Density-based inverse calibration with functional predictors

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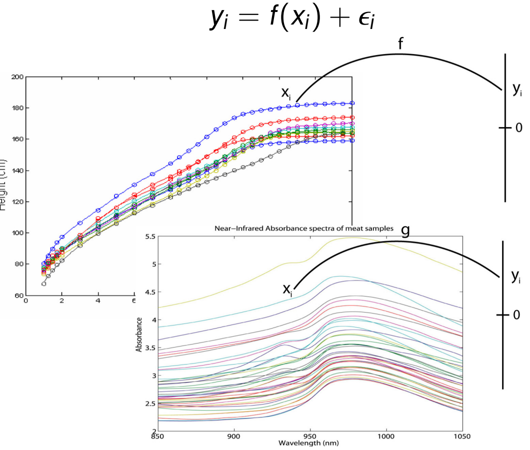
Joint work with **Noslen Hernández**, **Rolando J. Biscay** and **Isneri Talavera**

Introduction

The fast development of instrumental analysis equipment provides huge amount of data as **high-resolution digitized functions**.



Data

generally represented by **high-dimensional vectors** whose values at different coordinates are **strongly correlated**.

Curse of dimensionality

Usually the dimension of such vectors greatly exceeds the sample size.

Introduction

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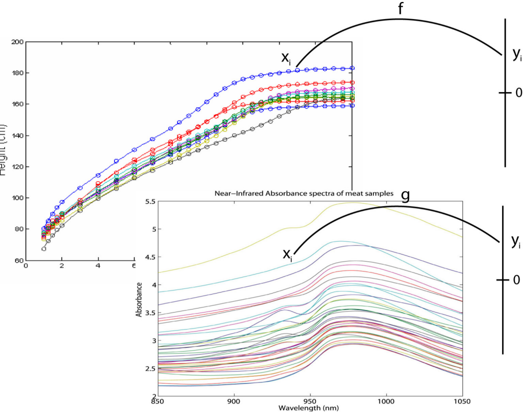
$$y_i = f(x_i) + \epsilon_i$$



ill-posed problem

The direct application of classical multivariate regression methods for this type of data often leads to the inversion of an ill-conditioned (variance) matrix

Functional Data Analysis

Functional Data Analysis (FDA): statistical techniques that take into account the **functional** nature of the data.

- first developed by **[Ramsay and Silverman, 1997]**
- **Idea**: think about observed data as **one or more continuous real-valued functions**, rather than as finite-dimensional vectors.
- also integrate some **functional processing techniques** (derivation, integration, etc).

Example of FDA methods: $X \in L_2([0,1])$, $Y \in \mathbb{R}$

Purpose: approximate the regression function: $\gamma(x) = \mathbb{E}(Y|X = x)$

a) Functional linear methods

- [Cardot et al., 1999]

b) Functional nonparametric regression methods

- Functional Kernel (NWK) [Ferraty and Vieu, 2006]
- Functional Neural Networks (NN, NN-RBF) [Rossi et al., 2005]
- Functional regression in RKHS (RBF, FSVR) [Preda, 2007, Hernández et al., 2007]

c) Functional inverse regression

- Functional sliced inverse regression (FIR) [Ferré and Yao, 2003, Ferré and Yao, 2005]

Outline

1. Functional Density-Based Inverse Regression (DBIR)
2. Simulations
3. Concluding Remarks

Definition of DBIR

Data:

(X, Y)	random variables taking values in $\mathcal{X} \times \mathbb{R}$
$\mathcal{D} = (x_1, y_1), ..., (x_n, y_n)$	independent realizations of (X, Y)

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The "true" physical model is

$$X = F(Y) + \epsilon, \qquad F : \mathbb{R} \to \mathcal{X}$$

where ϵ: stochastic process with zero mean, independent of Y.

Assumptions for DBIR

1. There exists a probability measure P_0 on $\mathcal{X}$ (not depending on Y) such that $P(.|y)$ is absolutely continuous with respect to P_0 ($P \ll P_0$).

$$\Downarrow$$

$\exists\, f(.|y) = \frac{dP(A|y)}{dP_0}$ such that $P(A|y) = \int_A f(.|y)dP_0$, $\forall\, A \subset \mathcal{X}$ measurable.

2. Y is a continuous random variable.

$$\Downarrow$$

$\exists\, f_Y(y)$

Proposal

$$\begin{aligned}\gamma(x) &= \mathbb{E}(Y|X=x)\\ &= \int_{\mathbb{R}} y f(y|x) dy\\ &= \int_{\mathbb{R}} y \frac{f(x|y) f_Y(y)}{f_X(x)} dy\\ &= \boxed{\frac{1}{f_X(x)} \int_{\mathbb{R}} y f(x|y) f_Y(y) dy}\end{aligned}$$

$$f(y|x) = \frac{f(x|y) f_Y(y)}{f_X(x)}$$

$$f_X(x) = \int_{\mathbb{R}} f(x|y) f_Y(y) dy$$

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General estimator

$$\hat{\gamma}(x) = \frac{\sum_{i=1}^n \hat{f}(x|y_i) y_i}{\sum_{i=1}^n \hat{f}(x|y_i)}$$

Gaussian case

Additional assumption with $\mathcal{X} = L_2([0, 1])$

- For a fixed y, $P(.|y)$ is a Gaussian measure on $\mathcal{X}$ with mean $\mu(y)$ and covariance operator Γ.

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Consequences

for $(\varphi_j, \lambda_j)_j$ eigenfunctions and eigenvalues of Γ:

- $$\sum_{j=1}^{\infty} \frac{\mu_j^2(y)}{\lambda_j} < \infty, \qquad \mu_j(y) = \langle \mu(y), \varphi_j \rangle$$
- $$f(x|y) = \exp\left\{ \sum_{j=1}^{\infty} \frac{\mu_j(y)}{\lambda_j} \left(x_j - \frac{\mu_j(y)}{2} \right) \right\}, \qquad x_j = \langle x, \varphi_j \rangle, \ \forall j \geq 1$$

Specification in the Gaussian case

1. Obtain an estimate $\hat{\mu}(y)$ of $\mu(y)$

Nadaraya-Watson kernel estimate for $\mu(y,t) = \mathbb{E}(X(t)|Y=y)$

$$\hat{\mu}(y,t) = \frac{\sum_{i=1}^n x_i(t) K\left(\frac{y_i - y}{h}\right)}{\sum_{i=1}^n K\left(\frac{y_i - y}{h}\right)}$$

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2. Obtain estimates $(\hat{\lambda}_i, \hat{\varphi}_i)_i$ of $(\lambda_i, \varphi_i)_i$ on the basis of the empirical covariance of the residuals

Functional PCA

$$\hat{\epsilon}_i = x_i - \hat{\mu}(y_i), \qquad i = 1, ..., n$$

$$\hat{\Gamma} = \frac{1}{n} \sum_{i=1}^n (\hat{\epsilon}_i - \overline{\epsilon}) \otimes (\hat{\epsilon}_i - \overline{\epsilon}), \qquad \overline{\epsilon} = \frac{1}{n} \sum_{i=1}^n \epsilon_i$$

Specification in the Gaussian case II

3. Chose $p = p(n) \in \mathbb{N}$,

Estimate $f(x|y)$

$$\hat{f}(x|y) = \exp\left\{\sum_{j=1}^{p} \frac{\hat{\mu}_j(y)}{\hat{\lambda}_j}\left(\hat{x}_j - \frac{\hat{\mu}_j(y)}{2}\right)\right\}, \text{ with } \left\{\begin{array}{l} \hat{\mu}_j(y) = \langle \hat{\mu}(y), \hat{\varphi}_j \rangle \\ \text{and } x_j = \langle x, \hat{\varphi}_j \rangle \end{array}\right.$$

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DBIR estimator

$$\hat{\gamma}(x) = \frac{\sum_{i=1}^{n} \hat{f}(x|y_i) y_i}{\sum_{i=1}^{n} \hat{f}(x|y_i)}$$

Consistency DBIR

Theorem [Hernández et al., 2014]

Under assumptions (A1)-(A12), we have, for all $x \in \mathcal{X}$ such that $f_X(x) > 0$,

$$\lim_{n \to +\infty} \hat{\gamma}(x) =^{\mathbb{P}} \gamma(x).$$

Outline

Simulations

- (X, Y): random pair taking values in $\mathcal{X} = L_2([0,1]) \times \mathbb{R}$
- $(v_j)_{j\geq 1}$: the trigonometric basis of $\mathcal{X}$:

$$\begin{aligned} v_{2k-1} &= \sqrt{2}\cos(2\pi k) \\ v_{2k} &= \sqrt{2}\sin(2\pi k) \quad \text{for} \quad k = 1, 2, \ldots \end{aligned}$$

- $X = \mu(Y) + \epsilon$ with ϵ: Gaussian process (independent of Y) with zero mean and covariance operator

$$\Gamma_\epsilon = \sum_{j\geq 1} \frac{1}{j} v_j \otimes v_j$$

Simulated models

M2

$$X = Yv_1 + 2Yv_2 + 3Yv_{10} + \epsilon$$

M2

$$X = \sin(Y)v_1 + \log(Y + 1)v_5 + \epsilon$$

M3

$$X = Yq_1 + 5Yq_2 + \epsilon$$

where $q_1 = 2t^3$ and $q_2 = t^4$

M4

$$X = \sin(Y)q_1 + 20\log(Y + 1)q_2 + \epsilon$$

Computational aspects of the simulations

- $n_L = 300$ (number of samples in the training)
- $n_T = 200$ (number of samples in the test)
- $t \in \tau$, where τ equally spaced into $[0, 1]$
- $Y \sim \mathcal{U}(0, 10)$;
- ϵ was simulated by using a truncation of Γ_ϵ:

$$\Gamma_\epsilon(s, t) \simeq \sum_{j=1}^{N_j} \frac{1}{j} v_j(t) v_j(s)$$

with $N_j = 500$.

Performances compared to standard nonparametric estimate

Model	DBIR	NWK	DBIR (linear est. of the mean)
$M1$	0.23	0.28	0.22
$M2$	1.71	1.91	X
$M3$	0.07	0.19	0.02
$M4$	0.35	0.47	X

Outline

Conclusion and Remarks

- DBIR based on **estimation of the "inverse" regression model** $f(x|y)$ but (contrary to FSIR) no need to choose the effective dimension d and only 1-dimensional regression (instead of d);
- **computationally simple** and performs well on the simulated data;
- $P(.|y)$ assumed Gaussian but no assumption on the distribution of X or Y or Y given X.

Thank you for your attention...

...any question?

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Consistency of the DBIR estimator (notations)

- m st $\mu(.|y) = \frac{m(y)}{f_Y(y)}$;
- $(\eta_n)_n \subset \mathbb{R}^{+*}$, $\eta_n \searrow 0$;
- $r : y \rightarrow \mu(.|y)$, $r_{\eta_n}(y) = \frac{m(y)}{f_{Y,\eta_n}(y)}$ with $f_{Y,\eta_n}(y) = \max(f_Y(y), \eta_n)$;
- $\hat{m}(y) = \sum_{i=1}^n x_i K\left(\frac{y_i - y}{h}\right)$;
- $\hat{r}_{\eta_n} : y \rightarrow \hat{\mu}(.|y), \quad \hat{r}_{\eta_n}(y) = \frac{\hat{m}(y)}{\hat{f}_{Y,\eta_n}(y)}, \quad \hat{f}_{Y,\eta_n}(y) = \max(\hat{f}_Y(y), \eta_n)$;
- $\hat{f}_Y(y) = \sum_{i=1}^n K\left(\frac{y_i - y}{h}\right)$.

Consistency of the DBIR estimator (part 1)

(A1) f_Y has support $\Omega_Y \subset \mathbb{R}$, and f_Y and r are $\mathcal{C}^k$, for a $k \geq 2$, on Ω_Y;

(A2) K is an order k kernel with compact support;

(A3) there exists d_1 and d_2 such that $\sup_{y\in\Omega_Y} \left|f_Y^{(k)}(y)\right| < d_1$ and $\sup_{y\in\Omega_Y} \left\|r^{(k)}(y)\right\| < d_2$;

(A4) $h = O\left(n^{-c_1}\right)$, where $\frac{1}{4+2k} < c_1 < \frac{1}{4}$;

(A5) there exists $b_1 > 0$ such that $\inf_{y\in\Omega_Y} f_Y(y) \geq b_1$;

(A6) there exists $b_2 > 0$ such that $\sup_{y\in\Omega_Y} \left\|r(y)\right\| \leq b_2$.

Proposition 1

Under assumptions (A1)-(A6) we have:
$\sup_{y\in\Omega_Y} \left\|\hat{r}(y) - r(y)\right\| = O_P\left(n^{-c_1 k} + \left(\frac{\log n}{n^{1-2c_1}}\right)^{1/2}\right)$.

Consistency of the DBIR estimator (part 2)

(A7) $\mathbb{E}\left(\|\epsilon\|^4\right) < +\infty$;

Proposition 2

Under assumptions (A1)-(A7) we have:

$$\left\|\Gamma - \hat{\Gamma}\right\| = O_P\left(\frac{1}{n^{1/2-2c_1}}\right).$$

Consistency of the DBIR estimator (part 3)

(A8) $\sum_{j=1}^{\infty} \sup_{y\in\Omega_Y} \frac{|r_j(y)|}{\sqrt{\lambda_j}} < \infty$;

(A9) The $(\lambda_j)_j$ are all distinct;

(A10) $\lim_{n\to+\infty} p = +\infty$;

(A11) $\lim_{n\to+\infty} \frac{\sum_{j=1}^{p} a_j}{\lambda_p n^{1/2-2c_1}} = 0$;

(A12) $\frac{p}{\lambda_p^2} = O\left(n^q\right)$ for some $0 < q < \min(c_1 k, \frac{1}{2} - c_1)$.

Proposition 3

Under Assumptions (A1)-(A12), for any $x \in \mathcal{X}$ we have:
$\sup_{y\in\Omega_Y} \left|\hat{f}(x|y) - f(x|y)\right| = o_P\left(1\right)$.