Statistical Depth Functions

Satvik Saha Supervised by Dr. Anirvan Chakraborty 17 May, 2024

Department of Mathematics and Statistics, Indian Institute of Science Education and Research, Kolkata

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 $\mathbf{x} \in \mathcal{X}$ is with respect to a distribution F.

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

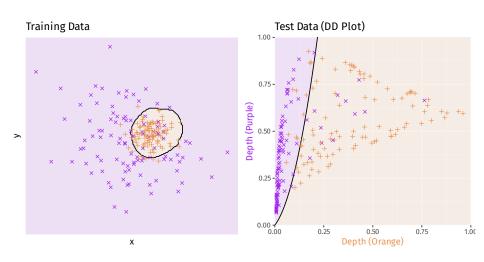
Depth Functions in \mathbb{R}^d

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

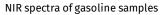
- P1. Affine invariance: $D(Ax + b, F_{Ax+b}) = D(x, F_X)$.
- P2. Maximality at centre: $D(\theta, F_X) = \sup_{\mathbf{x} \in \mathbb{R}^d} D(\mathbf{x}, F)$.
- P3. Monotonicity along rays: $D(x, F) \le D(\theta + \alpha(x \theta), F)$.
- P4. Vanish at infinity: $D(x, F) \to 0$ as $||x|| \to \infty$.

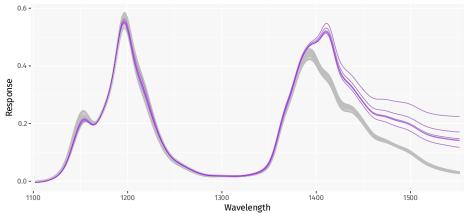
Zuo, Y., & Serfling, R. (2000) General notions of statistical depth function

The DD classifier



Depth Functions for Functional Data





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

Let \mathscr{X} be a class of functions of the form $\mathbf{x} \colon [0,1] \to \mathbb{R}^d$, 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 $D: \mathcal{X} \times \mathcal{F} \to \mathbb{R}$.

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

Let X be a class of functions of the form $x \in [0, 1] \to X'$, equipped with $x + \cos x = 1 + 1$. In specially chosen x([0, 1] + x'). Quality of which x([0, 1] + x') is wast to generalize the 2.o.-furfling properties (P - x) in this setting for dayth functions $D: X \times P \to X$.

Quality, i.e. X = ([0, 1] + x').

Depth Functions in Banach spaces 30

Properties *P*3 (Monotonicity along rays) and *P*4 (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

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

is degenerate for a wide class of distributions \mathcal{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

P0. Non-degeneracy: $\inf_{x \in X} D(x,F) < \sup_{x \in X} D(x,F)$.
The naïve generalization of the halfspace/Tukey depth
$D_H(x,F) = \inf_{v \in X^-} P_{X \sim F}(v^*(X) \le v^*(x)),$
s degenerate for a wide class of distributions \mathcal{F} . For instance, $\mathcal{E} = \mathcal{E}[0,1]$, Gaussian processes with positive definite covariance kernels.

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

Non-degeneracy

The functional analogue of the spatial depth

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

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 $x \in \mathcal{X}$,

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

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

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

Maximality at Center

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

- P2C. Maximality at center of central symmetry: For $F \in \mathcal{X}$ centrally symmetric about $\theta \in \mathcal{X}$, $D(\theta, F) = \sup_{\mathbf{x} \in \mathcal{X}} D(\mathbf{x}, F)$.
- P2H. Maximality at center of halfspace symmetry: For $F \in \mathcal{X}$ halfspace symmetric about $\theta \in \mathcal{X}$, $D(\theta, F) = \sup_{\mathbf{x} \in \mathcal{X}} D(\mathbf{x}, F)$.

The Integrated and Infimal Depths

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

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

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

The J-th order Integrated and Infimal Depths

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

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

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

$$D_B^J(\mathbf{x},F) = \sum_{j=2}^J P_{\mathbf{X}_i^{\text{iid}}_i \sim F}(\mathbf{x} \in \text{conv}(\mathbf{X}_1,\ldots,\mathbf{X}_j)).$$

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

The band depth becomes degenerate for $\mathcal{X} = \mathcal{C}[0,1]$, 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

The Modified Band Depth

Define the enveloping time

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

The modified band depth is defined as

$$D_{\text{MBD}}(\mathbf{x}, F) = \sum_{j=2}^{J} \mathbb{E}_{\mathbf{X}_{i}^{\text{iid}} \in F} \left[\text{ET}(\mathbf{x}; \mathbf{X}_{1}, \dots, \mathbf{X}_{j}) \right].$$

The Half-Region Depth

We say that y is in the hypograph (resp. epigraph) of x, denoted $y \in H_x$ (resp. E_x), if $y(t) \le x(t)$ (resp. \ge) for all $t \in [0,1]$.

The half-region depth is defined as

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

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

$$MHI_F(x) = \mathbb{E}_{X \in F}[m_1\{t \in [0, 1] : x(t) \ge X(t)\}],$$

$$MEI_F(x) = \mathbb{E}_{X \in F}[m_1\{t \in [0, 1] : x(t) \le X(t)\}].$$

The modified half-region depth is defined as

$$D_{MHR}(x, F) = \min \{ MHI_F(x), MEI_F(x) \}.$$

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 $\mathfrak{D} = \{(X_i, O_i)\}_{i=1}^n$ where $(X_i, O_i) \stackrel{\text{iid}}{\sim} F_X \times Q$, we keep track of the indices observed at time $t \in [0, 1]$ as $\mathscr{J}(t) = \{j \colon t \in O_j\}$, 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

$$D_{POIFD}((\mathbf{x}, o), F_{\mathbf{X}} \times Q) = \int_{O} D(\mathbf{x}(t), F_{\mathbf{X}(t)}) w_{o}(t) dt,$$

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

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

The Functional Reconstruction Problem

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

We may search for a reconstruction operator $\mathcal{R}: L^2(O) \to L^2(M)$ 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 \mathcal{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 \mathcal{I} .

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

Additionally, we want \mathcal{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

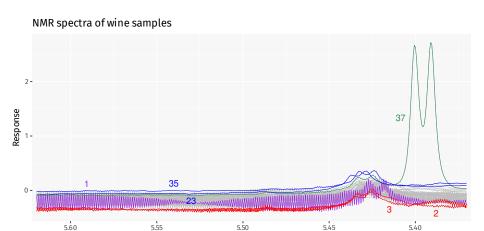
A Naïve Outlier Detection Scheme

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

For instance, we may choose

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

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



5.50

Wavelength

5.45

5.40

Functional Outliers

A curve $x: [0,1] \to \mathbb{R}$ 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

Statistical Depth Functions

Control

C



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 x is to bundle it with its derivatives $x^{(j)}$.

$$\int_{[0,1]} D((\mathbf{x}^{(0)}(t),\ldots,\mathbf{x}^{(l)}(t))^{\top},F_{(\mathbf{X}^{(0)}(t),\ldots,\mathbf{X}^{(l)}(t))^{\top}}) w(t) dt.$$

Shape Outliers and Derivatives

—Shape Outhers and Derivatives

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

$$D_{FM}^{J}(\mathbf{x}, F_{\mathbf{X}}) = \int_{[0,1]^{J}} D((\mathbf{x}(t_{1}), \dots, \mathbf{x}(t_{J}))^{\top}, F_{(\mathbf{X}(t_{1}), \dots, \mathbf{X}(t_{J}))^{\top}}) w(\mathbf{t}) d\mathbf{t}.$$

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

We say that a curve \mathbf{x} is a \mathbf{j} -th order outlier with respect to $F_{\mathbf{x}}$ there exists $\mathbf{t} \in [0,1]$ such that the vector $[\mathbf{x}(t_1),\dots,\mathbf{x}(t_j))^T$ is outlying with respect to $F_{(\mathbf{x}(t_1),\dots,\mathbf{x}(t_j))}$. $\mathcal{O}_{los}(\mathbf{x},F_{\mathbf{x}}) = \int_{\mathbb{R}^{n-1}} \mathcal{O}(\mathbf{x}(t_1),\dots,\mathbf{x}(t_j))^{T}, F_{(\mathbf{x}(t_1),\dots,\mathbf{x}(t_j))^T}) \cdot \mathbf{w}(\mathbf{t}) \, d\mathbf{t}.$

Shape Outliers and the I-th order Integrated Depth

Shape Outliers and the *J*-th order Integrated
Depth

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

The Centrality-Stability Scheme

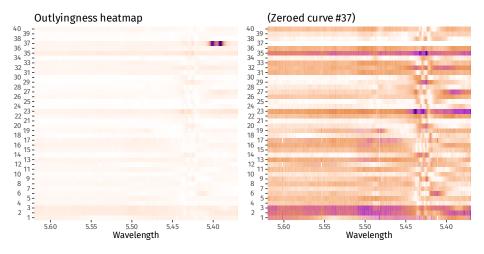
Consider an outlyingness function O(x(t)) which measures the outlyingness of x(t) with respect to $F_{X(t)}$. For instance, we may choose

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

Then, we may define a depth function

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

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



The Centrality-Stability Scheme

Define

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

Then, Cauchy-Schwarz gives

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

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

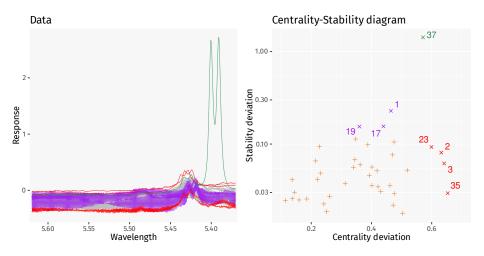
The Centrality-Stability scheme

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

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

The centrality deviation is measured as

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



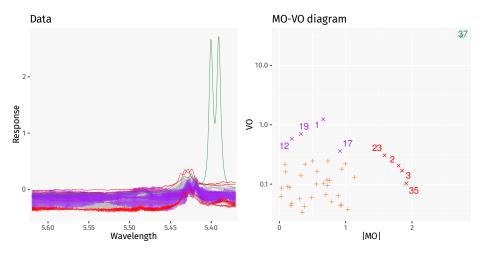
The MO-VO Scheme

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

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

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

Dai, W., & Genton, M. G. (2018) An outlyingness matrix for multivariate functional data classification



The Outliergram

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

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

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 x_i as an outlier if d_i exceeds a cutoff such as $Q_3 + 1.5 \, \text{IQR}$.

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

Statistical Depth Functions 2024-05-17 Outlier Detection for Functional Data └─The Outliergram

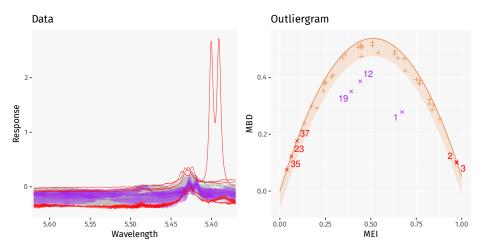
The numbers d_i are always positive!

The Outliergram

Given a dataset of curves $\mathfrak{D} = \{x_i\}_{i=1}^n$, the distances $d_i = a_0 + a_1 MEI(\mathbf{x}_i) + a_2 n^2 MEI(\mathbf{x}_i)^2 - MBD(\mathbf{x}_i),$

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 x_i as an outlier if d_i exceeds a cutoff such as Q1 + 1.5 IQR.



Local Depth Functions

Elliptical Distributions

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

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

for some strictly decreasing function h. Write $F \in EII(h; \mu, \Sigma)$.

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

└─Elliptical Distributions

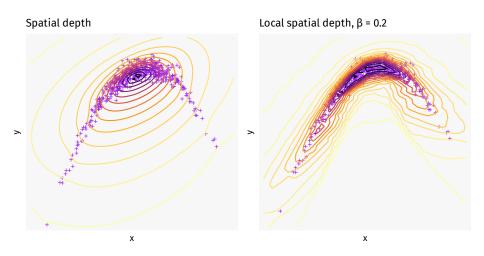
We say that a distribution F is elliptical if it admits a density of the form $f_E(\mathbf{x}) = c|\Sigma|^{-1/2}h\left((\mathbf{x}-\mathbf{\mu})^T\Sigma^{-1}(\mathbf{x}-\mathbf{\mu})\right)$

for some strictly decreasing function h. Write $F \in Ell(h; \mu, \Sigma)$. An affine invariant depth function continuous in x uniquely

Elliptical Distributions

determines F within EN(h; ., -). The depth and density contours coincide.

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



Local Depth Neighbourhoods

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

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

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

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

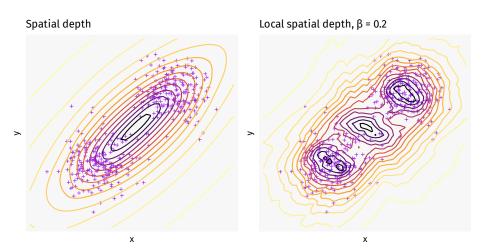
Local Depth

Let $F_{\beta}^{\mathbf{x}}$ denote the distribution $F_{\mathbf{X}}$ conditioned on $N_{\beta}^{\mathbf{x}}(F_{\mathbf{X}})$.

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 $LD_1 = D$.



Local Depth based Regression

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

Given $\mathbf{x} \in \mathcal{X}$, 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 $N_{\beta}^{\mathbf{x}}(F_{\mathbf{X}})$.

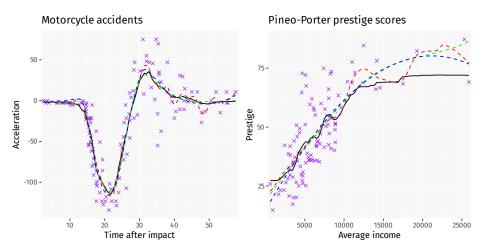
Local Depth based Regression

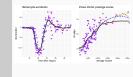
We propose a linear estimator of the form

$$\hat{\mathbf{y}}_{\beta}(\mathbf{x}) = \sum_{i} w_{i}(\mathbf{x})\mathbf{y}_{i}, \qquad w_{i}(\mathbf{x}) = \frac{K_{\beta}^{\mathbf{x}}(\mathbf{x}_{i})}{\sum_{j} K_{\beta}^{\mathbf{x}}(\mathbf{x}_{j})}.$$

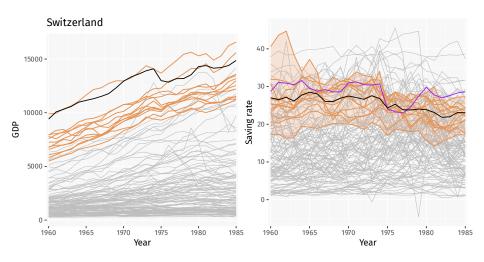
This may be interpreted as a weighted KNN estimator, or a variable bandwidth kernel estimator.

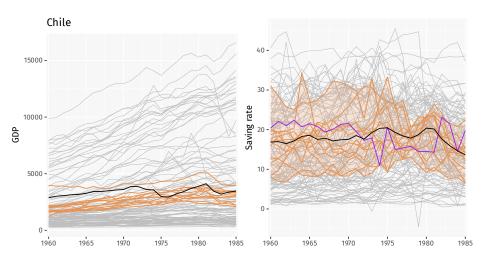
We only have one tuning parameter $\beta \in (0,1]$.

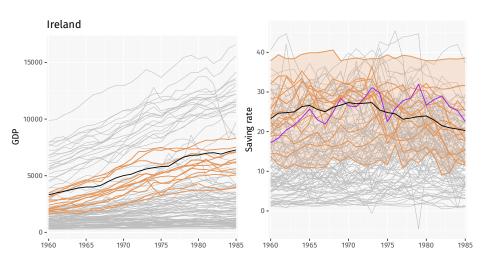


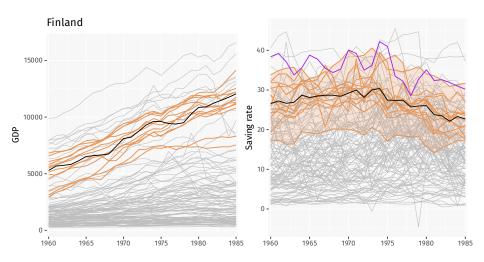


The methods used are local depth based regression (black), Nadaraya-Watson kernel (red), local linear (green) and quadratic (blue).









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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