Statistical Depth Functions

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17 May, 2024

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Outline

1. Depth Functions for Functional Data
2. Outlier Detection for Functional Data
3. Local Depth Functions
4. Concluding Remarks

Depth Functions

A *depth function* quantifies how *central* a point $\mathbf{x} \in \mathscr{X}$ is with respect to a distribution F.

This induces a *center-outwards* ordering on the space $\mathscr{X}$.

Depth Functions in $\mathbb{R}^d$

We want $D\colon \mathbb{R}^d \times \mathscr{F} \to \mathbb{R}$ to be bounded, non-negative, continuous, and satisfy the following properties.

P1. **Affine invariance:** $D(A\mathbf{x} + b, F_{A\mathbf{x}+b}) = D(\mathbf{x}, F_X)$.

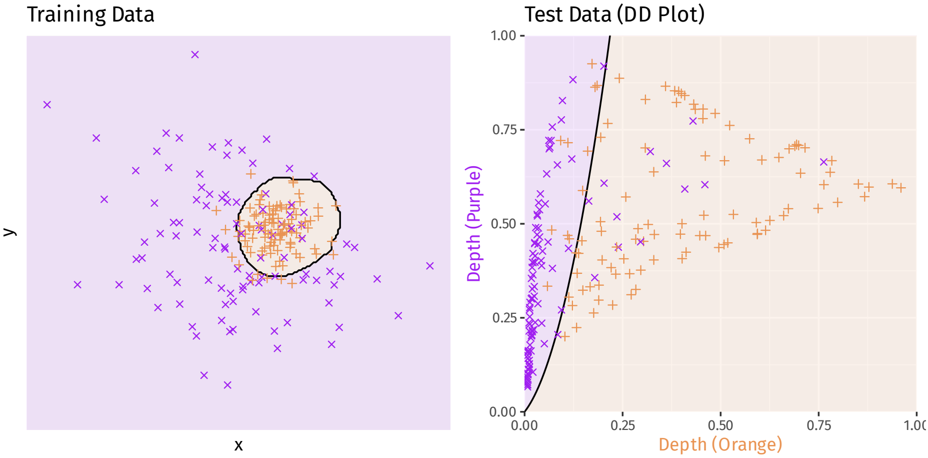
P2. **Maximality at centre:** $D(\theta, F_X) = \sup_{\mathbf{x}\in\mathbb{R}^d} D(\mathbf{x}, F)$.

P3. **Monotonicity along rays:** $D(\mathbf{x}, F) \leq D(\theta + \alpha(\mathbf{x} - \theta), F)$.

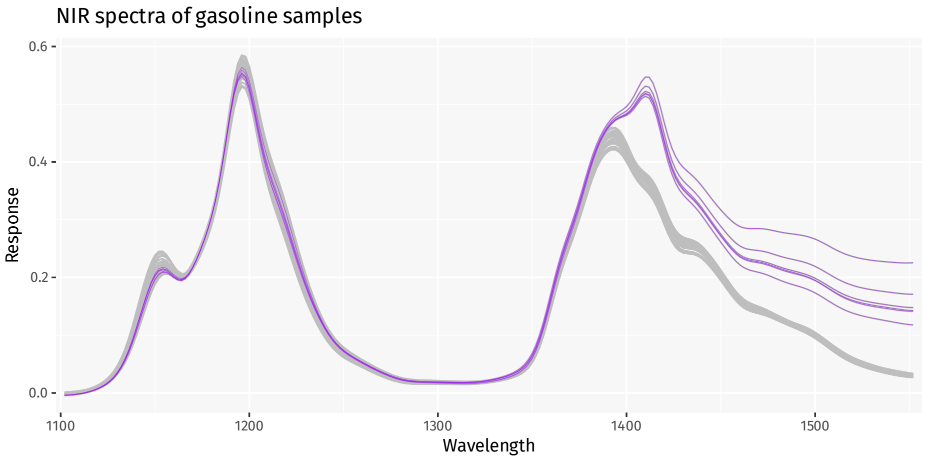
P4. **Vanish at infinity:** $D(\mathbf{x}, F) \to 0$ as $\|\mathbf{x}\| \to \infty$.

Zuo, Y., & Serfling, R. (2000) General notions of statistical depth function

The DD classifier



Depth Functions for Functional Data



NIR spectra of gasoline samples
0.6
0.4
0.2
0.0
Response
1100
1200
1300
1400
1500
Wavelength

Depth Functions in Banach spaces $\mathscr{X}$

Let $\mathscr{X}$ be a class of functions of the form $\boldsymbol{x}\colon [0,1] \to \mathbb{R}^d$, equipped with a norm $\|\cdot\|$. We typically choose $L^2[0,1]$ or $\mathcal{C}[0,1]$.

We want to generalize the Zuo-Serfling properties (P1-4) in this setting, for depth functions $D\colon \mathscr{X} \times \mathscr{F} \to \mathbb{R}$.

Gijbels, I., & Nagy, S. (2017) On a General Definition of Depth for Functional Data

2024-05-17

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Properties $P3$ (Monotonicity along rays) and $P4$ (Vanish at infinity) carry over naturally.

Non-degeneracy

P0. Non-degeneracy: $\inf_{x \in \mathcal{X}} D(x, F) < \sup_{x \in \mathcal{X}} D(x, F)$.

The naïve generalization of the halfspace/Tukey depth

$$D_H(x, F) = \inf_{v \in \mathcal{X}^*} P_{X \sim F}(v^*(X) \leq v^*(x)),$$

is degenerate for a wide class of distributions $\mathscr{F}$. For instance, $\mathcal{X} = \mathcal{C}[0, 1]$, Gaussian processes with positive definite covariance kernels.

Chakraborty, A., & and Chaudhuri, P. (2014) On data depth in infinite dimensional spaces

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Chakraborty, A., & and Chaudhuri, P. (2014) On data depth in infinite dimensional spaces

This also applies to the functional analogue of the projection depth.

Non-degeneracy

The functional analogue of the spatial depth

$$D_{Sp}(x, F) = 1 - \left\| \mathbb{E}_{X \sim F} \left[\frac{x - X}{\|x - X\|_2} \right] \right\|_2,$$

does not suffer from degeneracy.

Chakraborty, A., & and Chaudhuri, P. (2014) The spatial distribution in infinite dimensional spaces and related quantiles and depths

Affine Invariance

P1S. **Scalar-affine invariance:** For $a, b \in \mathbb{R}$ with a non-zero and $\mathbf{x} \in \mathscr{X}$,

$$D(a\mathbf{x} + b, F_{a\mathbf{X}+b}) = D(\mathbf{x}, F_{\mathbf{X}}).$$

P1F. **Function-affine invariance:** For $a, b, x \in \mathscr{X}$, with $ax \in \mathscr{X}$,

$$D(ax + b, F_{aX+b}) = D(x, F_X).$$

Maximality at Center

We say that F_X is symmetric about $\boldsymbol{\theta} \in \mathscr{X}$ if for all $\varphi \in \mathscr{X}^*$, we have $\varphi(X)$ symmetric about $\varphi(\boldsymbol{\theta})$.

P2C. **Maximality at center of central symmetry:** For $F \in \mathscr{X}$ centrally symmetric about $\boldsymbol{\theta} \in \mathscr{X}$, $D(\boldsymbol{\theta}, F) = \sup_{x \in \mathscr{X}} D(x, F)$.

P2H. **Maximality at center of halfspace symmetry:** For $F \in \mathscr{X}$ halfspace symmetric about $\boldsymbol{\theta} \in \mathscr{X}$, $D(\boldsymbol{\theta}, F) = \sup_{x \in \mathscr{X}} D(x, F)$.

The Integrated and Infimal Depths

$$D_{FM}(\mathbf{x}, F_{\mathbf{X}}) = \int_{[0,1]} D(\mathbf{x}(t), F_{\mathbf{X}(t)})\, w(t)\, dt.$$

$$D_{Inf}(\mathbf{x}, F_{\mathbf{X}}) = \inf_{t \in [0,1]} D(\mathbf{x}(t), F_{\mathbf{X}(t)}).$$

Fraiman, R., & and Muniz, G. (2001) Trimmed means for functional data
Mosler, K. (2013) Depth Statistics

The J-th order Integrated and Infimal Depths

$$D^J_{FM}(x, F_X) = \int_{[0,1]^J} D((x(t_1), \ldots, x(t_J))^\top, F_{(X(t_1),\ldots,X(t_J))^\top})\, w(\mathbf{t})\, d\mathbf{t}.$$

$$D^J_{Inf}(x, F_X) = \inf_{\mathbf{t}\in[0,1]^J} D((x(t_1), \ldots, x(t_J))^\top, F_{(X(t_1),\ldots,X(t_J))^\top}).$$

Nagy, S., Gijbels, I., & and Hlubinka, D. (2017) Depth-Based Recognition of Shape Outlying Functions

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Nagy, S., Gijbels, I., & and Hlubinka, D. (2017) Depth-Based Recognition of Shape Outlying Functions

These J-th order depths carry information about the derivatives of the curves, of orders $0, \ldots, J-1$.

The Band Depth

$$D_B^J(\mathbf{x}, F) = \sum_{j=2}^{J} P_{X_i \overset{\text{iid}}{\sim} F}(\mathbf{x} \in \operatorname{conv}(X_1, \ldots, X_j)).$$

This is the proportion of j-tuples of curves, for $2 \leq j \leq J$, which *completely* envelope $\mathbf{x}$.

The band depth becomes degenerate for $\mathscr{X} = \mathcal{C}[0, 1]$, Feller processes X (e.g. Brownian motion) with $P(X_0 = 0) = 1$ and each X_t for $t > 1$ non-atomic and symmetric about 0.

López Pintado, S., & Romo, J. (2009) On the concept of depth for functional data

Define the *enveloping time*

$$\mathrm{ET}(x; x_1, \ldots, x_j) = m_1(\{t \in [0,1] \colon x(t) \in \mathrm{conv}(x_1(t), \ldots, x_j(t))\})$$

The modified band depth is defined as

$$D_{\mathrm{MBD}}(x, F) = \sum_{j=2}^{J} \mathbb{E}_{X_i \overset{\mathrm{iid}}{\sim} F} \left[\mathrm{ET}(x; X_1, \ldots, X_j) \right].$$

The Half-Region Depth

We say that $\mathbf{y}$ is in the hypograph (resp. epigraph) of $\mathbf{x}$, denoted $\mathbf{y} \in H_{\mathbf{x}}$ (resp. $E_{\mathbf{x}}$), if $\mathbf{y}(t) \leq \mathbf{x}(t)$ (resp. $\geq$) for all $t \in [0, 1]$.

The half-region depth is defined as

$$D_{HR}(\mathbf{x}, F) = \min \left\{ P_F(H_{\mathbf{x}}),\ P_F(E_{\mathbf{x}}) \right\}.$$

This suffers from the same degeneracy problems as the band depth.

López Pintado, S., & Romo, J. (2011) A half-region depth for functional data

The Modified Half-Region Depth

Define the Modified Hypograph (MHI) and Epigraph (MEI) Indices as

$$\mathrm{MHI}_F(x) = \mathbb{E}_{X \in F}[m_1\{t \in [0,1] \colon x(t) \geq X(t)\}],$$
$$\mathrm{MEI}_F(x) = \mathbb{E}_{X \in F}[m_1\{t \in [0,1] \colon x(t) \leq X(t)\}].$$

The modified half-region depth is defined as

$$D_{MHR}(x, F) = \min\left\{\mathrm{MHI}_F(x),\ \mathrm{MEI}_F(x)\right\}.$$

Partially Observed Functional Data

Suppose that $X \sim F_X$ is not observed on the entire interval $[0, 1]$, but rather on some random compact subinterval $O \sim Q$ (independent of X).

Given a dataset $\mathscr{D} = \{(X_i, O_i)\}_{i=1}^n$ where $(X_i, O_i) \overset{\text{iid}}{\sim} F_X \times Q$, we keep track of the indices observed at time $t \in [0, 1]$ as $\mathscr{J}(t) = \{j : t \in O_j\}$, as well as their number $q(t) = |\mathscr{J}(t)|$.

The Partially Observed Integrated Functional Depth (POIFD)

We may define a depth function in this setting via

$$D_{POIFD}((\mathsf{X}, o), F_{\mathsf{X}} \times Q) = \int_{o} D(\mathsf{X}(t), F_{\mathsf{X}(t)})\, w_o(t)\, dt,$$

where $w_o(t) = q(t)/\int_0 q(t)\, dt$.

Elías, A., Jiménez, R., Paganoni, A. M., & Sangalli, L. M. (2023) Integrated depths for partially observed functional data

Given (X, O), can we estimate X on $M = [0, 1] \setminus O$?

We may search for a reconstruction operator $\mathcal{R}\colon L^2(O) \to L^2(M)$ that minimizes the mean integrated prediction squared error loss $\mathbb{E}[\|X_M - \mathcal{R}(X_O)\|^2]$. In this setup, the best predictor is the conditional expectation $\mathbb{E}[X_M \mid X_O]$.

We may also search for a continuous linear reconstruction operator $\mathscr{A}$, by estimating terms of the Karhunen-Loéve expansion of X.

Kneip, A., & Liebl, D. (2020) On the optimal reconstruction of partially observed functional data

The Functional Reconstruction Problem

Another approach is to take a convex linear combination of curves from a suitable curve envelope with indices $\mathscr{I}$.

The enveloping curves $\mathscr{I}$ may be chosen so that (X, O) is as deep as possible inside the curve envelope.

Additionally, we want $\mathscr{I}$ to envelope (X, O) for as long as possible (in the sense of the enveloping time ET), and contain as many near curves (in an appropriately modified norm $\|\cdot\|'$) to (X, O) as possible.

Elías, A., Jiménez, R., & Shang, H. L. (2023) Depth-based reconstruction method for incomplete functional data

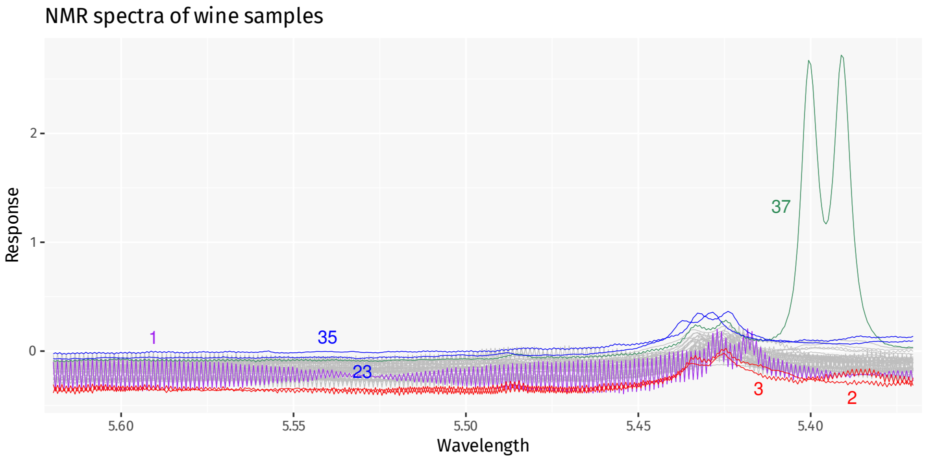
Outlier Detection for Functional Data

Given data $\mathscr{D} = \{\mathbf{x}_i\}_{i=1}^n$, we may extract ranks $r_i = R(\mathbf{x}_i, \hat{F}_n)$.

For instance, we may choose

$$R(\mathbf{x}, \hat{F}_n) \; = \; \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(D(\mathbf{x}_i, \hat{F}_n) \leq D(\mathbf{x}, \hat{F}_n)).$$

Declare those $\mathbf{x}_i$ with unusually high ranks r_i as outliers, say greater than a cutoff $Q_3 + 1.5\,\mathrm{IQR}$.



NMR spectra of wine samples
Response
Wavelength
2
1
0
5.60
5.55
5.50
5.45
5.40
1
35
23
37
3
2

Functional Outliers

A curve $x \colon [0,1] \to \mathbb{R}$ may exhibit outlying behaviour within a body of curves in many ways.

- **Isolated outlier:** Significant deviation over a short interval.
- **Persistent outlier:** Deviation over a large/entire interval.
  - Shape
  - Shift
  - Amplitude

Hubert, M., Rousseeuw, P. J., & Segaert, P. (2015) Multivariate functional outlier detection

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Hubert, M., Rousseeuw, P. J., & Segaert, P. (2015) Multivariate functional outlier detection

For a shape outlier, the slices $x(t)$ may all seem inconspicuous in the marginals $F_{X(t)}$.

Shape Outliers and Derivatives

One way of incorporating shape information of a curve $\boldsymbol{x}$ is to bundle it with its derivatives $\boldsymbol{x}^{(j)}$.

$$\int_{[0,1]} D((\boldsymbol{x}^{(0)}(t), \dots, \boldsymbol{x}^{(J)}(t))^\top, F_{(\boldsymbol{X}^{(0)}(t), \dots, \boldsymbol{X}^{(J)}(t))^\top})\, w(t)\, dt.$$

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This suffers from errors in approximating derivatives, and the assumption of differentiability in the first place.

Shape Outliers and the J-th order Integrated Depth

We say that a curve $\boldsymbol{x}$ is a J-th order outlier with respect to F_X if there exists $\boldsymbol{t} \in [0,1]^J$ such that the vector $(\boldsymbol{x}(t_1), \ldots, \boldsymbol{x}(t_J))^\top$ is outlying with respect to $F_{(X(t_1),\ldots,X(t_J))^\top}$.

$$D^J_{FM}(\boldsymbol{x}, F_X) = \int_{[0,1]^J} D((\boldsymbol{x}(t_1), \ldots, \boldsymbol{x}(t_J))^\top, F_{(X(t_1),\ldots,X(t_J))^\top})\, w(\boldsymbol{t})\, d\boldsymbol{t}.$$

Nagy, S., Gijbels, I., & and Hlubinka, D. (2017) Depth-Based Recognition of Shape Outlying Functions

Shape Outliers and the J-th order Integrated Depth

We say that a curve $\boldsymbol{x}$ is a J-th order outlier with respect to $F_{\boldsymbol{X}}$ if there exists $\boldsymbol{t} \in [0,1]^J$ such that the vector $(\boldsymbol{x}(t_1), \dots, \boldsymbol{x}(t_J))^\top$ is outlying with respect to $F_{(\boldsymbol{X}(t_1),\dots,\boldsymbol{X}(t_J))^\top}$.

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Nagy, S., Gijbels, I., & and Hlubinka, D. (2017) Depth-Based Recognition of Shape Outlying Functions

- This process looks at points of the form $(\boldsymbol{x}(t), \boldsymbol{x}(t+h), \dots)$, thus encoding information about the derivatives.
- One may choose the weight function $w(\cdot)$ to put emphasis on the diagonal.

The Centrality-Stability Scheme

Consider an outlyingness function $O(\boldsymbol{x}(t))$ which measures the outlyingness of $\boldsymbol{x}(t)$ with respect to $F_{X(t)}$. For instance, we may choose

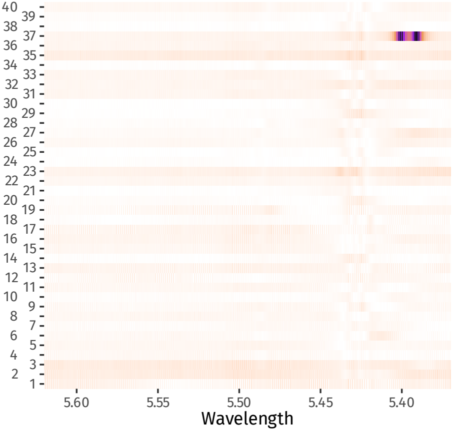
$$O(\boldsymbol{x}(t)) = \frac{\boldsymbol{x}(t) - \mathrm{med}(X(t))}{\mathrm{MAD}(X(t))}.$$

Then, we may define a depth function

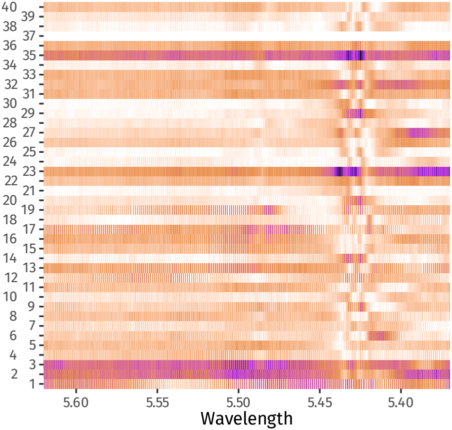
$$D(\boldsymbol{x}, F_X) = \int_{[0,1]} (1 + |O(\boldsymbol{x}(t))|)^{-1} \, dt.$$

Hubert, M., Rousseeuw, P. J., & Segaert, P. (2015) Multivariate functional outlier detection

Outlyingness heatmap



(Zeroed curve #37)



Define

$$\widetilde{MO}(\mathbf{x}, F_X) = \int_{[0,1]} |O(\mathbf{x}(t))| \, dt$$

Then, Cauchy-Schwarz gives

$$D(\mathbf{x}, F_X) \cdot (1 + \widetilde{MO}(\mathbf{x}, F_X)) \geq 1,$$

with equality when $O(\mathbf{x}(\cdot))$ remains constant over time.

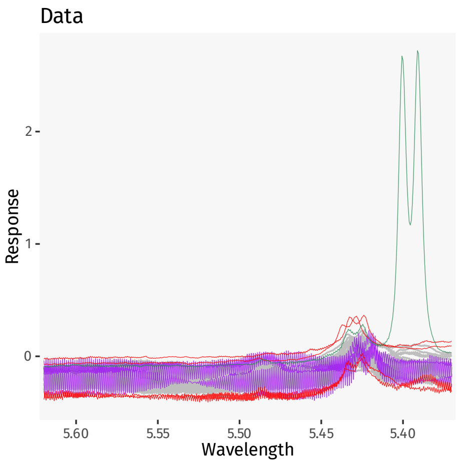
The Centrality-Stability scheme

Any sudden deviation in outlyingness will be detected by the *stability deviation*

$$\Delta S = (1 + \widetilde{MO}(\mathbf{x}, F)) - \frac{1}{D(\mathbf{x}, F)}.$$

The *centrality deviation* is measured as

$$\Delta C = 1 - D(\mathbf{x}, F).$$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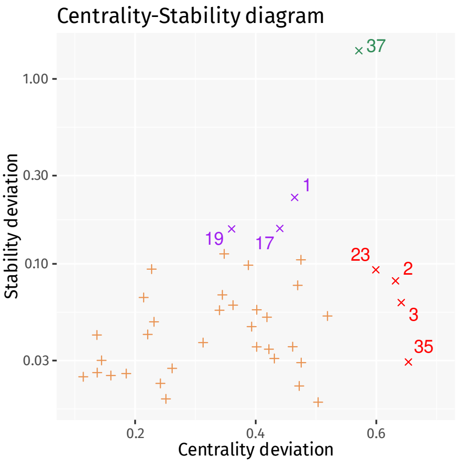
Wavelength


Centrality-Stability diagram
Stability deviation
1.00
0.30
0.10
0.03
0.2
0.4
0.6
Centrality deviation
37
1
19
17
23
2
3
35

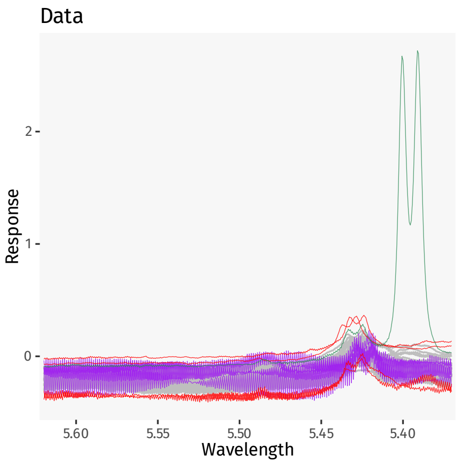
The MO-VO Scheme

We may measure the variability in outlyingness over time more simply via

$$\mathrm{MO}(\mathbf{x}, F) = \int_{[0,1]} O(\mathbf{x}(t))\, dt,$$

$$\mathrm{VO}(\mathbf{x}, F) = \int_{[0,1]} \|O(\mathbf{x}(t)) - \mathrm{MO}(\mathbf{x}, F)\|^2\, dt.$$

Dai, W., & Genton, M. G. (2018) An outlyingness matrix for multivariate functional data classification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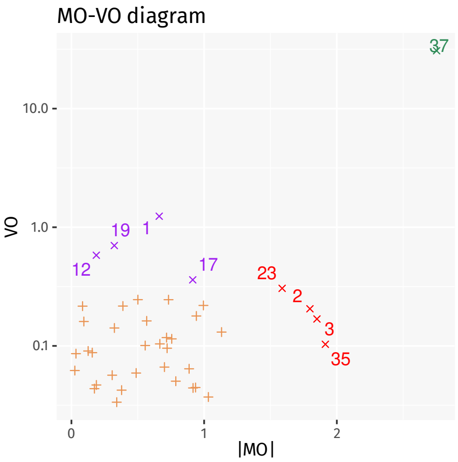
MO-VO diagram
VO
10.0
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|MO|
37
19
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12
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23
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3
35

The Outliergram

Given a dataset of curves $\mathscr{D} = \{\mathbf{x}_i\}_{i=1}^n$, the distances

$$d_i = a_0 + a_1 \,\mathrm{MEI}(\mathbf{x}_i) + a_2 n^2 \,\mathrm{MEI}(\mathbf{x}_i)^2 - \mathrm{MBD}(\mathbf{x}_i),$$

where $a_0 = a_2 = -2/n(n+1)$, $a_1 = 2(n+1)/(n-1)$, are indicative of shape outlyingness.

Thus, one may declare $\mathbf{x}_i$ as an outlier if d_i exceeds a cutoff such as $Q_3 + 1.5\,\mathrm{IQR}$.

Arribas-Gil, A., & Romo, J. (2014). Shape outlier detection and visualization for functional data: the outliergram

2024-05-17

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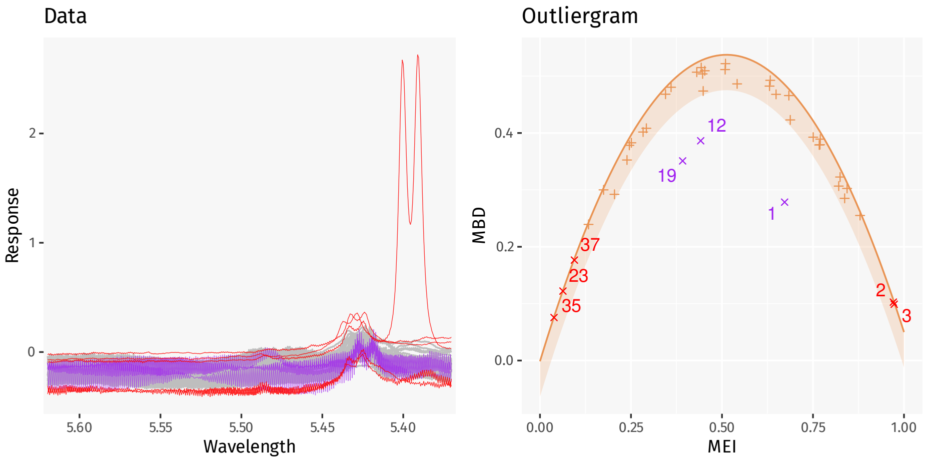
The numbers d_i are always positive!


Data
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Outliergram
MBD
0.4
0.2
0.0
12
19
1
37
23
35
2
3
0.00
0.25
0.50
0.75
1.00
MEI

Local Depth Functions

Elliptical Distributions

We say that a distribution F is elliptical if it admits a density of the form

$$f_X(x) = c|\Sigma|^{-1/2}h\left((x-\boldsymbol{\mu})^\top \Sigma^{-1}(x-\boldsymbol{\mu})\right)$$

for some strictly decreasing function h. Write $F \in \mathrm{Ell}(h; \boldsymbol{\mu}, \Sigma)$.

An affine invariant depth function continuous in $\boldsymbol{x}$ uniquely determines F within $\mathrm{Ell}(h; \cdot, \cdot)$. The depth and density contours coincide.

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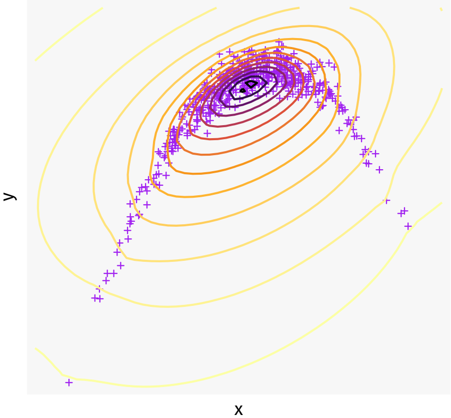
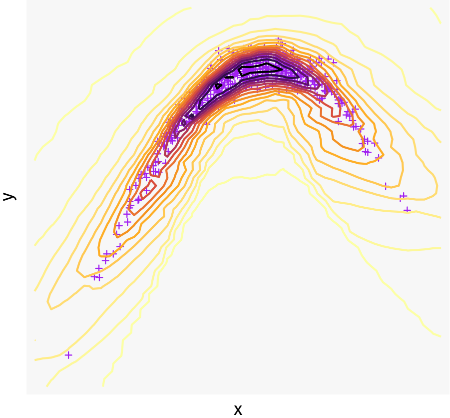
- The whitened random variable $Z = \Sigma^{-1/2}(X - \boldsymbol{\mu})$ has density $f_Z(\boldsymbol{z}) \propto h(\|\boldsymbol{z}\|^2)$.
- The halfspace, simplicial, projection depths satisfy this property.
- In general, depths such as the halfspace depth always produce convex central regions.

Spatial depth



Local spatial depth, β = 0.2



Local Depth Neighbourhoods

Given $\mathbf{x} \in \mathscr{X}$, we may symmetrize F_X as

$$F_X^{\mathbf{x}} = \frac{1}{2}F_X + \frac{1}{2}F_{2\mathbf{x}-X}.$$

The probability-β depth-based neighbourhood of $\mathbf{x}$ in F_X is simply the β-th central region of $F_X^{\mathbf{x}}$. This is denoted by $N_\beta^{\mathbf{x}}(F_X)$.

Paindaveine, D., & Van Bever, G. (2013) From depth to local depth: A focus on centrality

Local Depth

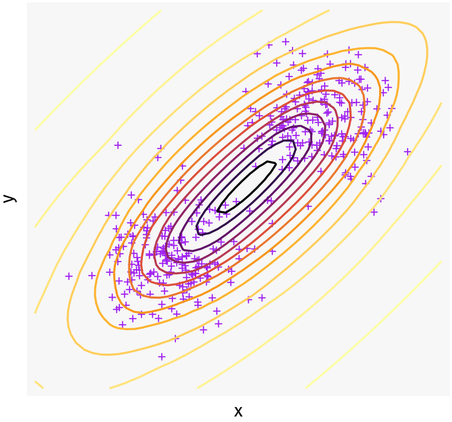
Let F_β^x denote the distribution F_X conditioned on $N_\beta^x(F_X)$.

The local depth function at locality level $\beta \in (0, 1]$ is defined as

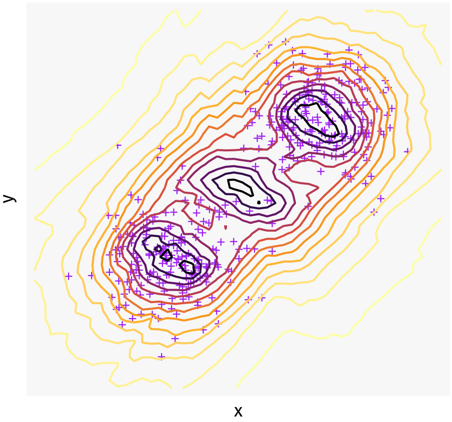
$$LD(x, F_X) = D(x, F_\beta^x).$$

When $\beta = 1$, we have $LD_1 = D$.

Spatial depth



Local spatial depth, β = 0.2



Let $\widetilde{F}_{\beta}^{\mathbf{x}}$ denote the distribution $F_{\mathbf{X}}^{\mathbf{x}}$ conditioned on $N_{\beta}^{\mathbf{x}}(F_{\mathbf{X}})$. Note that this is angularly symmetric about $\mathbf{x}$.

Given $\mathbf{x} \in \mathscr{X}$, we may define a local depth kernel, centered at $\mathbf{x}$, via

$$K_{\beta}^{\mathbf{x}} \colon N_{\beta}^{\mathbf{x}}(F_{\mathbf{X}}) \to \mathbb{R}, \qquad \mathbf{z} \mapsto D(\mathbf{z}, \widetilde{F}_{\beta}^{\mathbf{x}}).$$

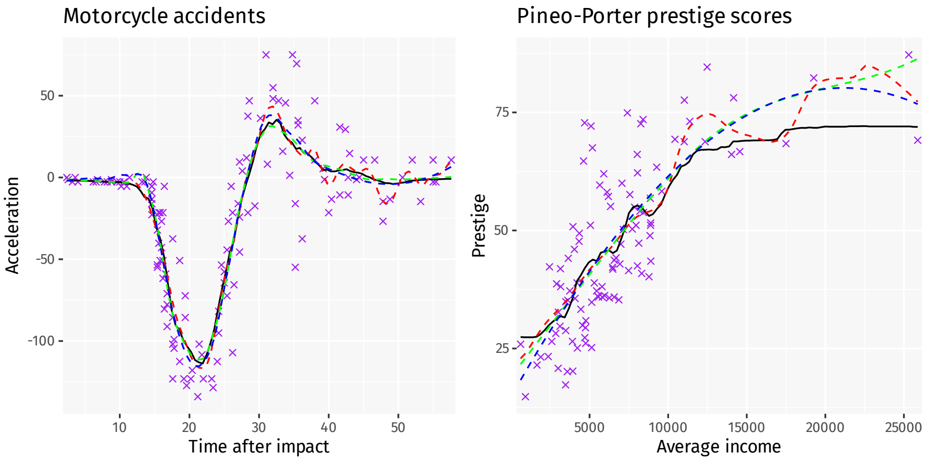
Extend this to $\mathscr{X}$ by setting $K_{\beta}^{\mathbf{x}}(\cdot) = 0$ outside $N_{\beta}^{\mathbf{x}}(F_{\mathbf{X}})$.

We propose a linear estimator of the form

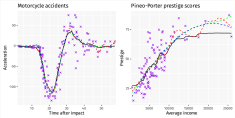
$$\hat{y}_\beta(x) = \sum_i w_i(x) y_i, \qquad w_i(x) = \frac{K_\beta^x(x_i)}{\sum_j K_\beta^x(x_j)}.$$

This may be interpreted as a weighted KNN estimator, or a variable bandwidth kernel estimator.

We only have one tuning parameter $\beta \in (0, 1]$.

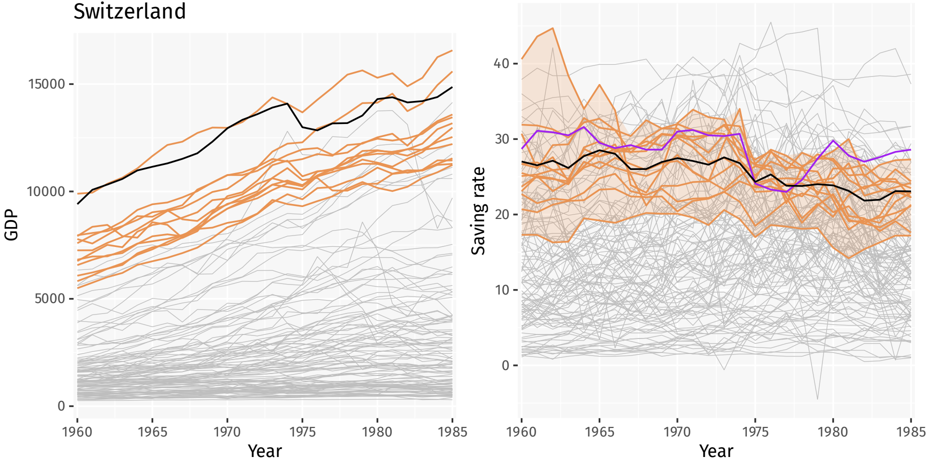


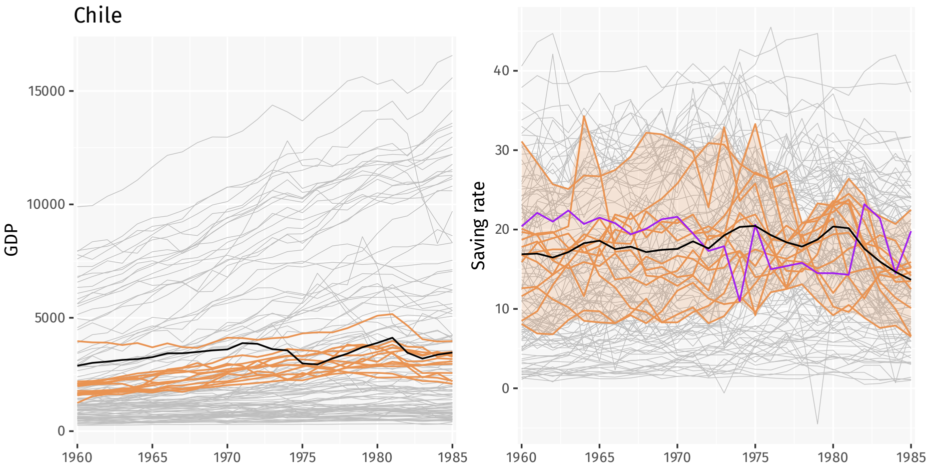
Motorcycle accidents
Acceleration
Time after impact
50
0
-50
-100
10
20
30
40
50
Pineo-Porter prestige scores
Prestige
Average income
75
50
25
5000
10000
15000
20000
25000

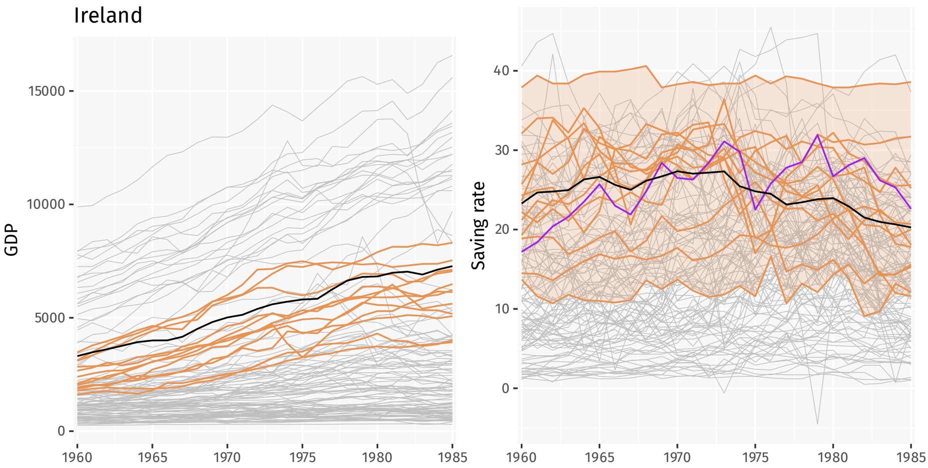


The methods used are local depth based regression (black), Nadaraya-Watson kernel (red), local linear (green) and quadratic (blue).

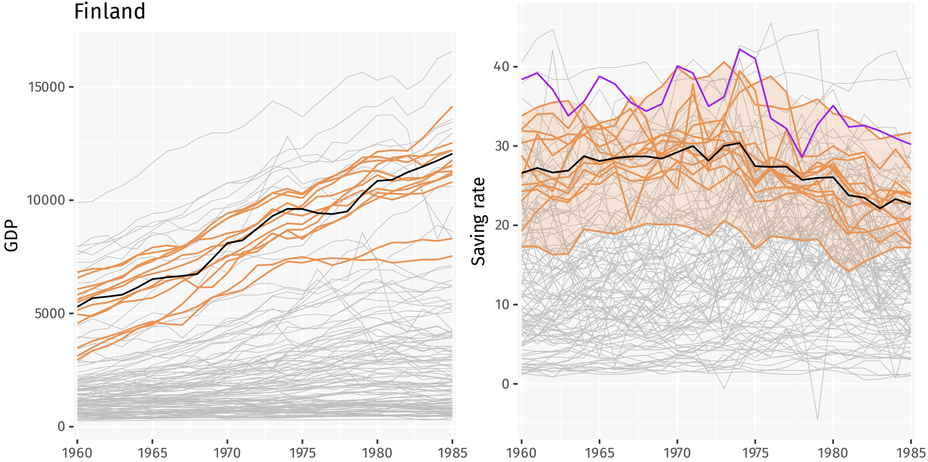
Switzerland




Chile
GDP
15000
10000
5000
0
1960
1965
1970
1975
1980
1985
Saving rate
40
30
20
10
0
1960
1965
1970
1975
1980
1985


Ireland
GDP
15000
10000
5000
0
1960
1965
1970
1975
1980
1985
Saving rate
40
30
20
10
0
1960
1965
1970
1975
1980
1985

Finland


GDP
15000
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1960
1965
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Saving rate
40
30
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1965
1970
1975
1980
1985

Concluding Remarks

- Formulation and Properties of Depth Functions
    - Multivariate Data
    - Functional Data
- Extensions of Depth Functions
    - Partially Observed Functional Data
    - Local Depth
- Applications
    - Exploratory Data Analysis
    - Testing
    - Classification
    - Clustering
    - Outlier Detection
    - Data Reconstruction
    - Regression ?

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