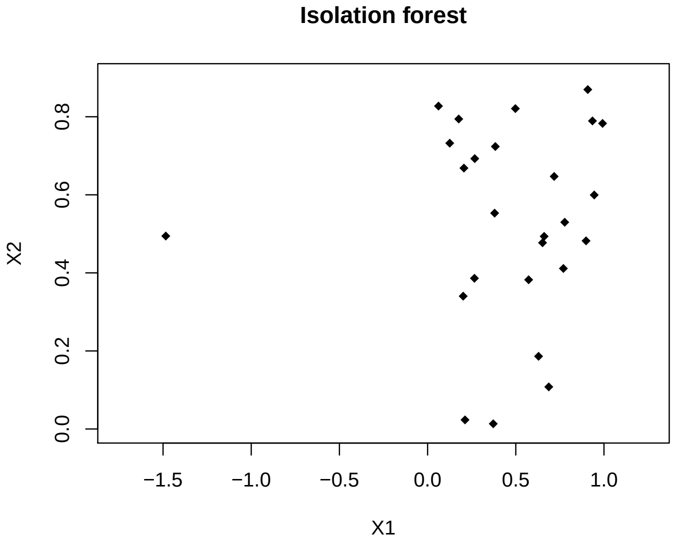
Illustration: Isolation tree



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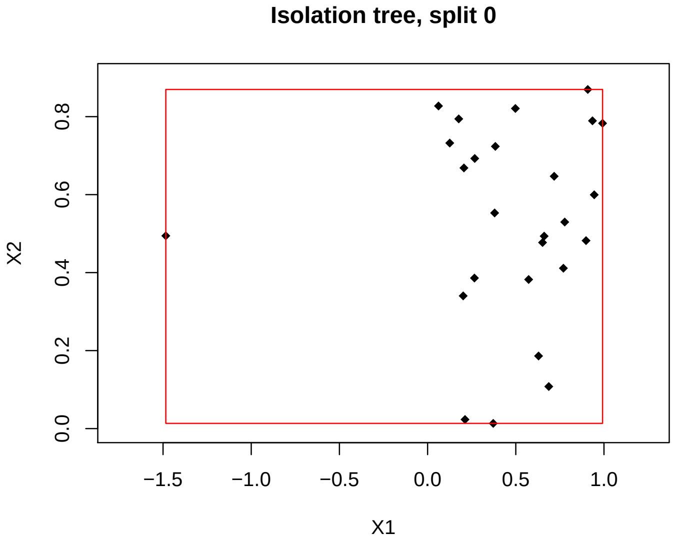

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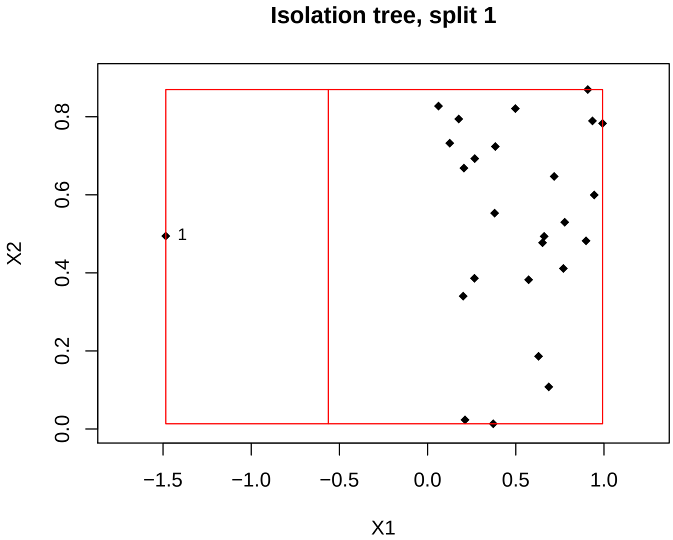

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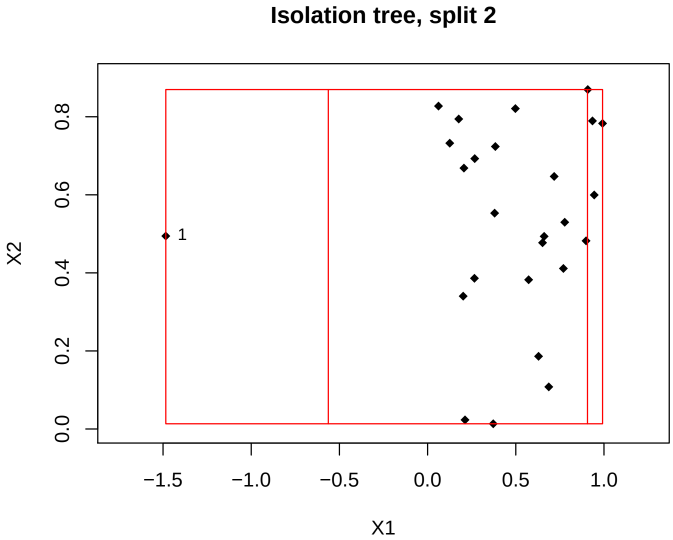

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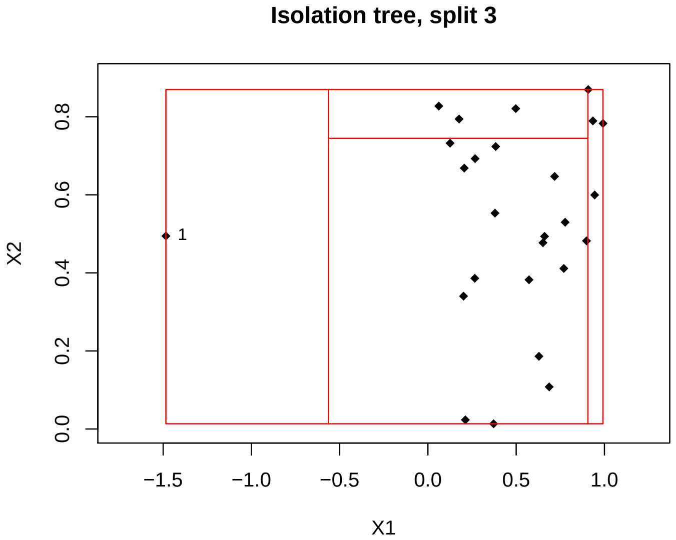

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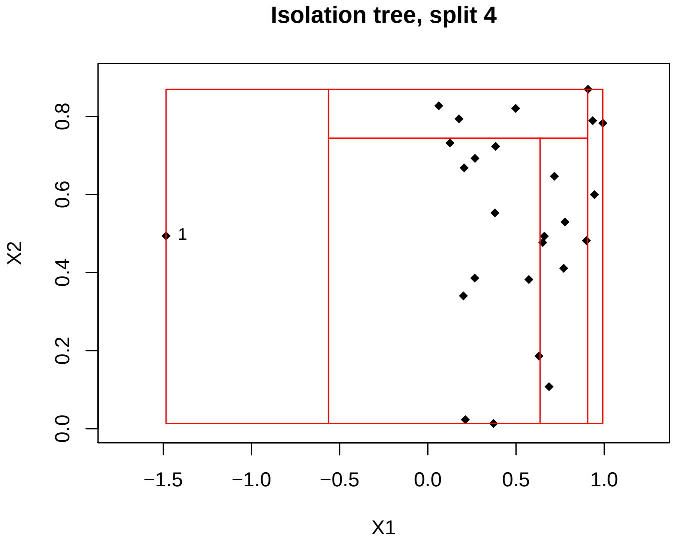

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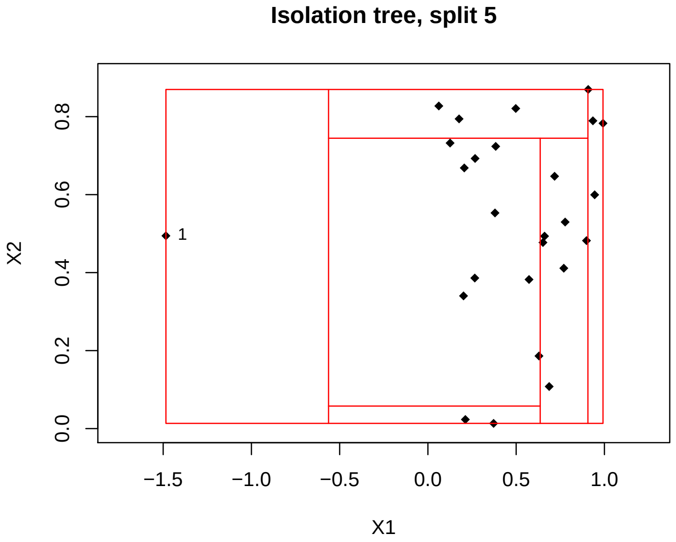

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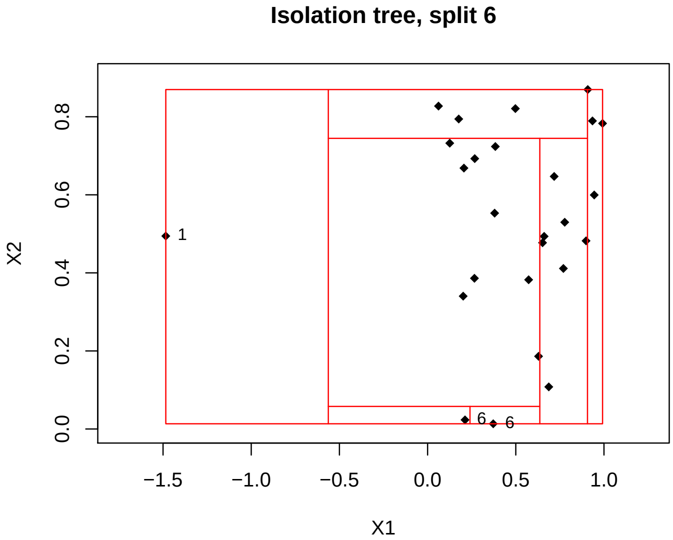

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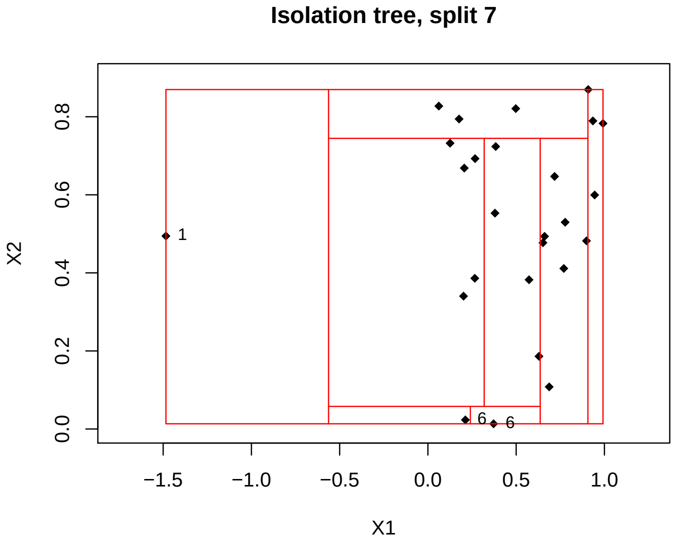

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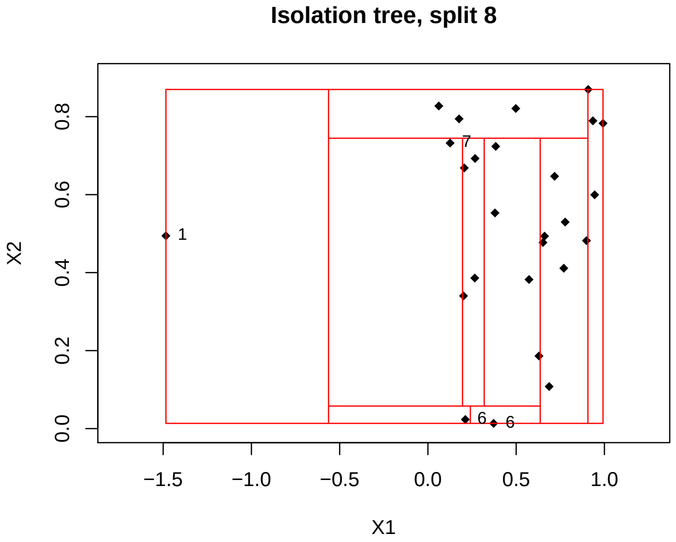

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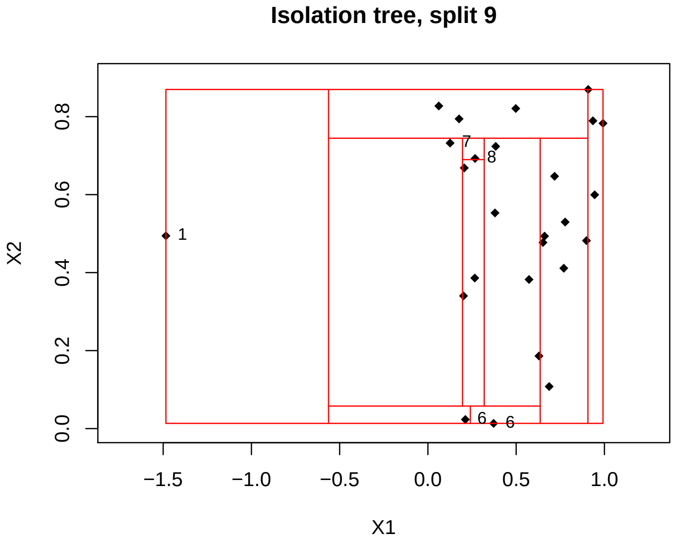

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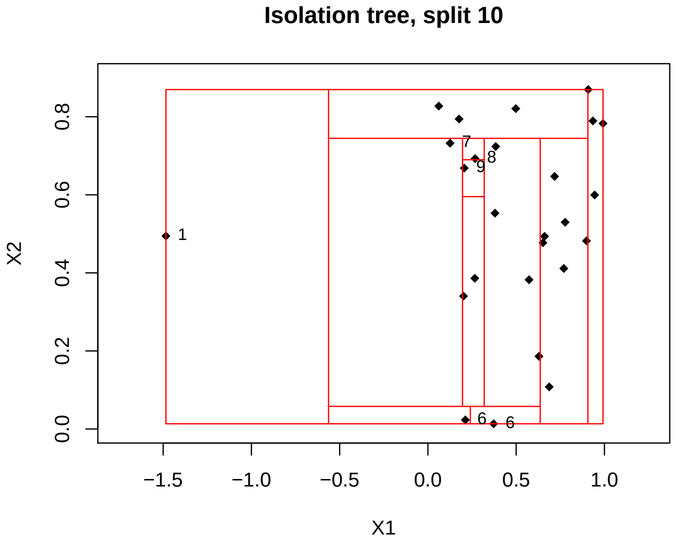

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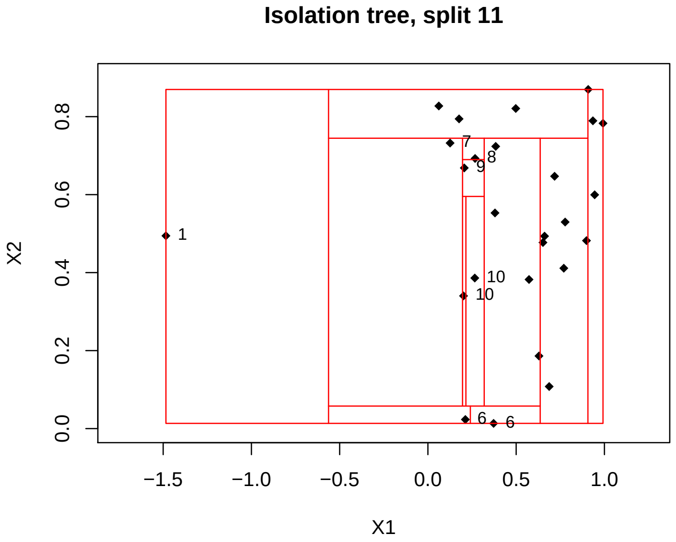

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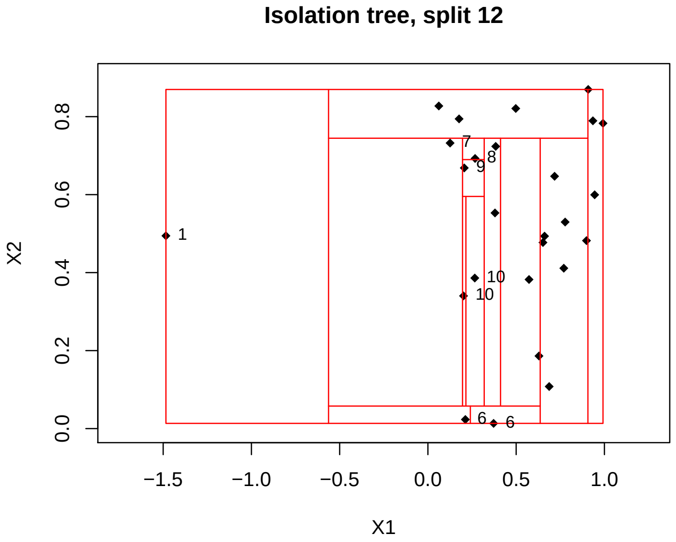

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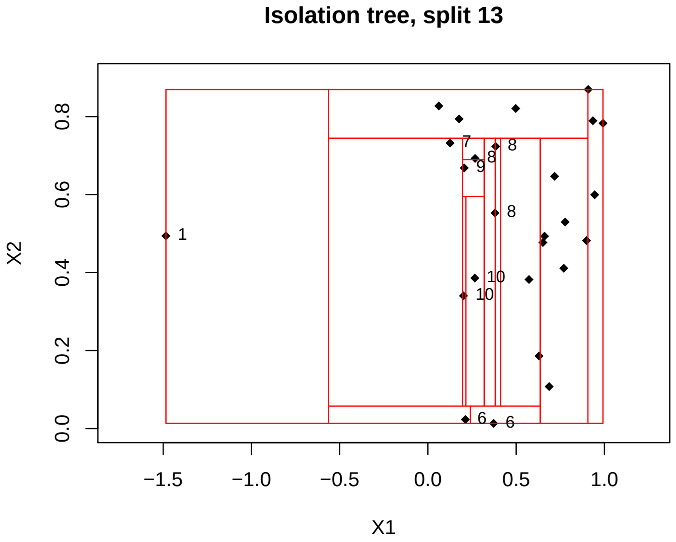

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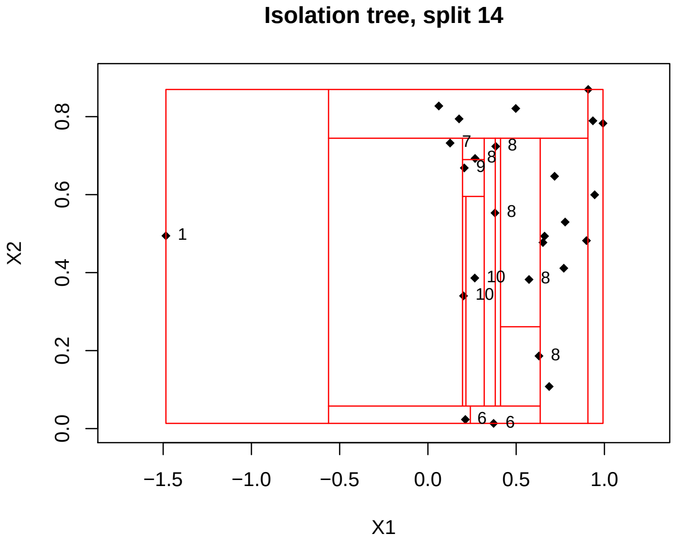

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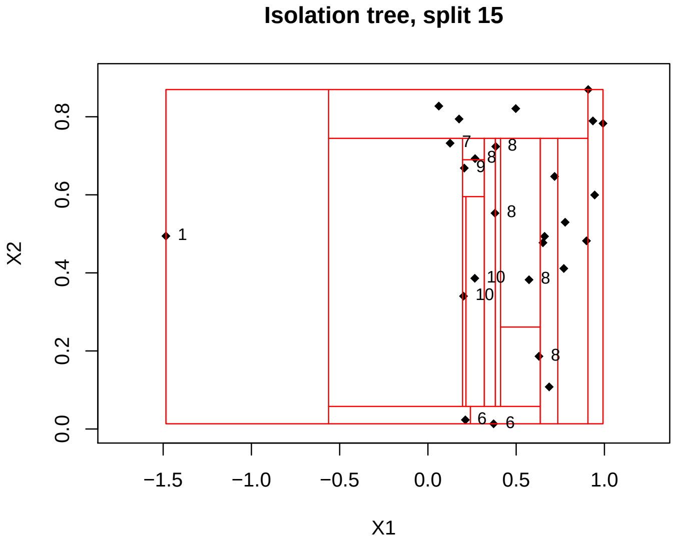

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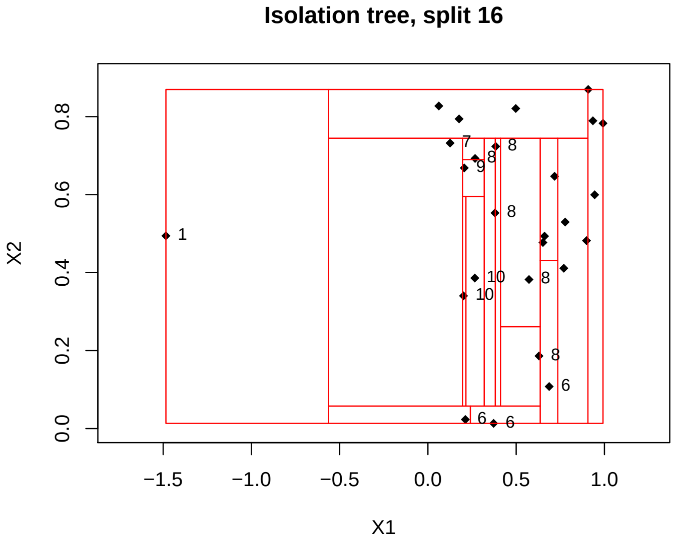

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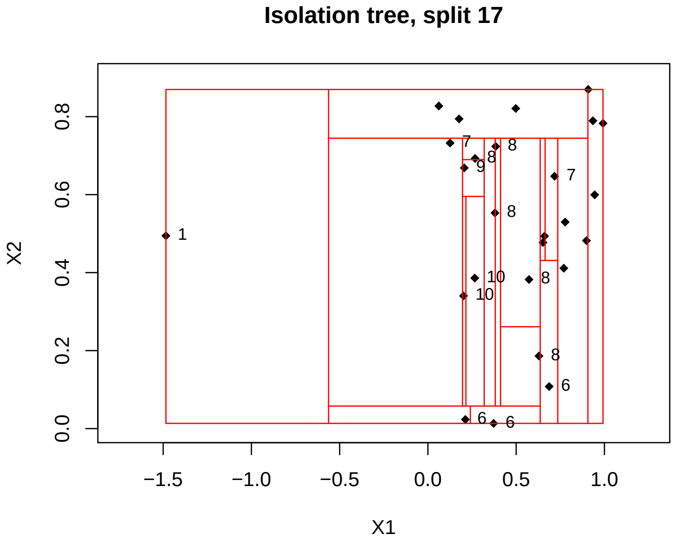

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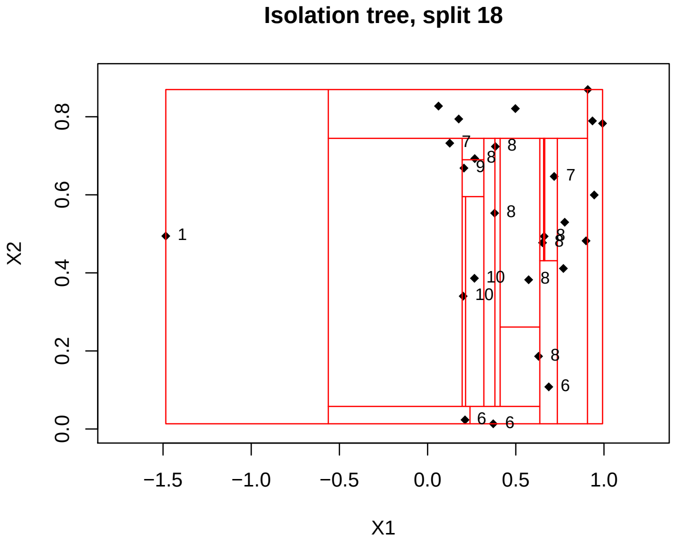

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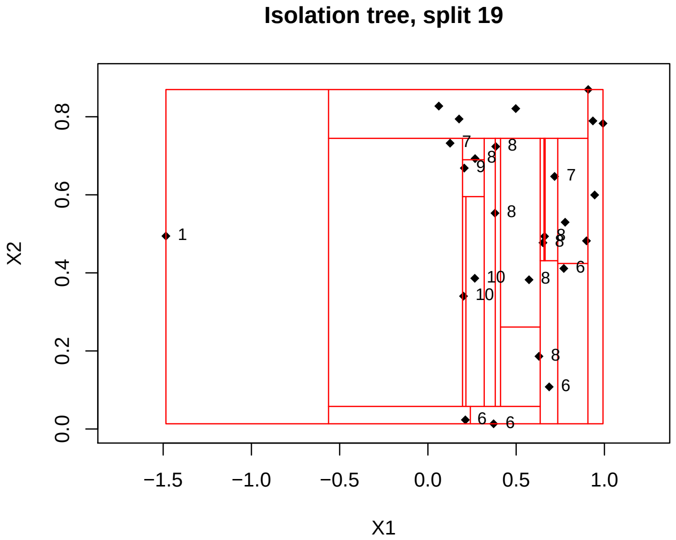

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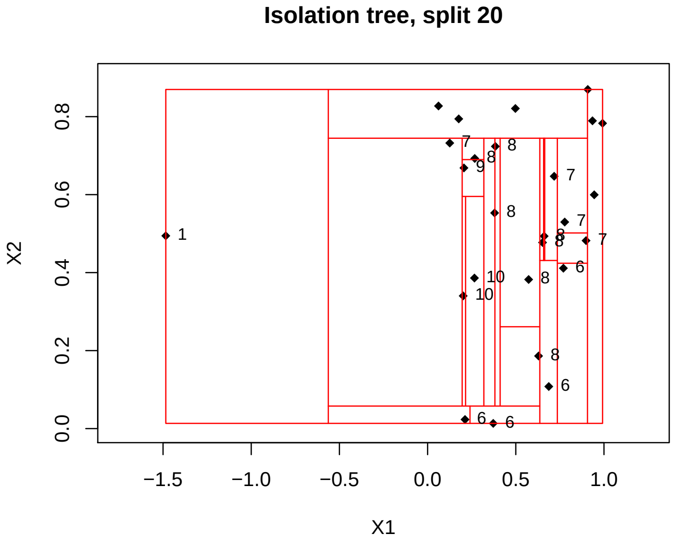

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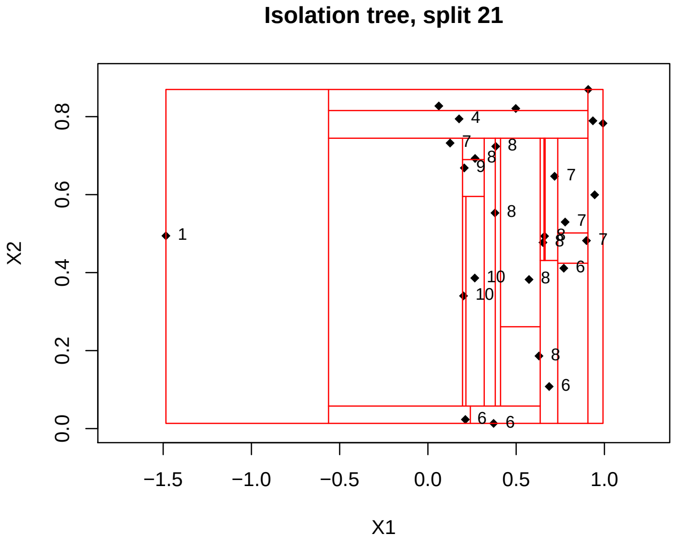

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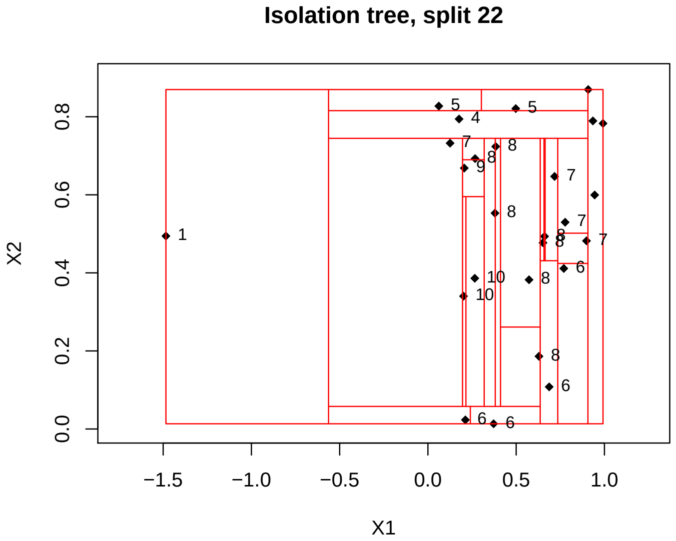

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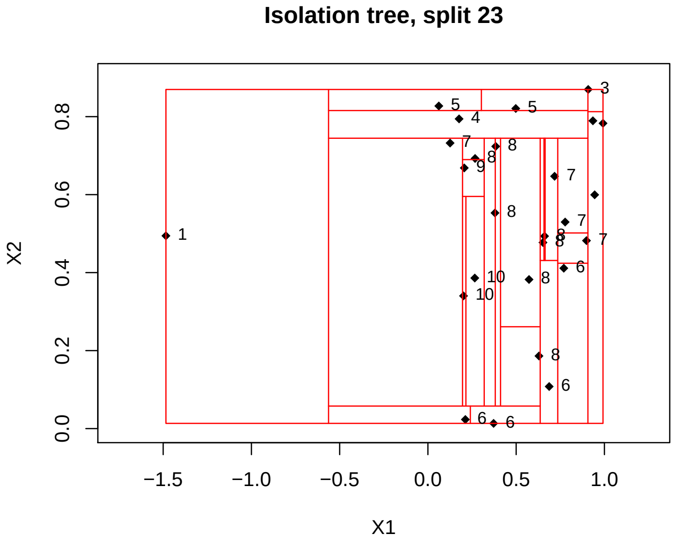

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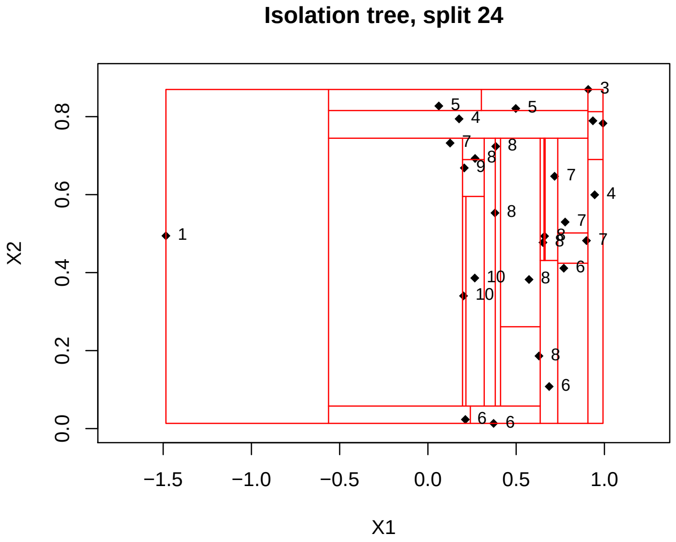

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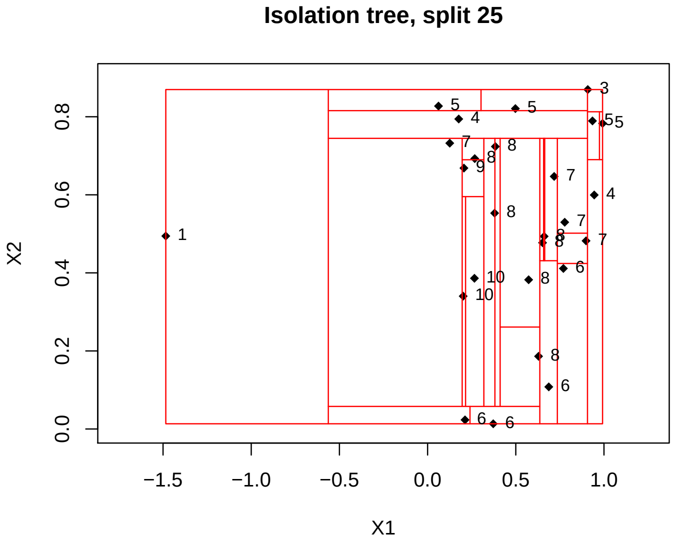

Isolation forest (Liu, Ting, Zhou; 2008)

Anomaly score calculation for observation $\boldsymbol{x}$:

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

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

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

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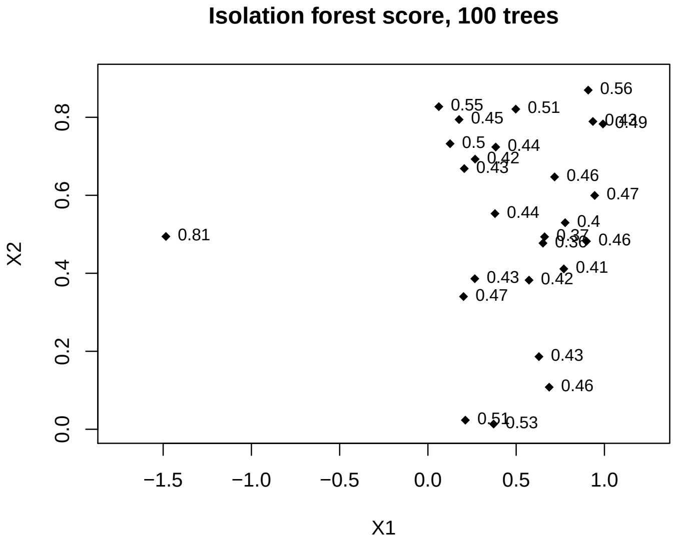
Illustration: Anomaly score



Contents

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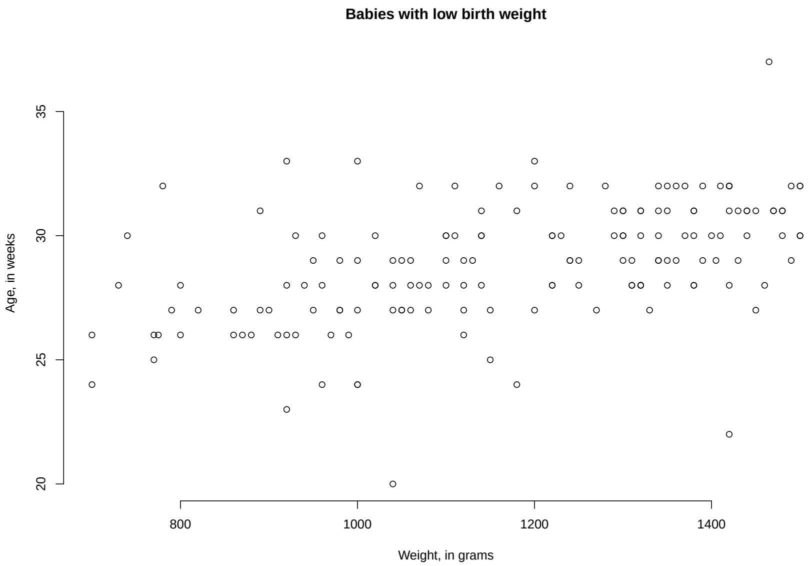
Data depth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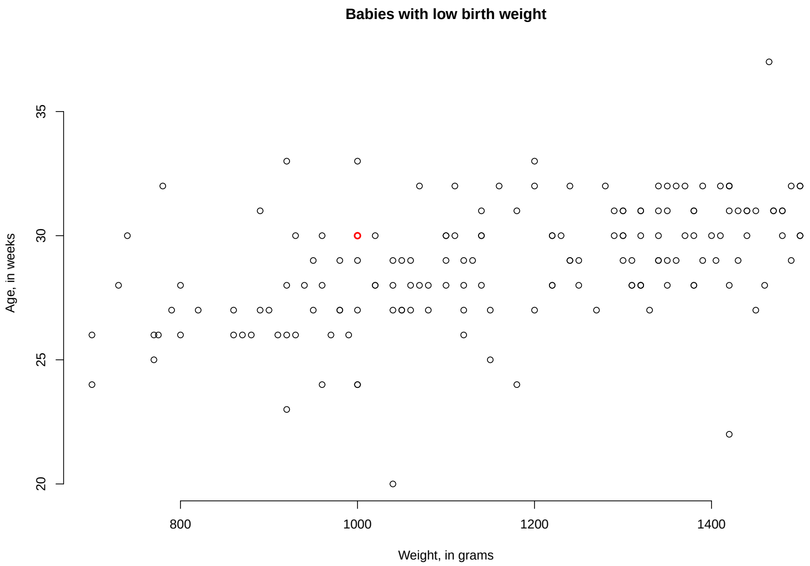

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Statistical data depth

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

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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.

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

Contents

Tukey (=halfspace, location) depth

Tukey (1975) — "Mathematics and the picturing of data"

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

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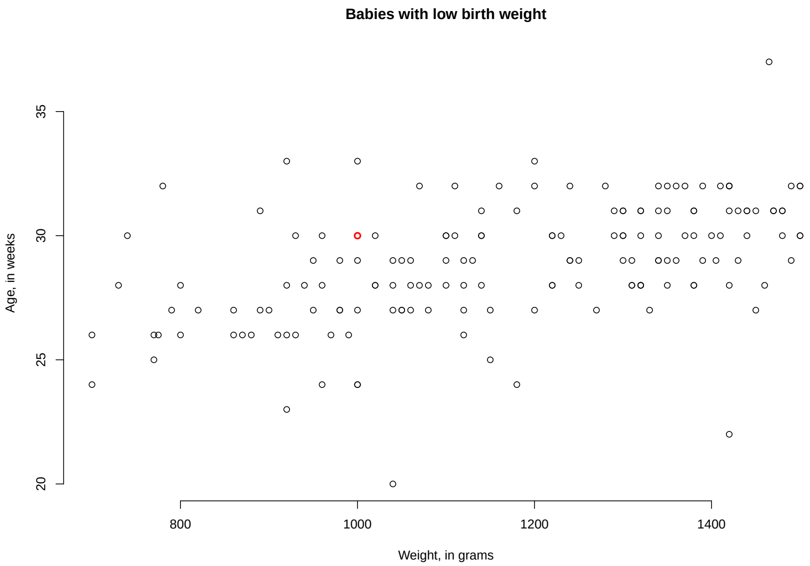
Tukey depth

- 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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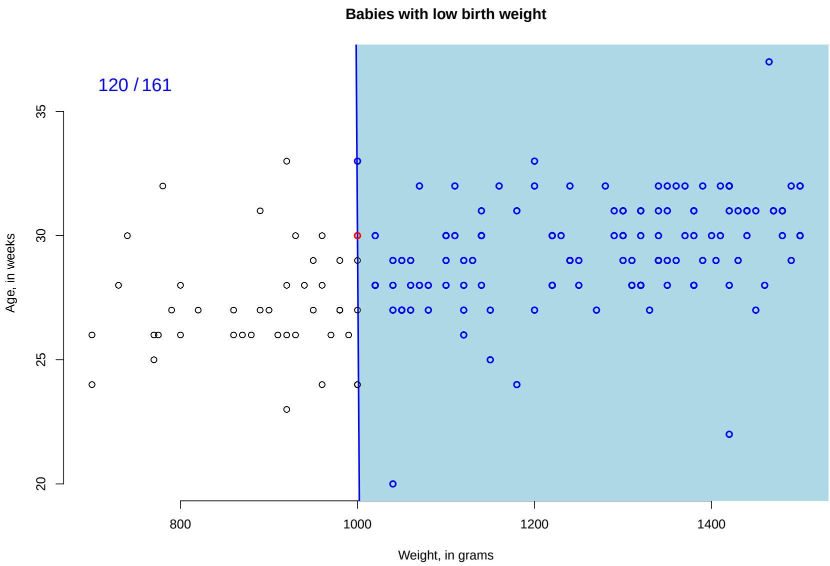

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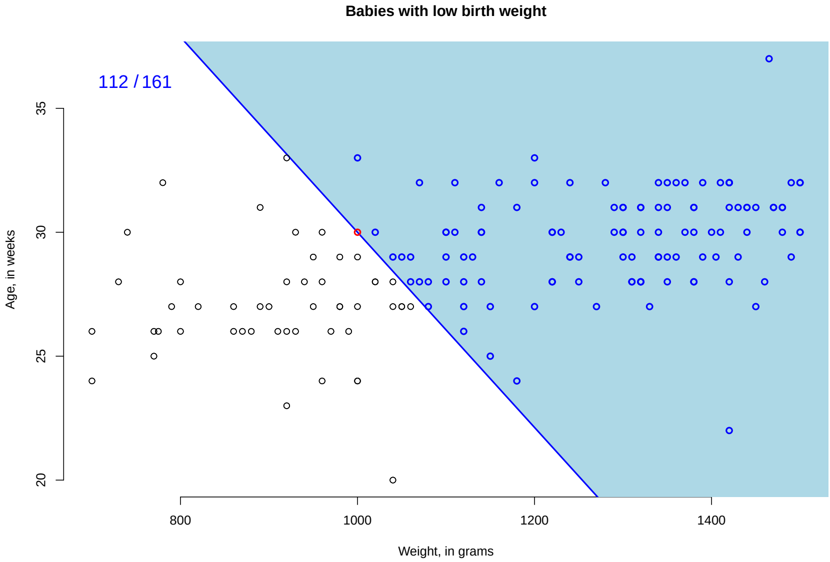

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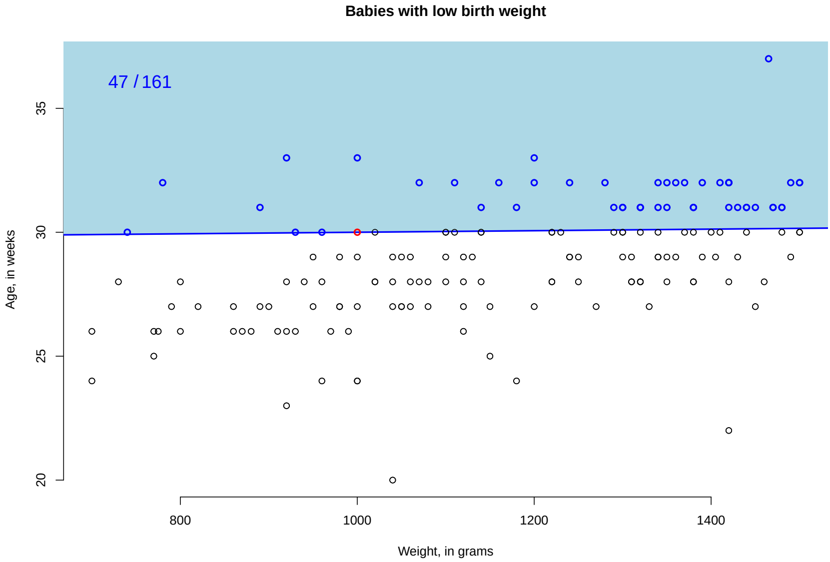

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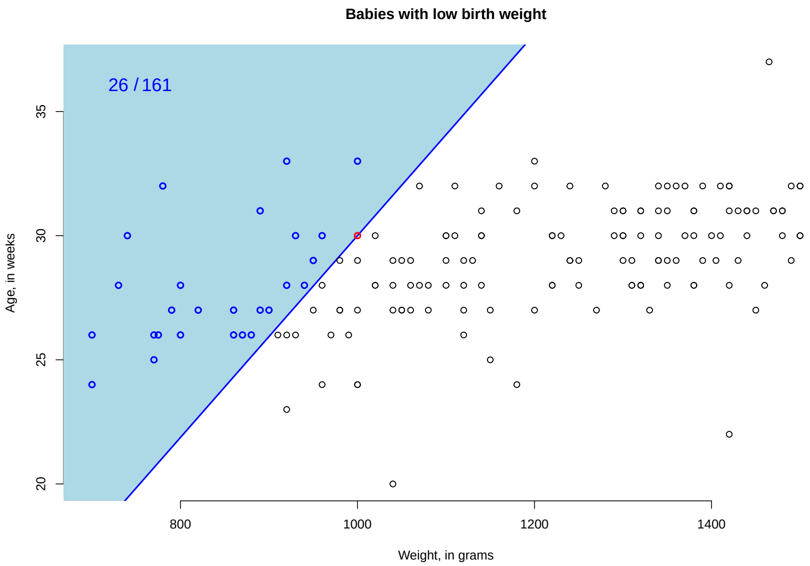

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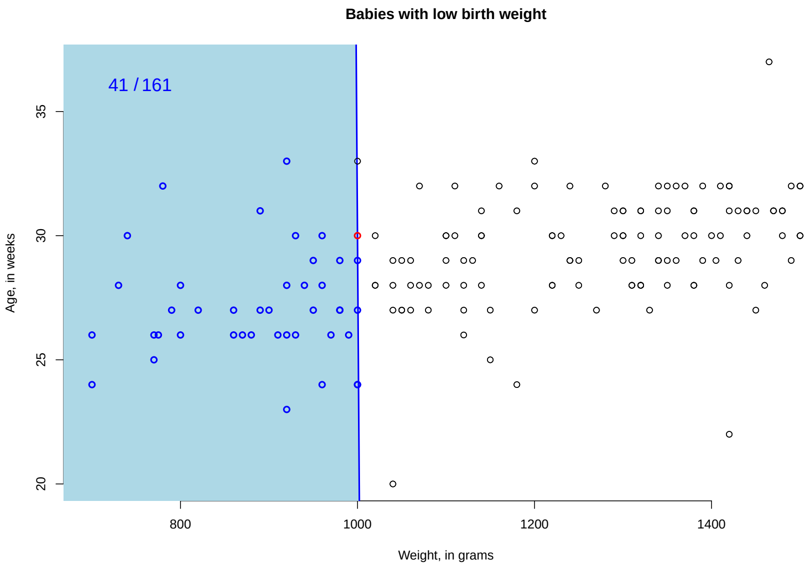

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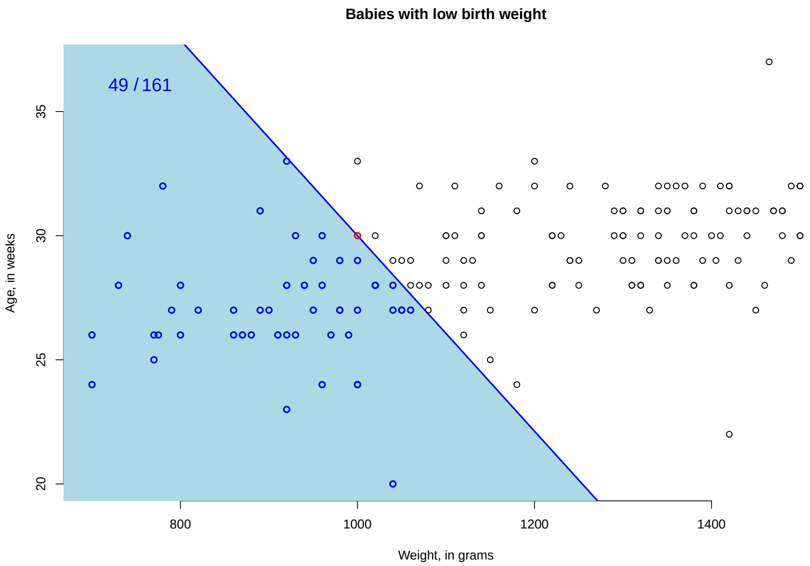

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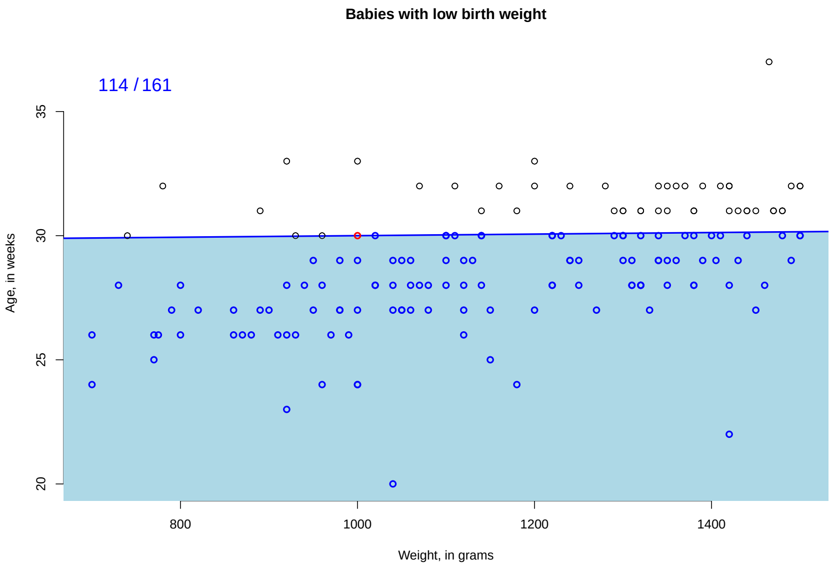

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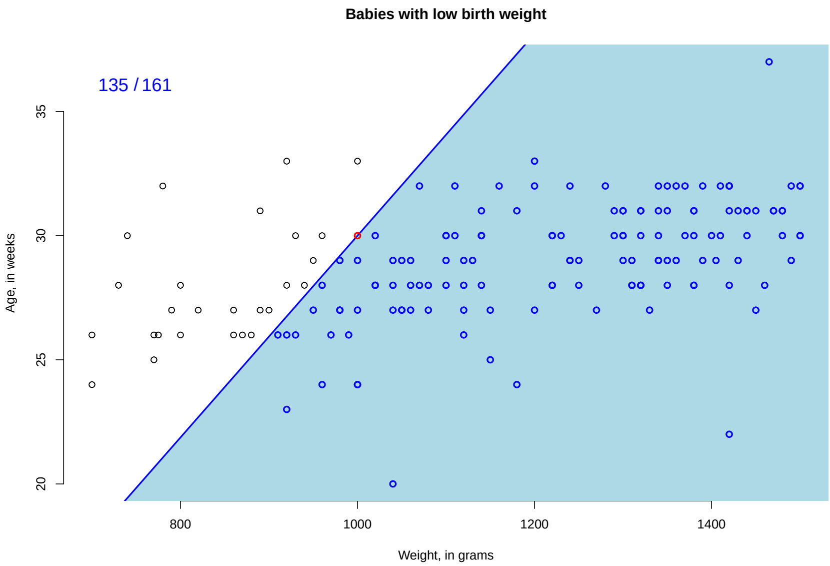

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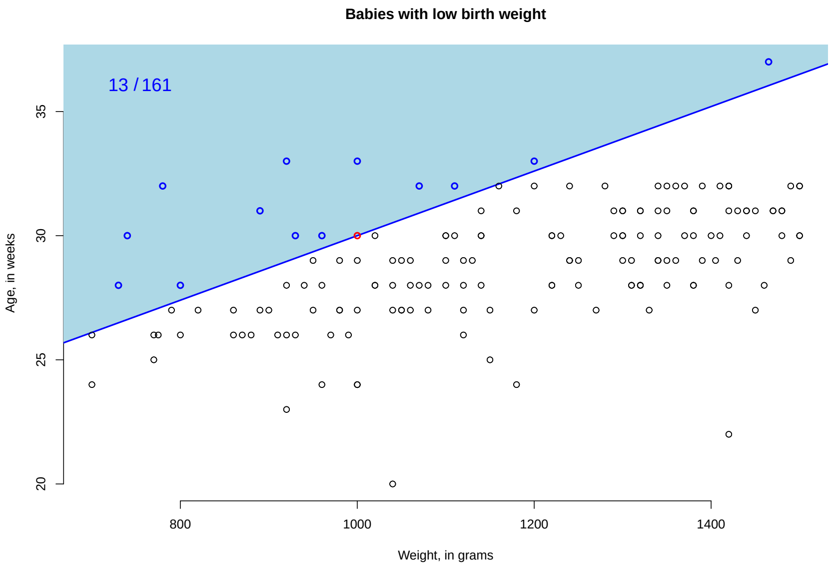

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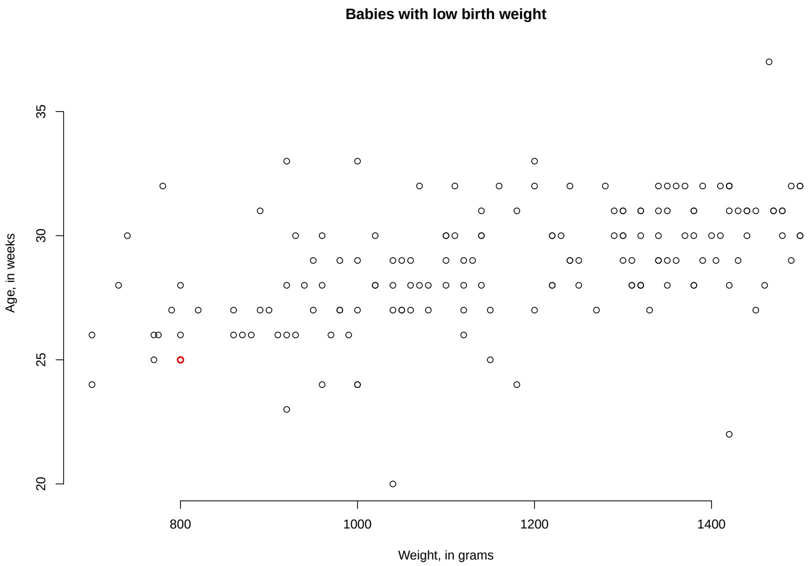

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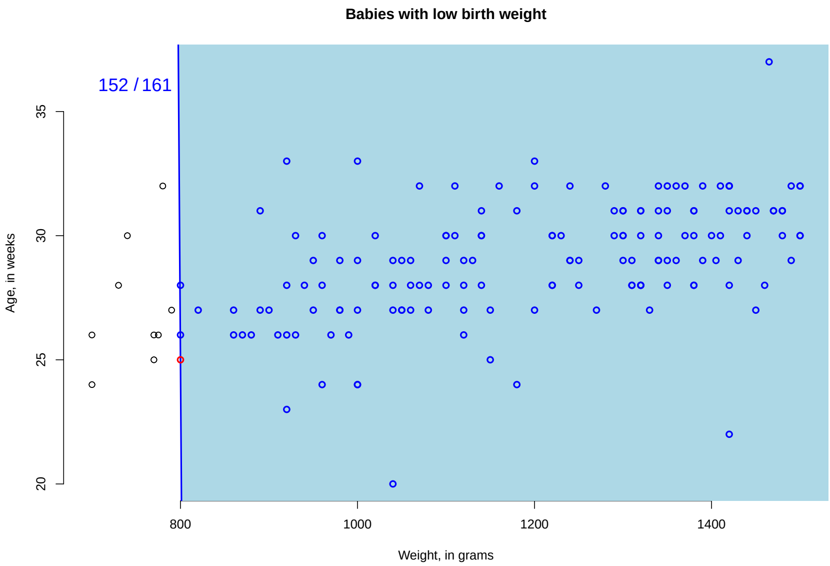

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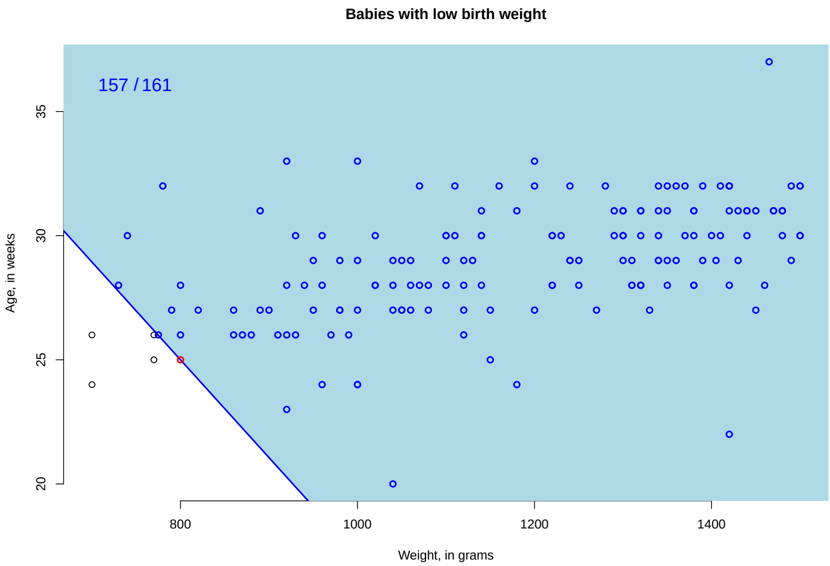

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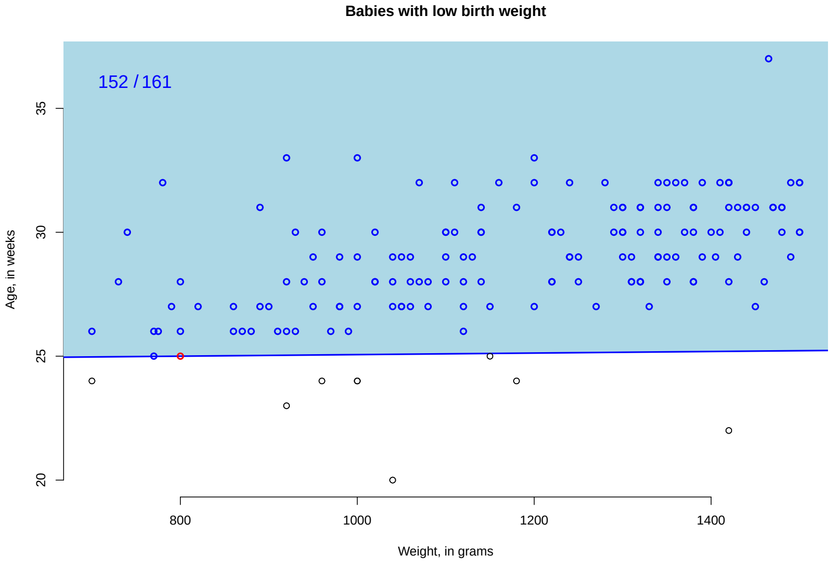

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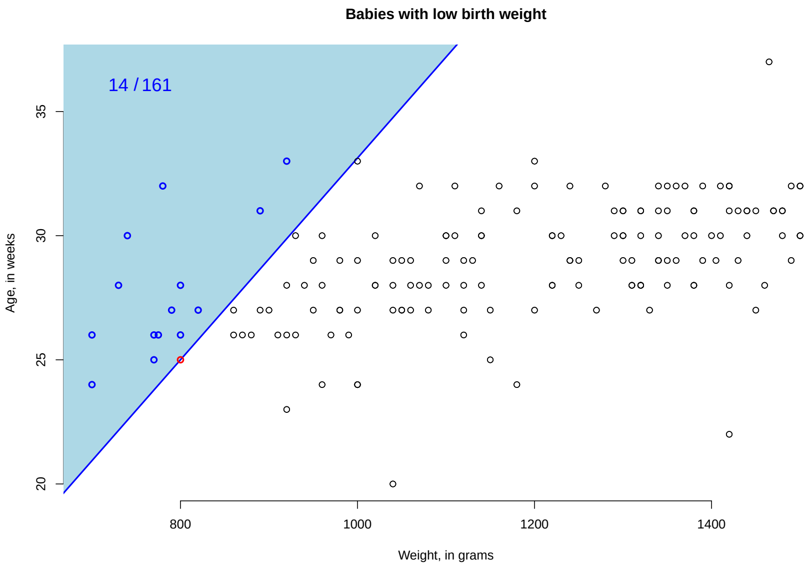

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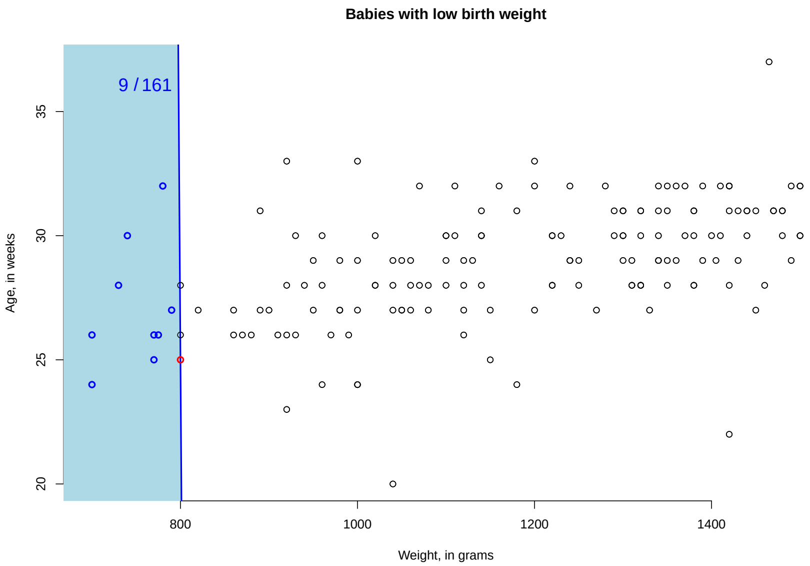

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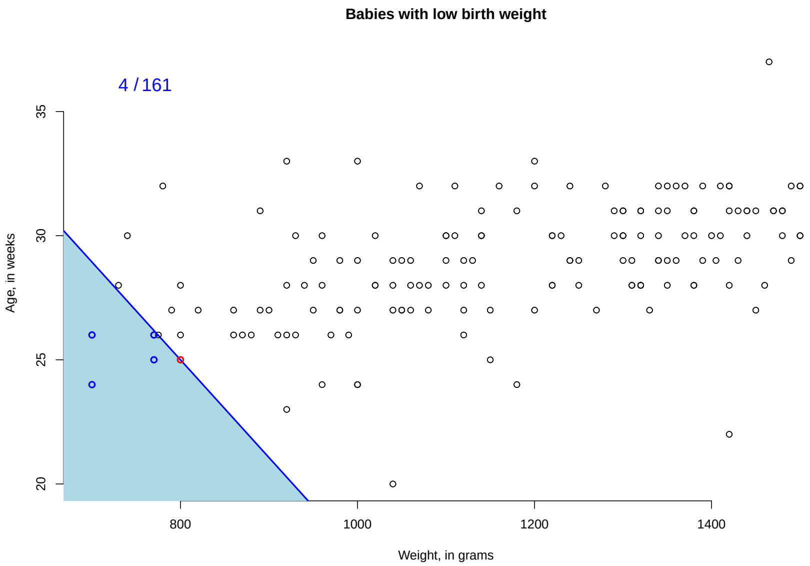

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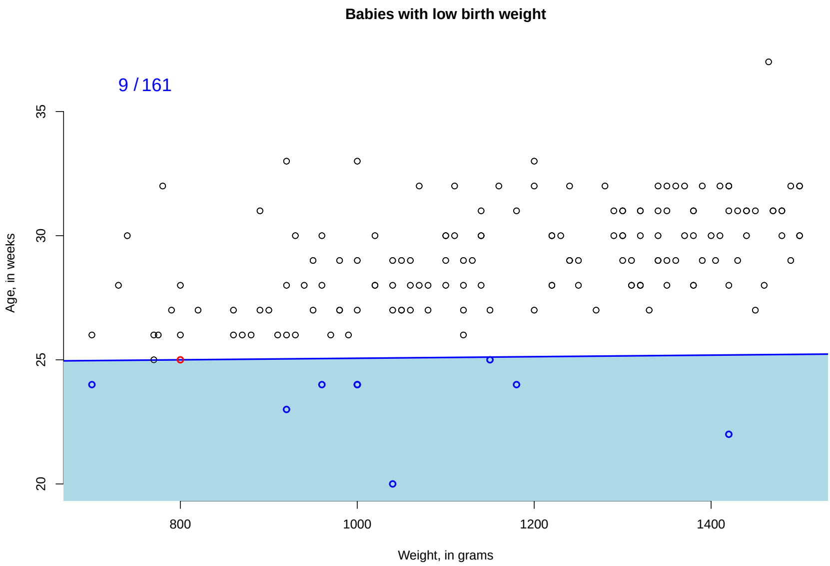

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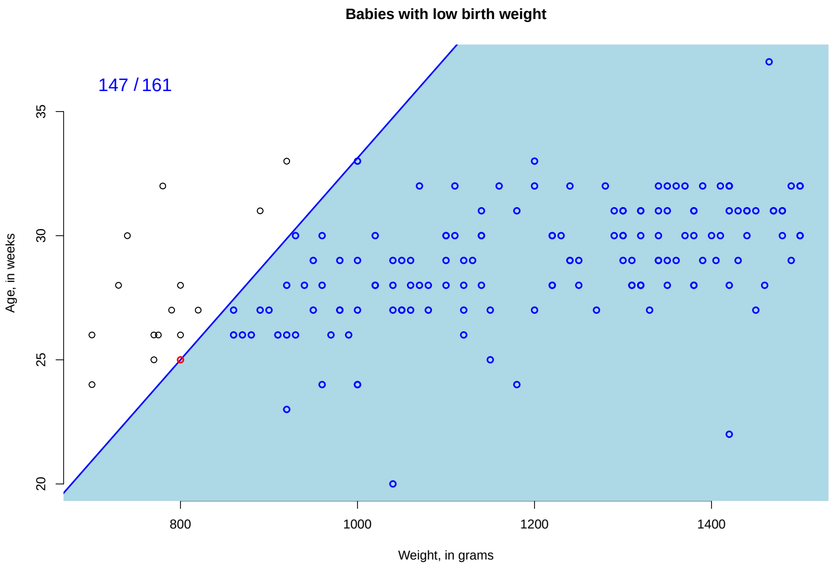

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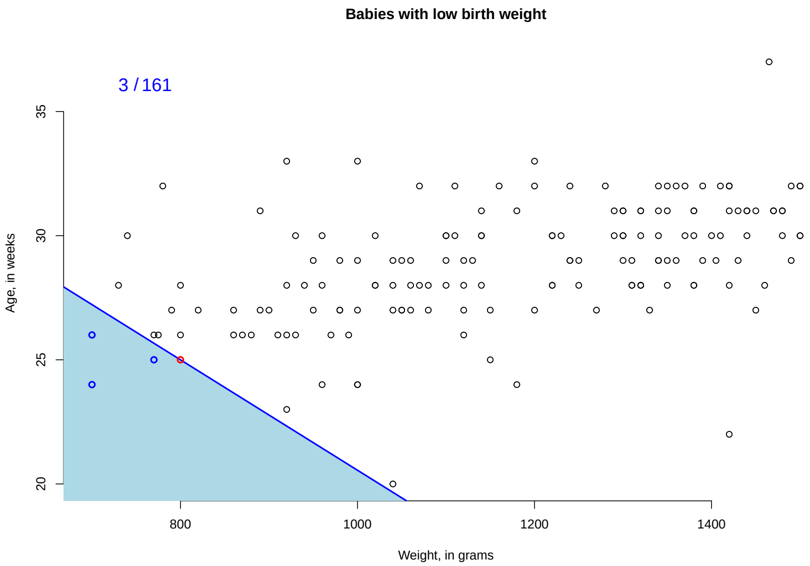

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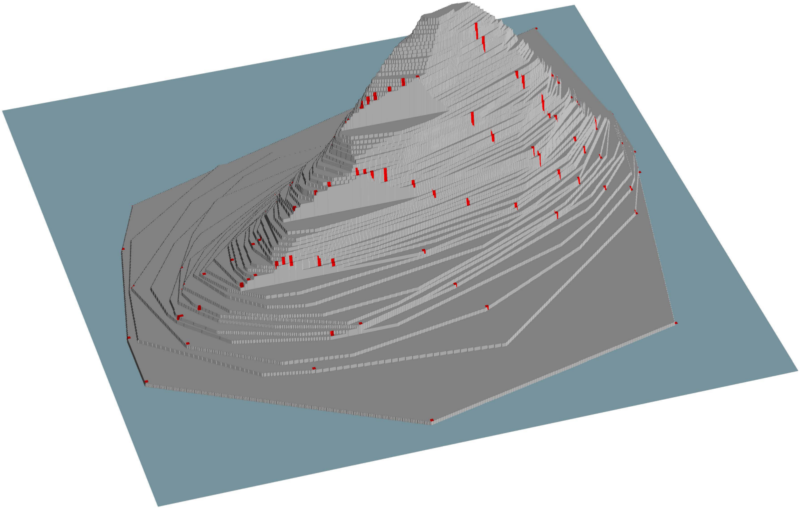

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▶ Quasiconcave.	Convex.

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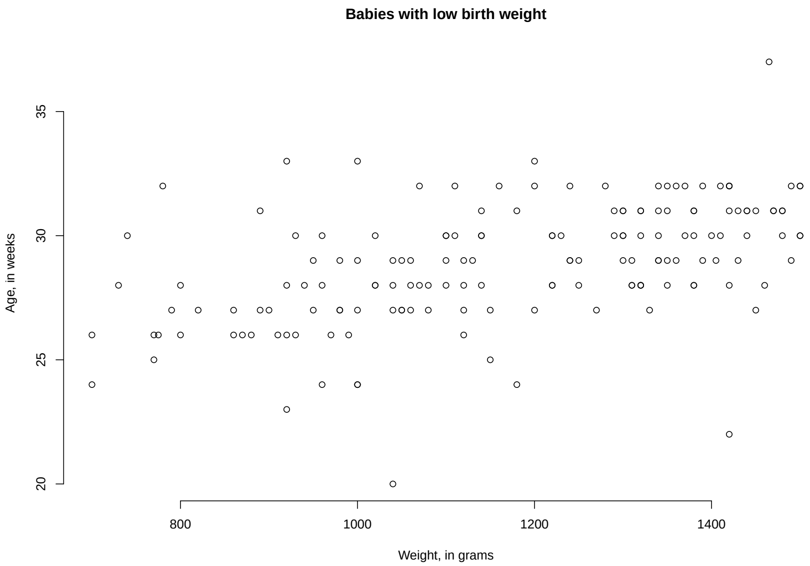

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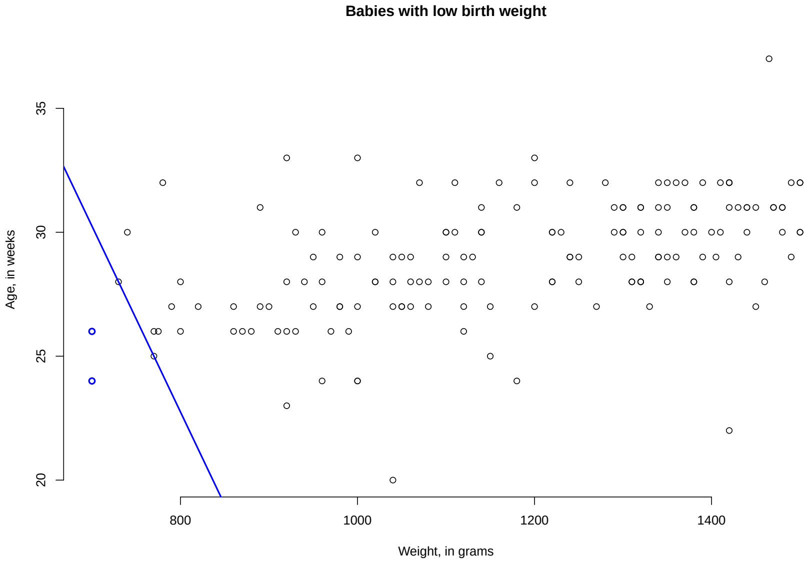

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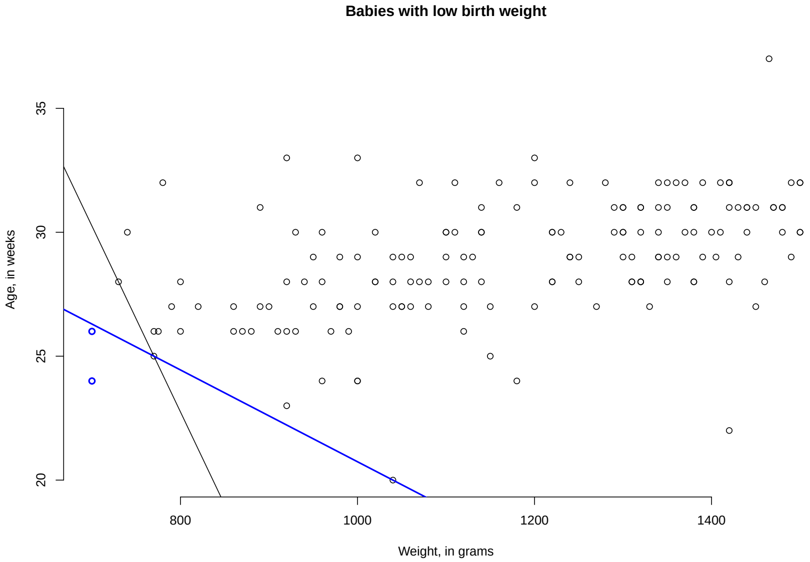

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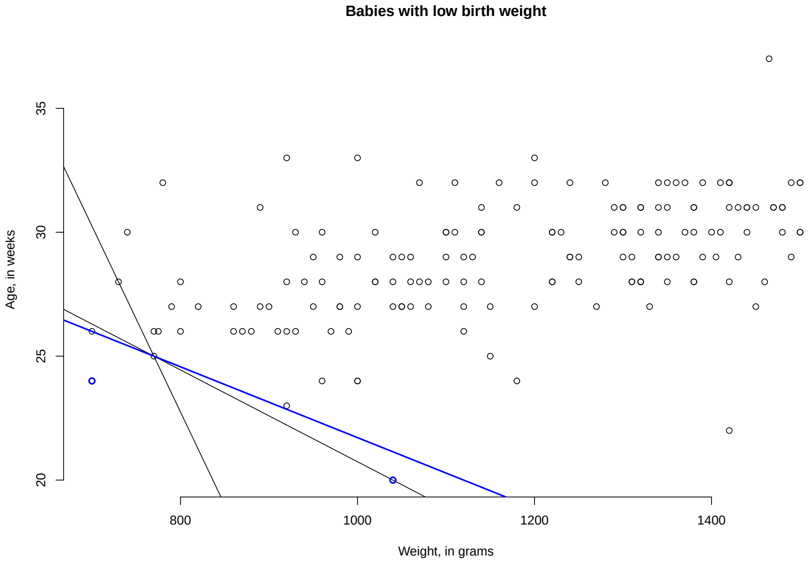

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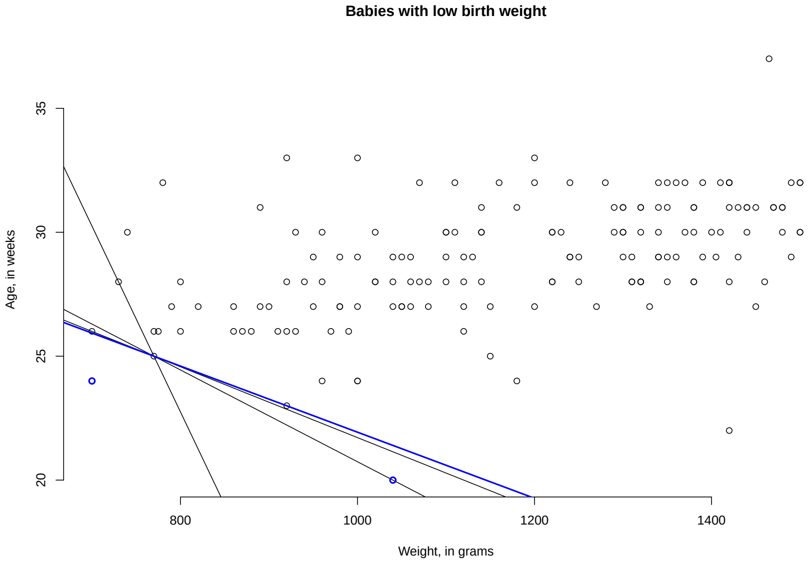

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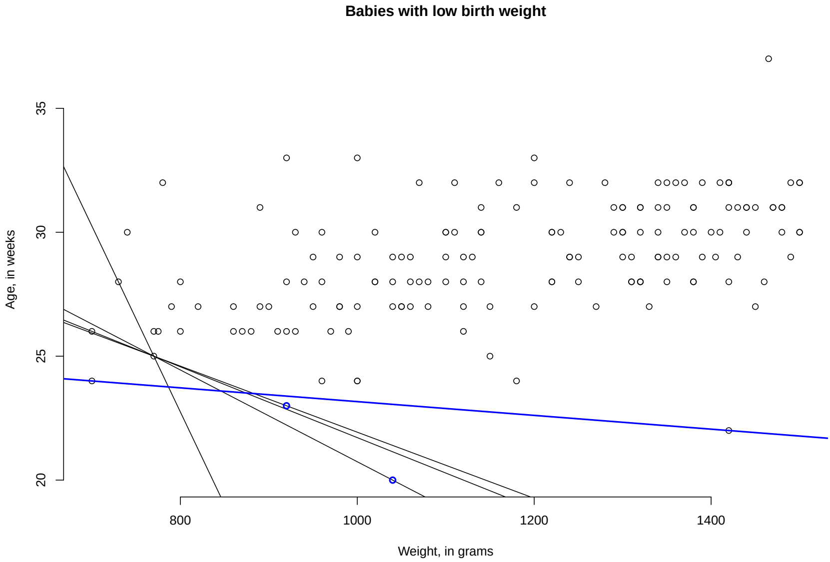

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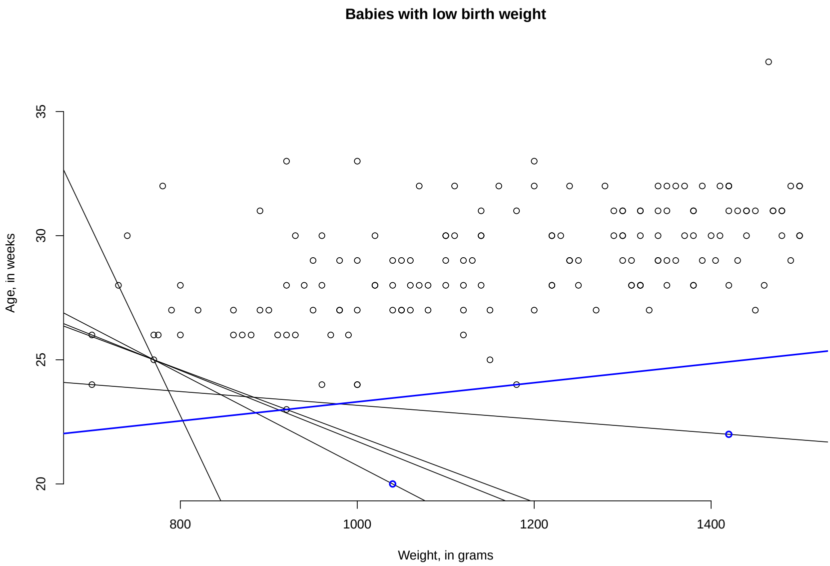

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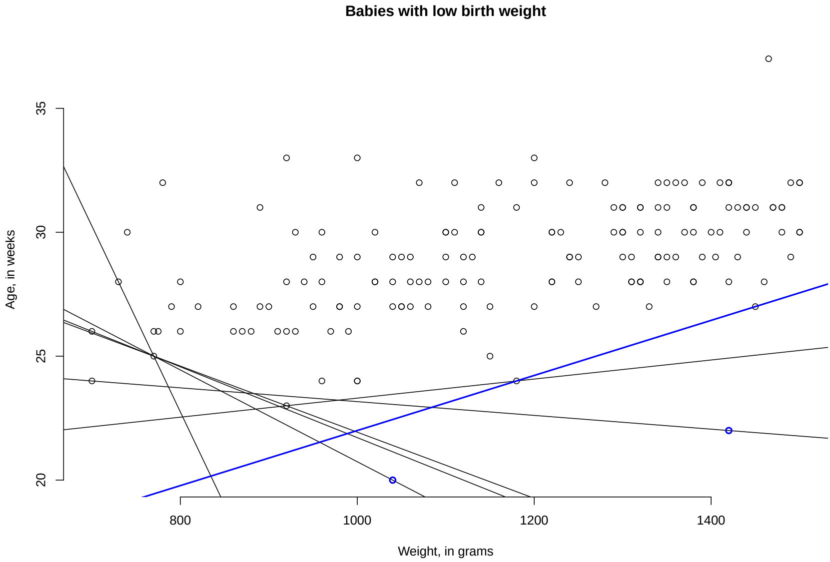

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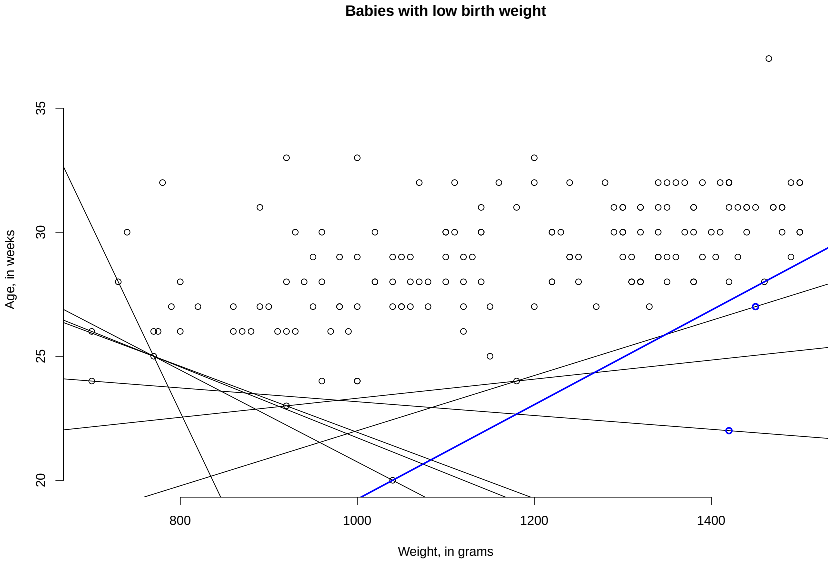

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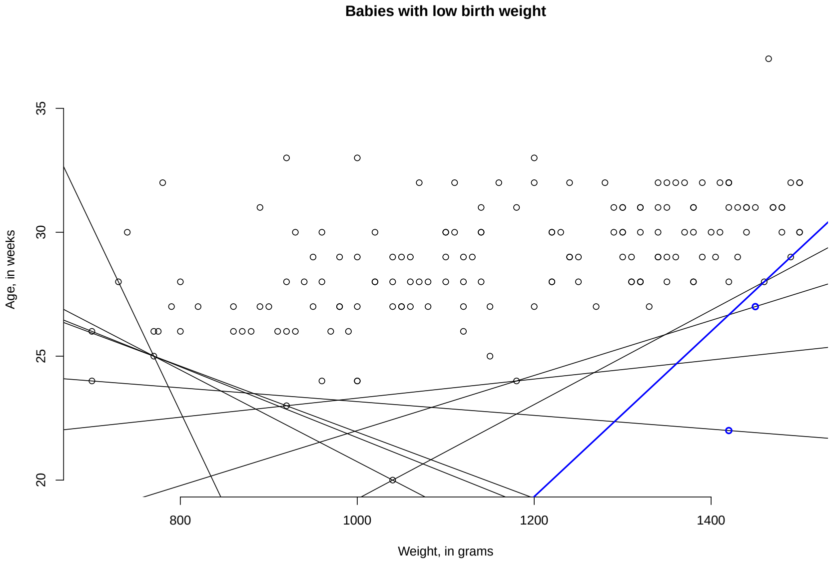

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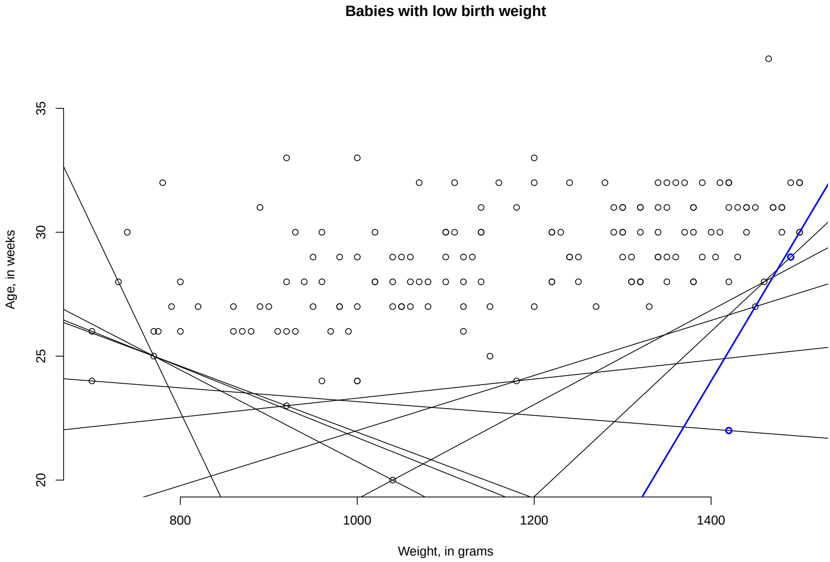

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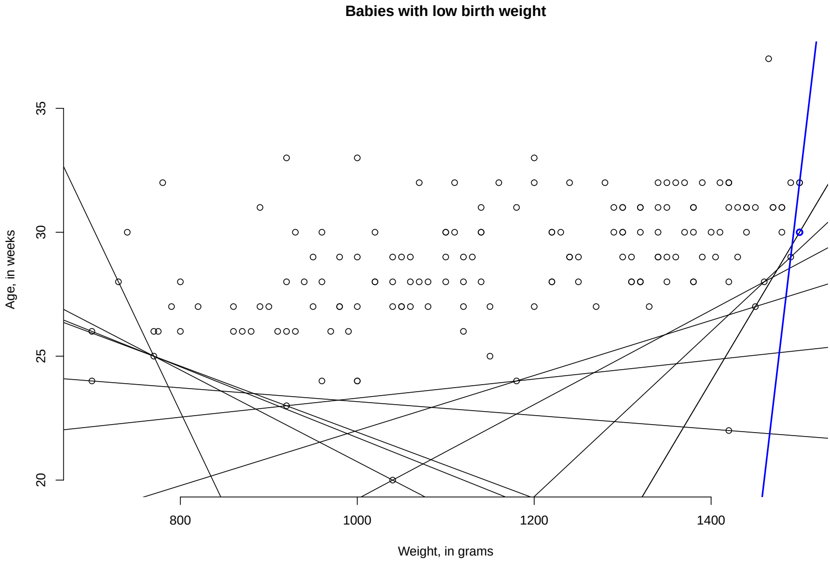

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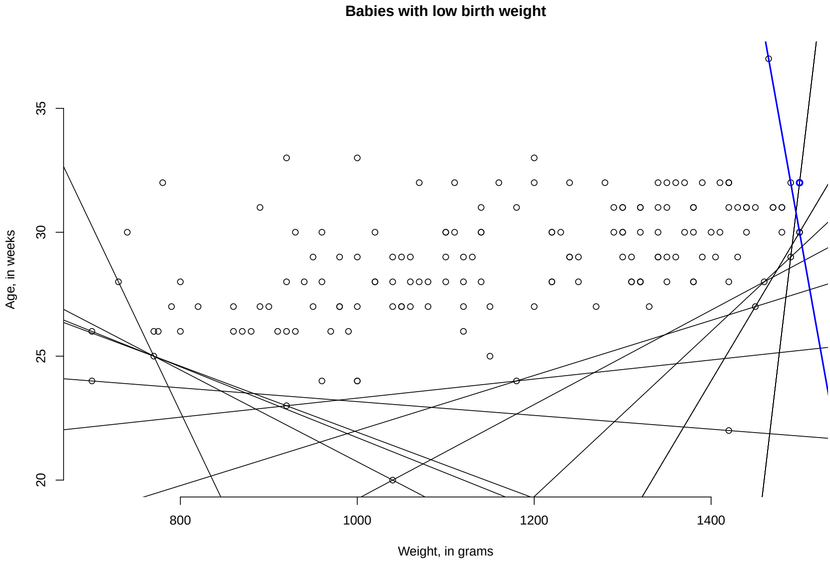

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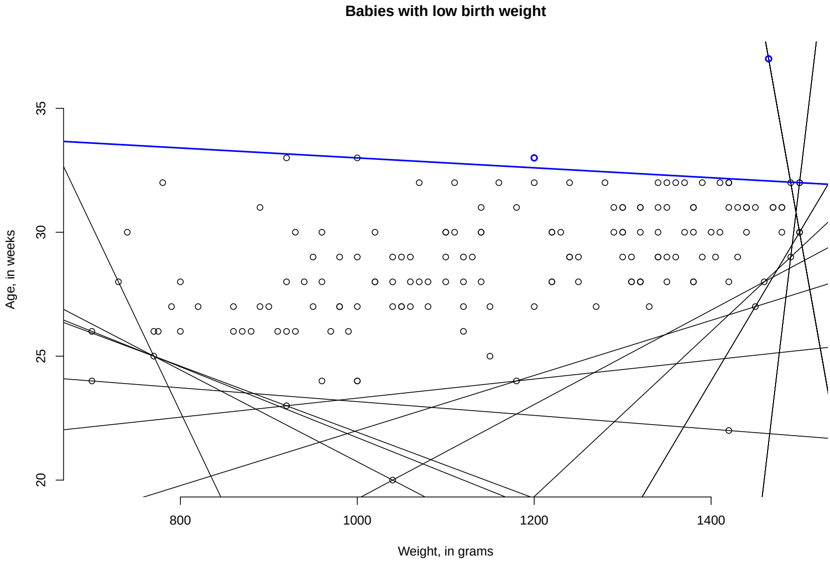

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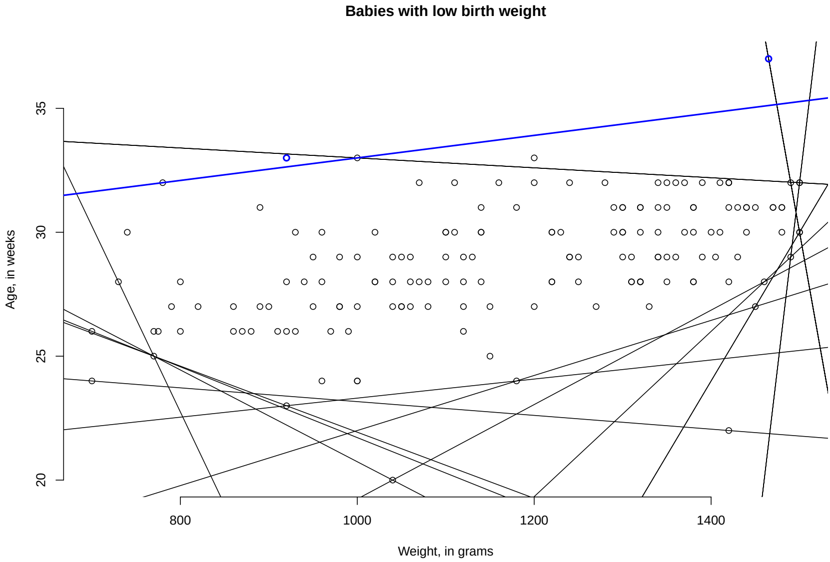

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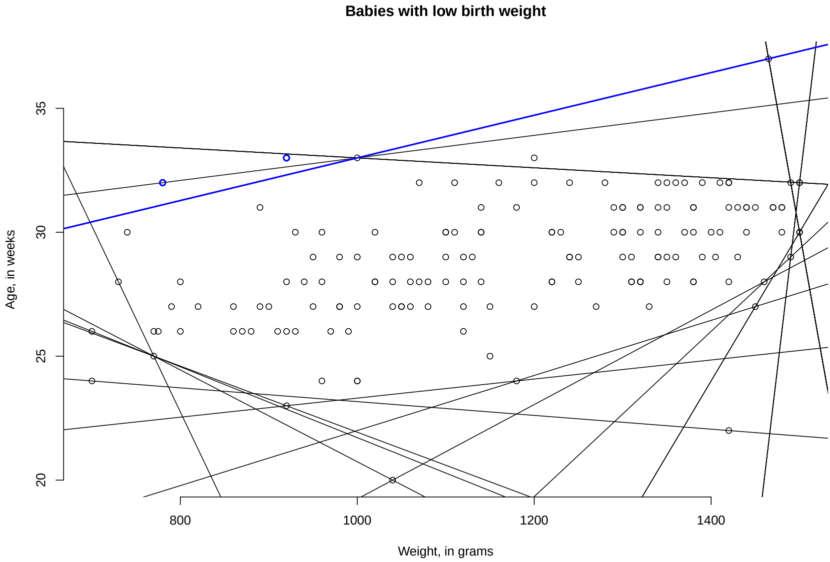

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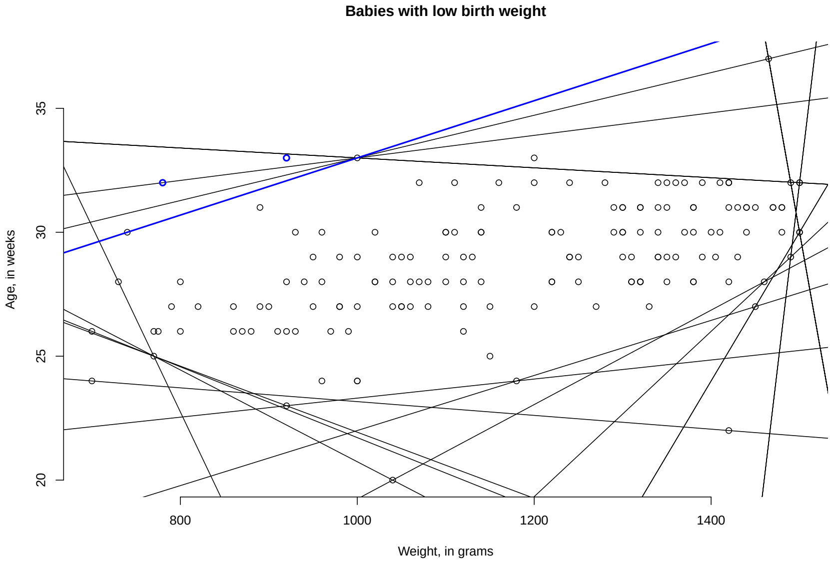

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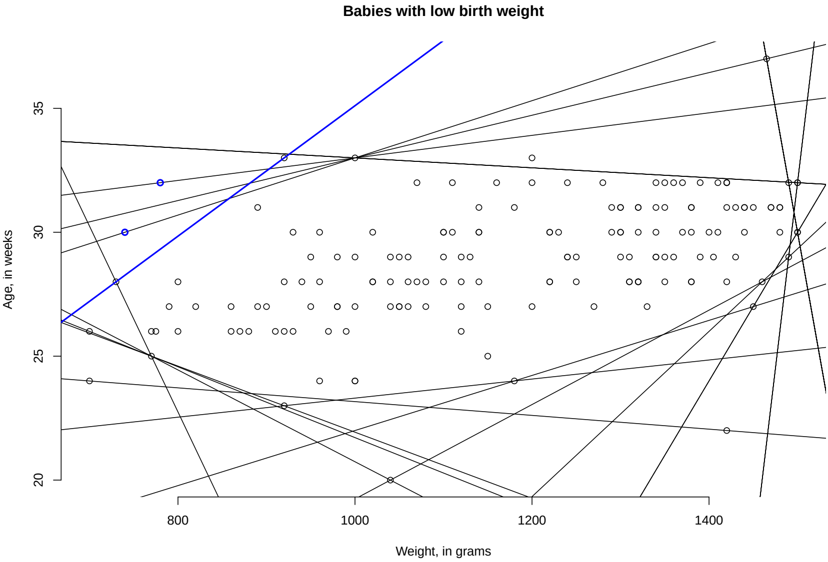

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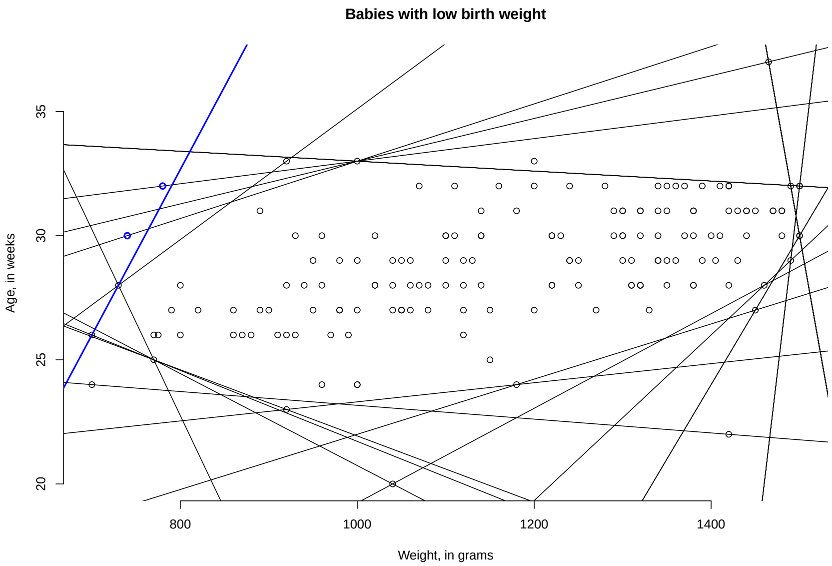

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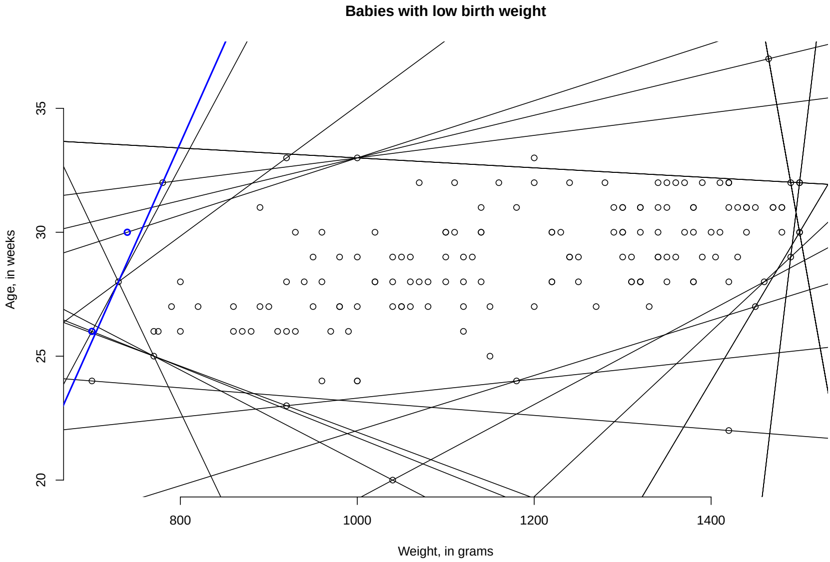

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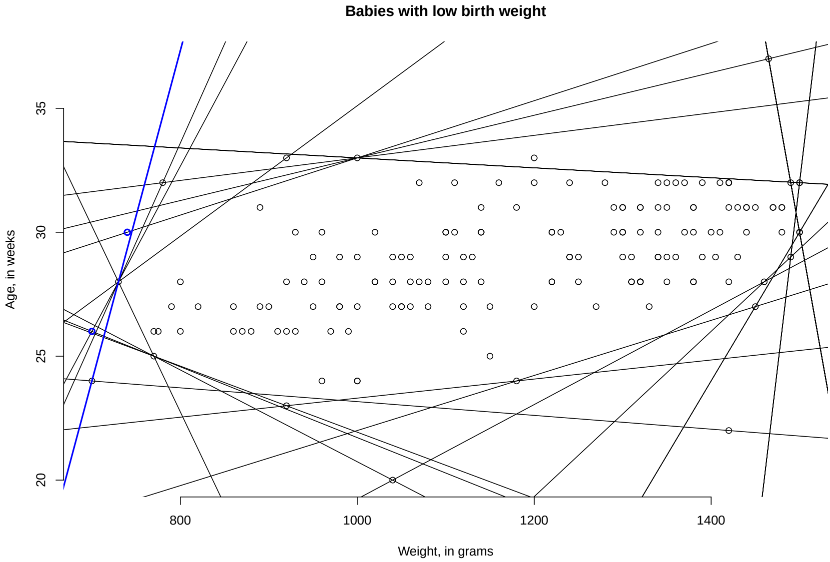

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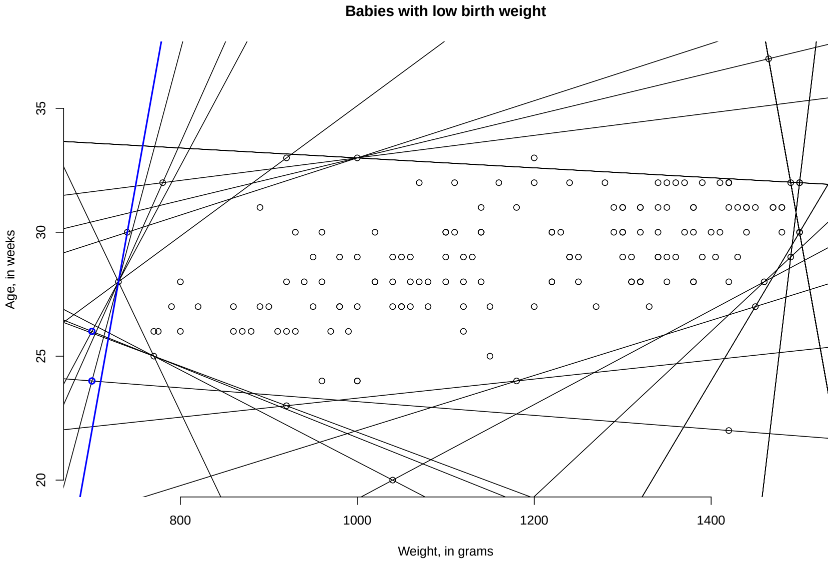

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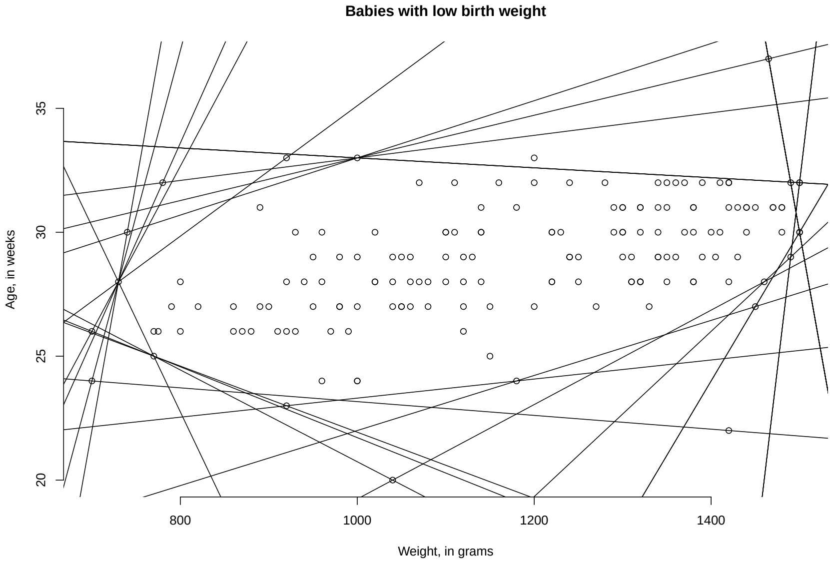

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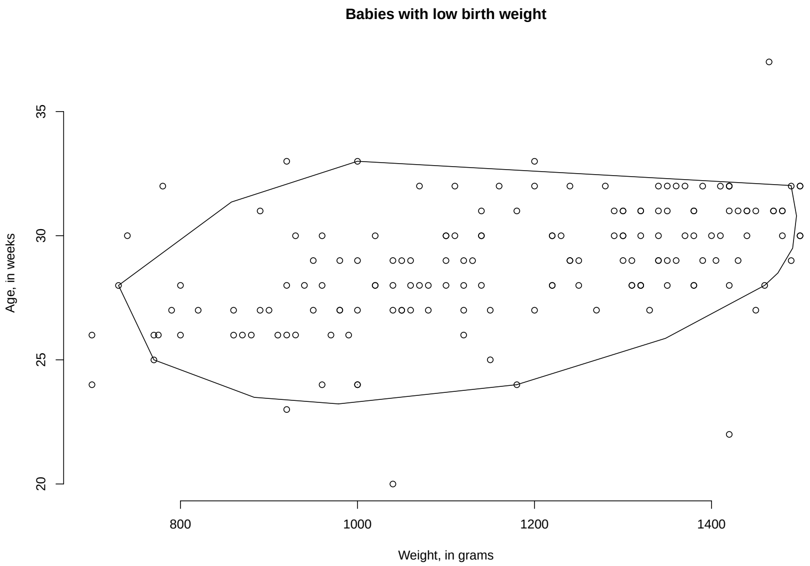

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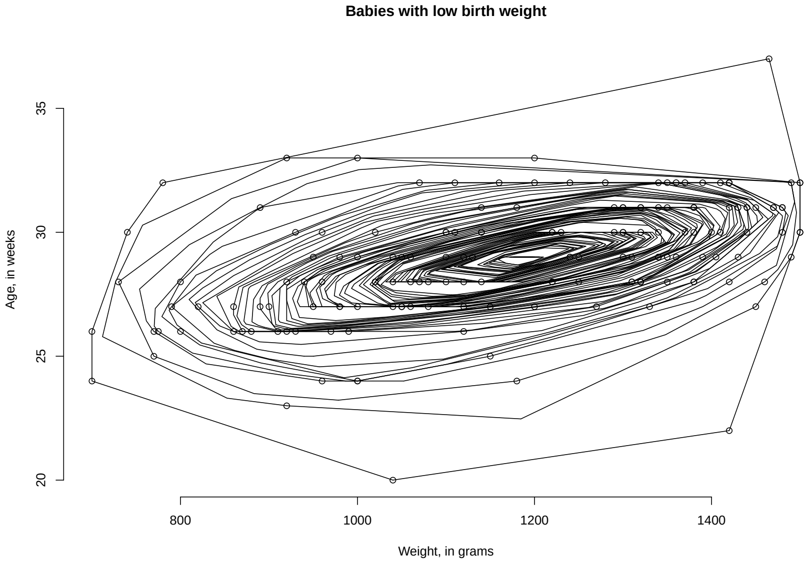

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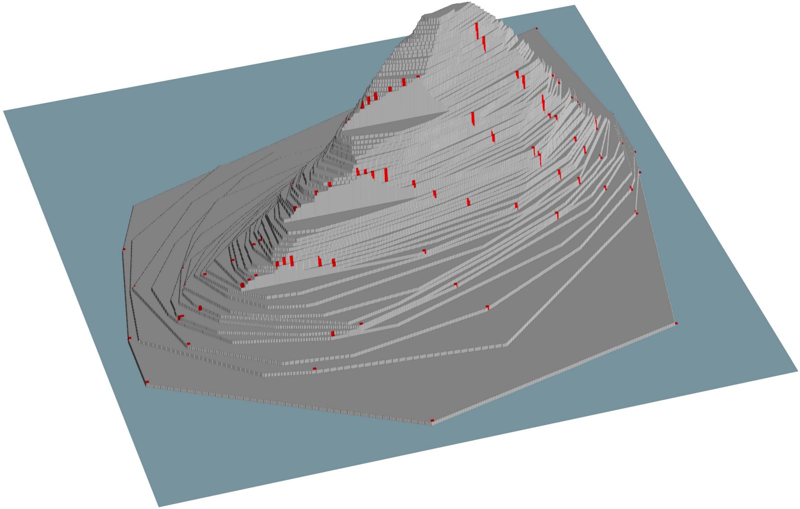

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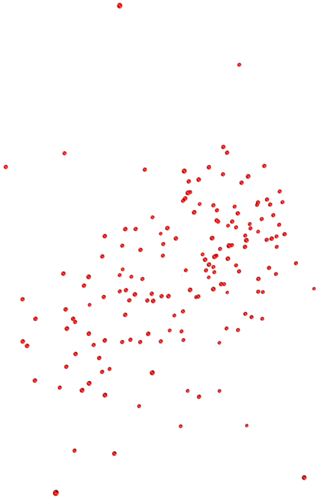
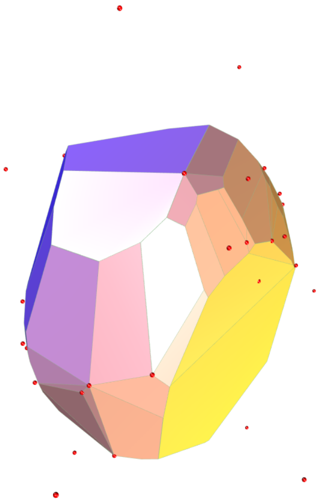


Tukey (=halfspace, location) depth region: $\tau = 2/161$



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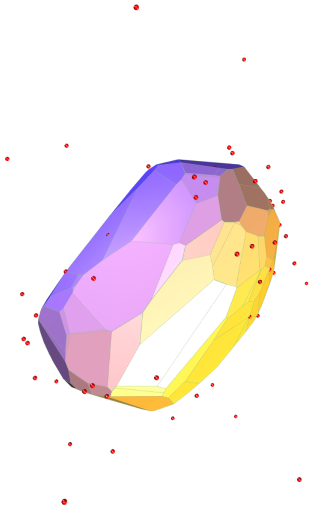

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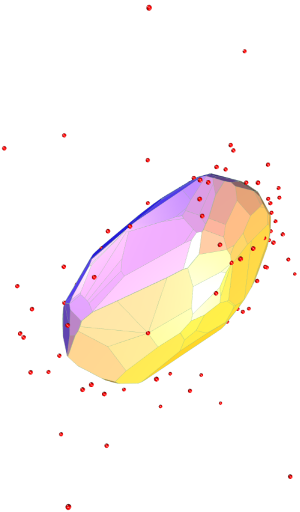
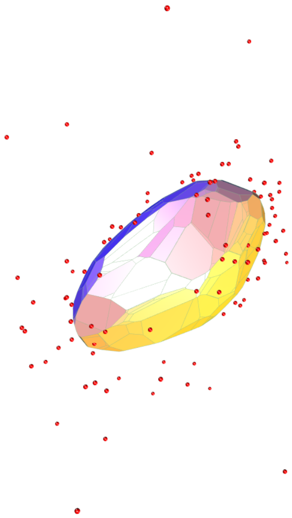
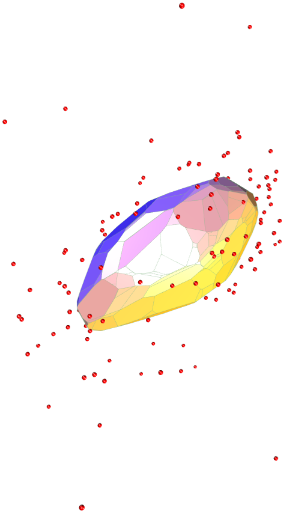


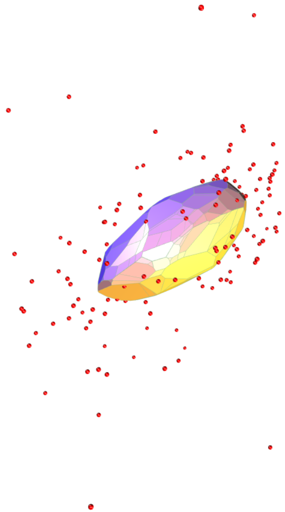
Tukey (=halfspace, location) depth region: τ =13/161



Tukey (=halfspace, location) depth region: τ =17/161



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



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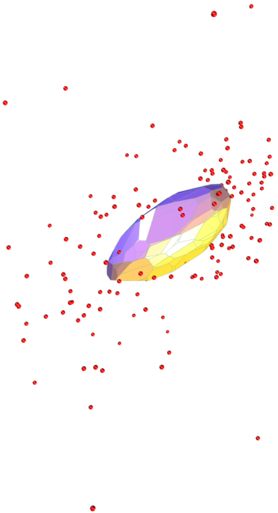

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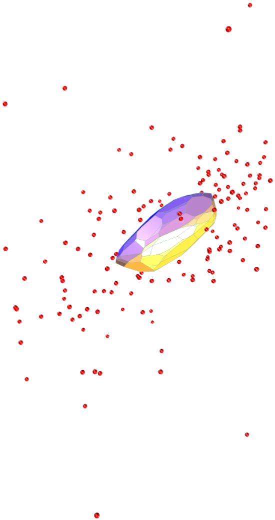
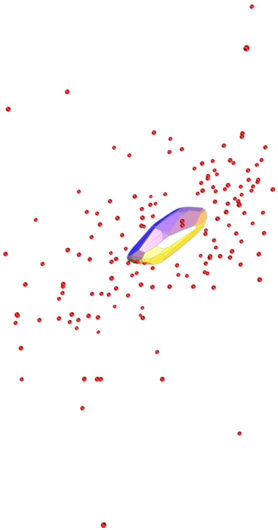


Tukey (=halfspace, location) depth region: τ =49/161



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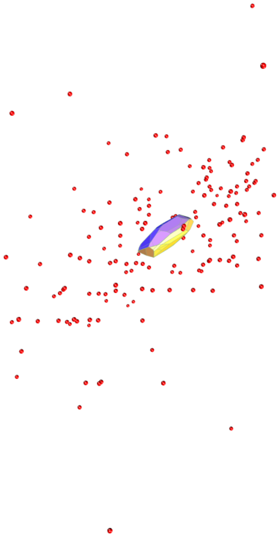

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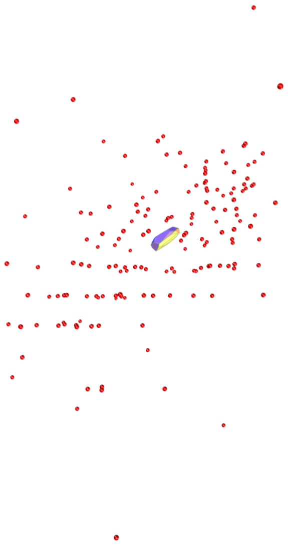

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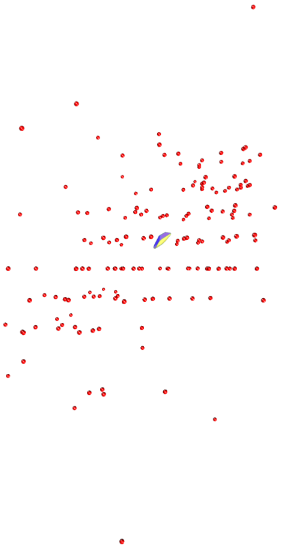

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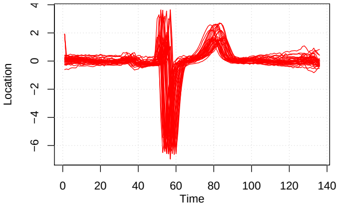
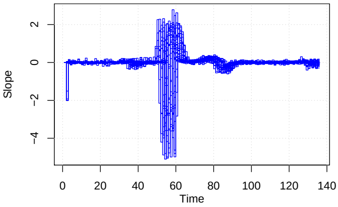
ECG five days data





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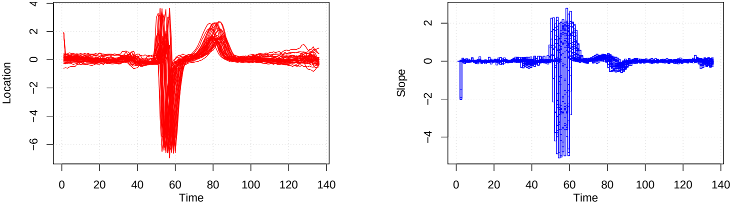

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with $\hat{f}_i(t)$ being the function obtained by connecting the points $(t_{ij},\, f_i(t_{ij})), j = 1, \ldots, N_i$ with line segments, $\hat{f}_i'(t)$ its derivative.

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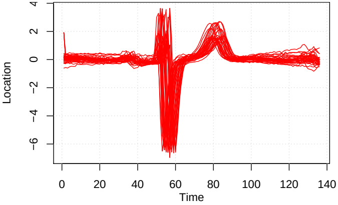

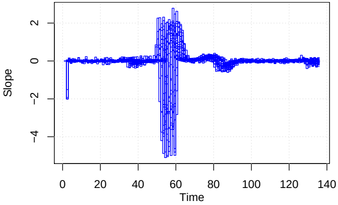

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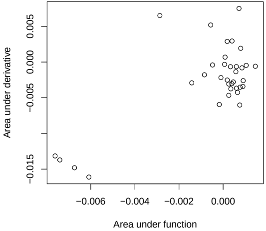

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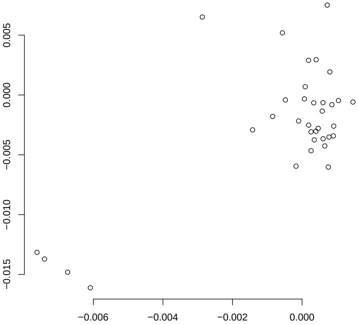

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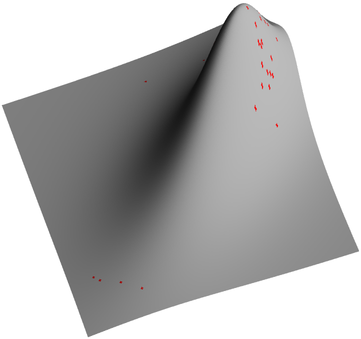
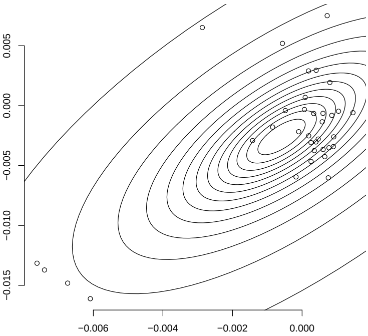
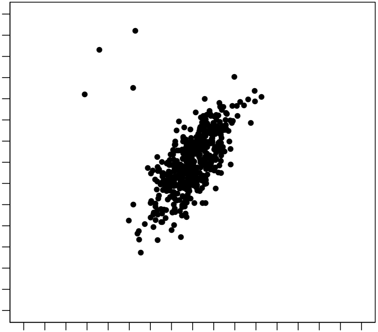




Multivariate anomaly detection: an example



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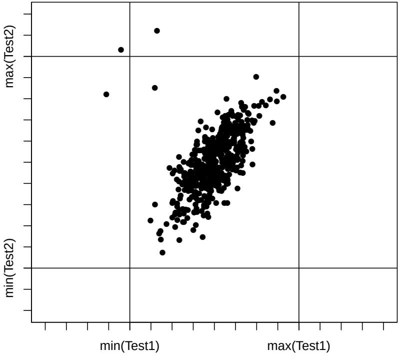

- Checking for **minimum** and **maximum** in each test result.

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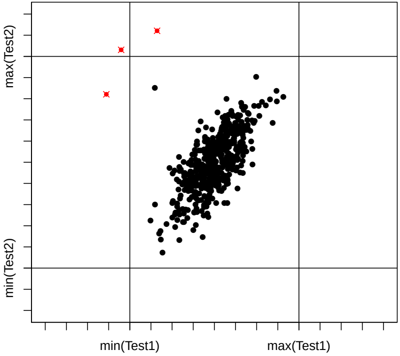

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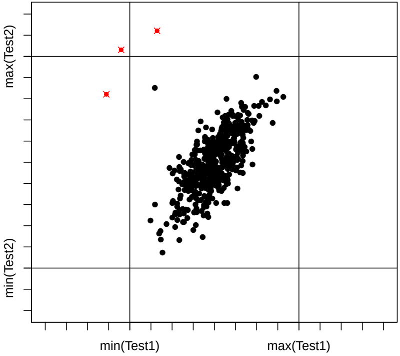

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- **Not all** anomalies can be detected.

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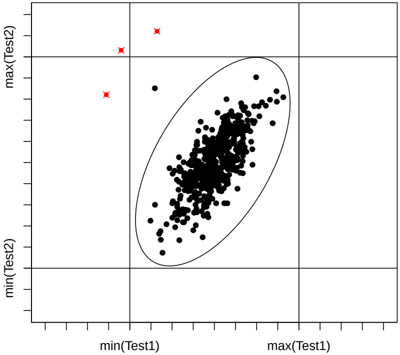

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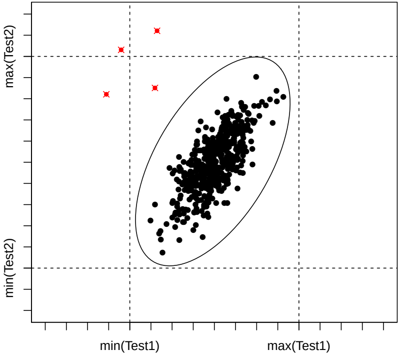

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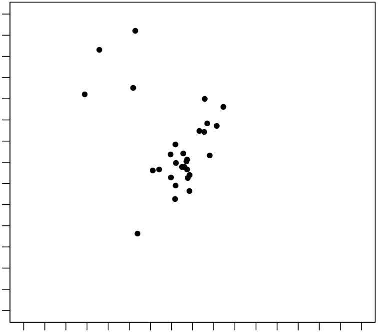

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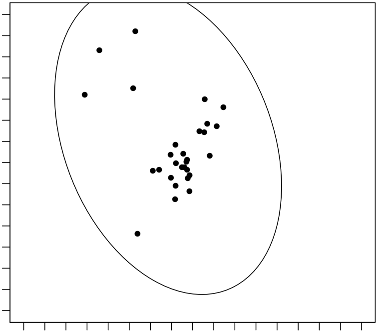

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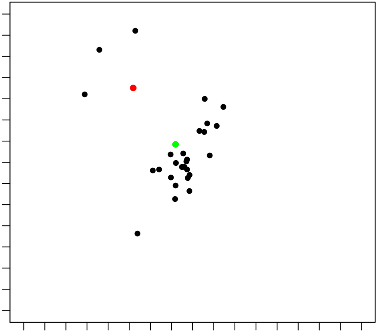

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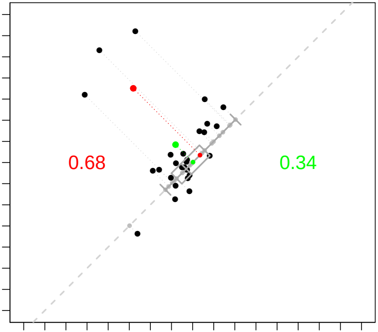

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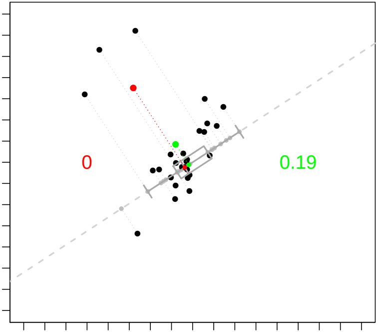

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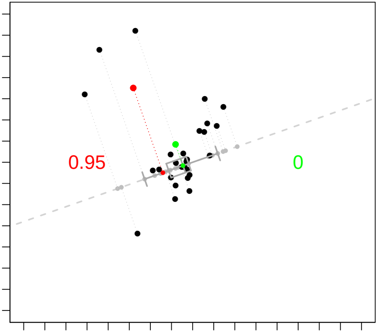

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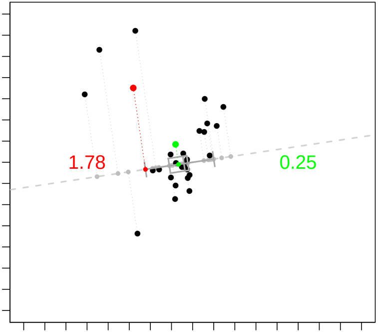

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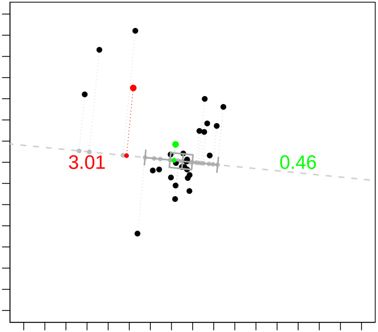

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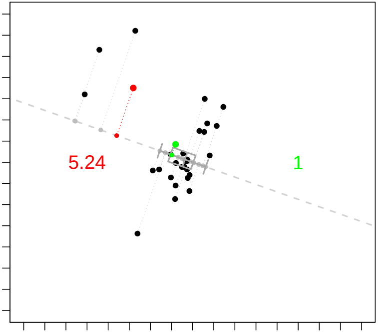

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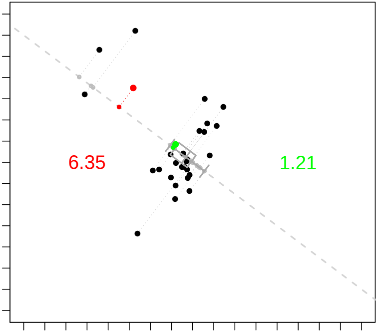

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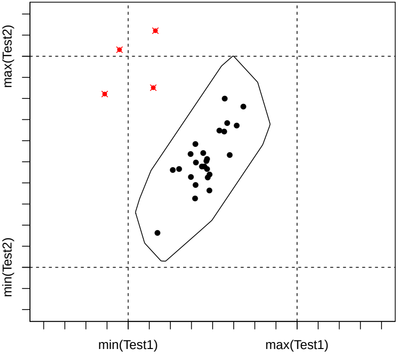

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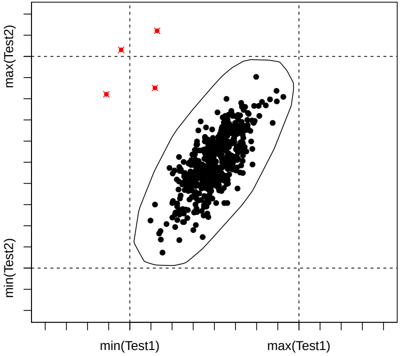

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is the **projected outlyingness** (Stahel, 1981; Donoho, 1982), $\mathrm{med}(Y)$ and $\mathrm{MAD}(Y) = \mathrm{med}\big(\big|Y - \mathrm{med}(Y)\big|\big)$ are the univariate median and median absolute deviation from the median, respectively.

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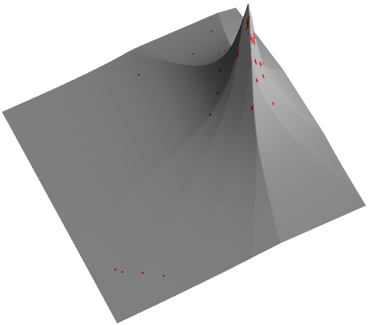

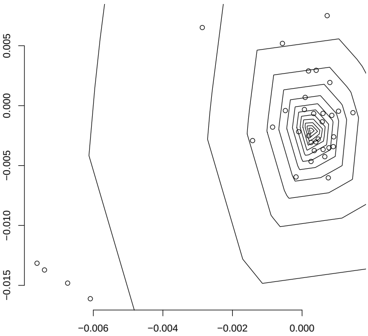

Spatial depth (Vardi & Zhang, 2000; Serfling 2002)

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

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

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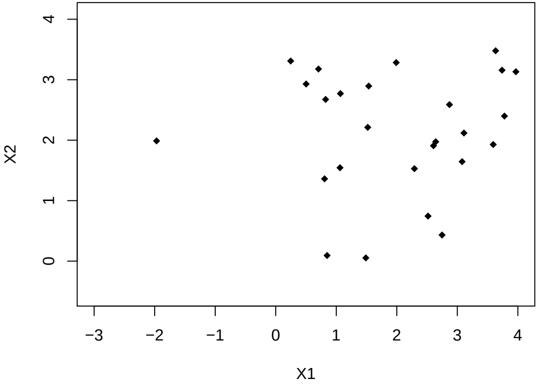

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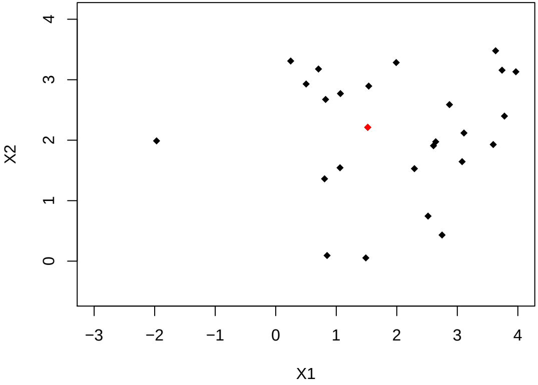

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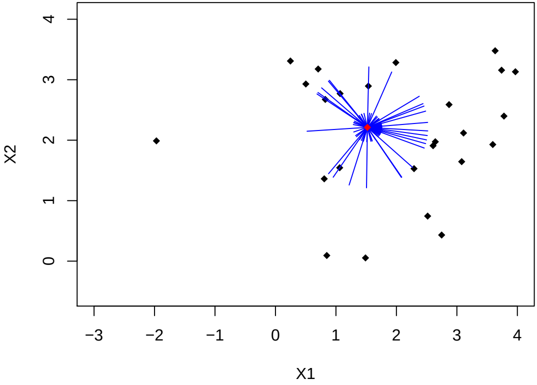

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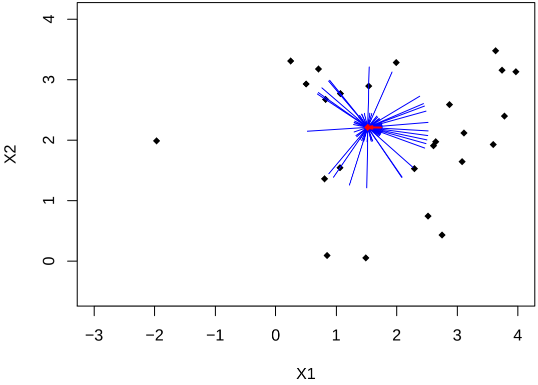

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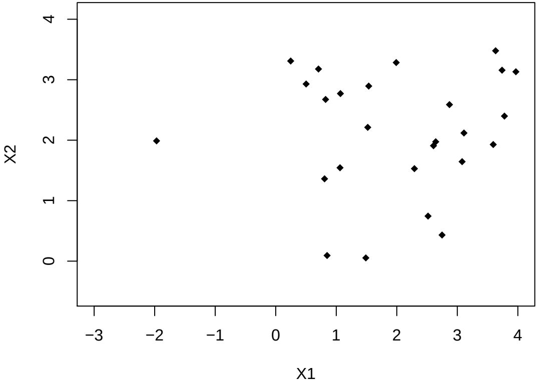

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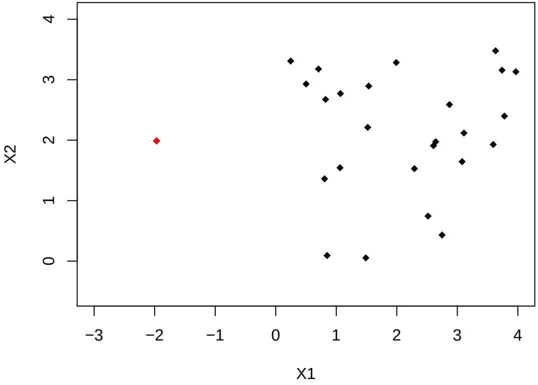

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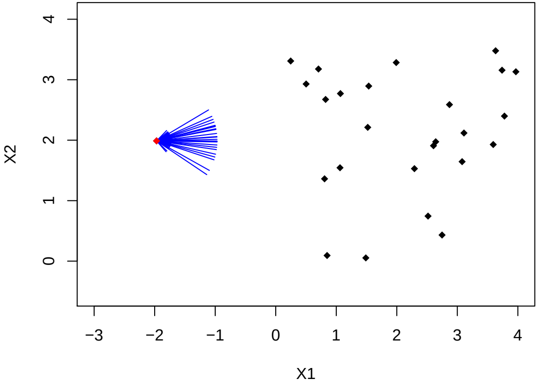

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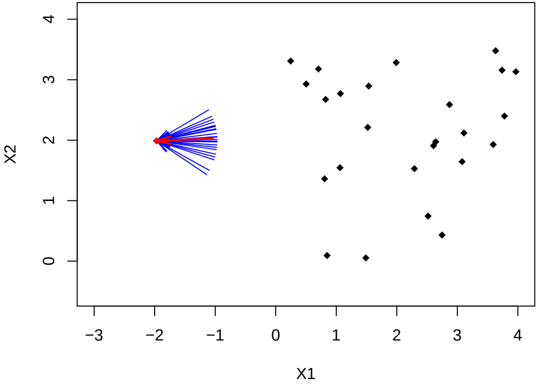

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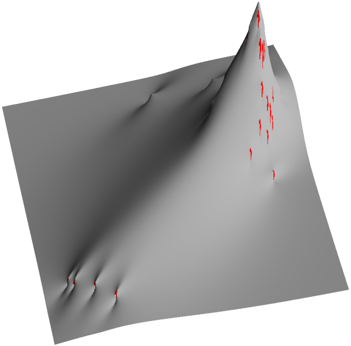
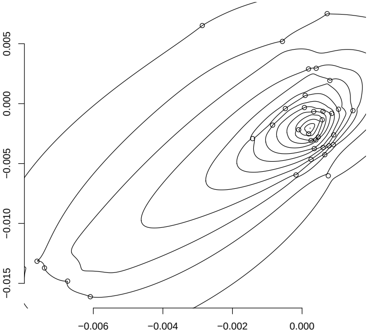
- satisfies **D1 – D5**, but not **D4con**, is continuous;
- if $\boldsymbol{\Sigma}$ is orthogonal, satisfies **D2iso** only;
- with **D2iso** its maximum (say $\boldsymbol{x}^*$) is referred to as **spatial median**, a multivariate location estimator having asymptotic breakdown point of 0.5.

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





Contents

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

- Chandola, V., Banerjee, A., and Kumar, V. (2009). Anomaly detection: A survey. ACM *Computing Surveys (CSUR)*, 41(3):15, 1–58.
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Practical session (part I)

Notebooks:

- `anomdet_simulation1.Rmd`,
- `anomdet_hurricanes.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.

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.

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