Deciding the Dimension of Effective Dimension Reduction Space for Functional Data

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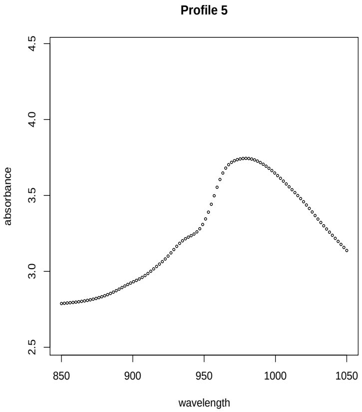
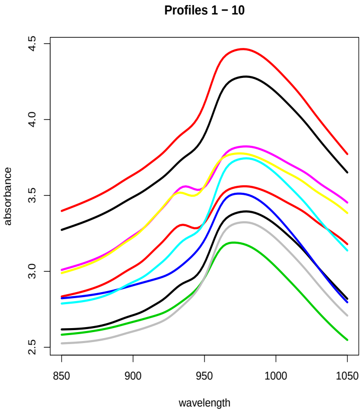
Near infrared spectroscopy data

- Meat samples were analyzed using near-infrared spectroscopy, which uses the near infrared region of the electromagnetic spectrum from 850 nm to 1050 nm. Each sample contains finely chopped pure meat with different moisture, fat and protein contents.
- For each meat sample the contents of water, fat and protein (in percent) were determined by analytic chemistry.
- See `http://lib.stat.cmu.edu/datasets/tecator` for details.

Near infrared spectroscopy data





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Data description

- number of meat samples: 215
- functional variable: absorbances
- multivariate data: moisture, fat and protein contents
- data size
  - absorbance: 100×215
  - moisture, fat and protein contents: 3×215

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Problem of interest

- estimating moisture, fat and protein contents based on absorbance

Basics of FDA

Let $\{X(t) : t \in T\}$ be a stochastic process with

- $\mu(t) = \mathbb{E}\{X(t)\}$ and $R(s,t) = \text{cov}\{X(s), X(t)\}$
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Data

- independent realizations $X_1, X_2, \ldots, X_n$ of X, (usually) densely observed, or
- independent realizations $(X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n)$ where Y is a covariate

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Inference

- distributional properties of X
- relationship between X and Y

Hilbert space and covariance operator

Let $\mathscr{H}$ be a Hilbert space of functions on T and $\langle \cdot, \cdot \rangle$ be the inner product of $\mathscr{H}$. Assume that $X \in \mathscr{H}$ a.s.

We will focus on $\mathscr{H} = L^2[a, b]$, the space of square-integrable functions on $[a, b]$, for some finite a, b, where

$$\langle f, g \rangle = \int_a^b f(t)g(t)dt.$$

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The *covariance operator* is

$$\Gamma_X : f \mapsto \int_a^b R(s,\cdot)f(s)ds, \;\; L^2[a,b] \mapsto L^2[a,b].$$

Eigen decomposition

Assume that $\mathbb{E}\|X\|^2 < \infty$. It follows that

- $\Gamma_X = \sum_{j=1}^{\infty} \omega_j \psi_j \otimes \psi_j$,
  - $\psi_1, \psi_2, \ldots$ are orthonormal
  - $\psi_j \otimes \psi_j$ is projection operator
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- [Mercer's Theorem]

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  $R(s,t) = \sum_{j=1}^{\infty} \omega_j \psi_j(s) \psi_j(t)$
- [Karhunen-Loève expansion]

  $X(t) = \mu(t) + \sum_{j=1}^{\infty} \omega_j^{1/2} \eta_j \psi_j(t)$
  - mean square expansion
  - $\mathbb{E}(\eta_j) = 0, \mathrm{cov}(\eta_j, \eta_k) = \delta_{j,k}$

A general functional regression model

Consider the model

$$Y = f(\langle \beta_1, X \rangle, \cdots, \langle \beta_K, X \rangle, \varepsilon),$$

where ε is unobserved and $f, K, \beta_1, \ldots, \beta_K$ are unknown, and the β_k's are linearly independent.

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Goals:

- estimate K
- estimate $\text{span}(\beta_1, \ldots, \beta_K)$, effective dimension reduction (EDR) space
- estimate (a version of) f

Special cases

- linear regression model: $Y = \beta_0 + \langle \beta_1, X \rangle + \varepsilon$

  Cardot, Ferraty and Sarda (2003), Cai and Hall (2006), Li and Hsing (2007)

- generalized linear model: $Y = f(\langle \beta, X \rangle, \varepsilon)$

  Müller and Stadtmüller (2005), Cardot and Sarda (2005)

- projection pursuit model: $Y = \sum_{k=1}^{K} f_k(\langle \beta_k, X \rangle) + \varepsilon$

  James and Silverman (2005)

Assumption $\mathscr{L}$: For any $\beta \in \mathscr{H}$,

$$\mathbb{E}(\langle \beta, X\rangle | \langle \beta_1, X\rangle, \cdots, \langle \beta_K, X\rangle) = c_0 + \sum_{k=1}^{K} c_k \langle \beta_k, X\rangle$$

for some constants $c_0, \cdots, c_K$.

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Inverse regression

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Theorem

[Li 1991, Ferré and Yao 2003] Under Assumption $\mathscr{L}$,

$$IR(t) := \mathbb{E}(X(t) - \mu(t) | Y) \in span\ (\Gamma_X \beta_1, \cdots, \Gamma_X \beta_K).$$

Elliptically contoured distribution

- A process X has an elliptically contoured distribution if

$$\mathbb{E}e^{i\langle f, X-\mu\rangle} = \phi(\langle f, Tf\rangle),\ f \in \mathscr{H},$$

  for some self-adjoint operator T and characteristic function ϕ.

- In the infinite-dimensional case, X has an elliptically contoured distribution if $X \stackrel{d}{=} \mu + RZ$ where Z is a zero-mean Gaussian process and R is a nonnegative random variable independent of Z. This can be proved based on a result by Schoenberg.

- Examples: Gaussian process, t-process

Inverse regression

By the Ferré and Yao Theorem,

$$\mathrm{Im}(\Gamma_{IR}) \subset \text{span } (\Gamma_X \beta_1, \cdots, \Gamma_X \beta_K).$$

If

$$\mathrm{Im}(\Gamma_{IR}) = \text{span } (\Gamma_X \beta_1, \cdots, \Gamma_X \beta_K),$$

then the β_k's can be estimated through the estimation of Γ_X and Γ_{IR}.

Inverse regression via principal components

- $X = \mu + \sum_{j=1}^{\infty} \omega_j^{1/2} \eta_j \psi_j$
- $\beta_k = \sum_{j=1}^{\infty} \omega_j^{-1/2} b_{kj} \psi_j$

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- $\beta_k = \sum_{j=1}^{\infty} \omega_j^{-1/2} b_{kj} \psi_j$
- $$\begin{aligned} \langle X - \mu, \beta_k \rangle &= \sum_{j=1}^{m} \eta_j b_{kj} + \sum_{j=m+1}^{\infty} \eta_j b_{kj} \\ &=: \boldsymbol{\eta}_{(m)}^T \mathbf{b}_{k,(m)} + \zeta_{k,(m)} \end{aligned}$$

Inverse regression based on principal components

The model $Y = f(\langle \beta_1, X\rangle, \cdots, \langle \beta_K, X\rangle, \varepsilon)$ can be written as

$$\begin{aligned} Y &= f_1(\mathbf{b}_{1,(m)}^T \boldsymbol{\eta}_{(m)} + \zeta_{1,(m)}, \cdots, \mathbf{b}_{K,(m)}^T \boldsymbol{\eta}_{(m)} + \zeta_{K,(m)}, \varepsilon) \\ &= f_2(\mathbf{b}_{1,(m)}^T \boldsymbol{\eta}_{(m)}, \cdots, \mathbf{b}_{K,(m)}^T \boldsymbol{\eta}_{(m)}, \varepsilon_{(m)}) \end{aligned}$$

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- The EDR space of this problem is $\mathrm{span}(\mathbf{b}_{1,(m)}, \cdots, \mathbf{b}_{K,(m)})$.
- If $\mathbf{b}_{1,(m)}, \cdots, \mathbf{b}_{K,(m)}$ are linearly independent then the dimension of EDR space is K.
- Denote by $\Gamma_{IR,(m)}$ the inverse regression covariance matrix of this problem; namely

$$\Gamma_{IR,(m)} = \mathrm{cov}(\mathbb{E}(\boldsymbol{\eta}_{(m)} | Y)).$$

- The "pseudo-error", $\varepsilon_{(m)}$, is equal to

$$(\varepsilon, \zeta_{1,(m)}, \ldots, \zeta_{K,(m)}),$$

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- What's the role of m?

An example

- $$X(t) = \sum_{k=1}^{\infty} \omega_{2k-1}^{1/2} \eta_{2k-1} \sqrt{2} \cos(2k\pi t) + \sum_{k=1}^{\infty} \omega_{2k}^{1/2} \eta_{2k} \sqrt{2} \sin(2k\pi t), \quad t \in [0,1],$$

  where $\omega_k = 20(k+1.5)^{-3}$ and η_k's $\sim N(0,1)$.

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- The principal components are

  $$\sqrt{2}\cos(2\pi t), \sqrt{2}\sin(2\pi t), \sqrt{2}\cos(4\pi t), \sqrt{2}\sin(4\pi t), \ldots$$

- $$\begin{aligned}\beta_1(t) &= 0.9\sqrt{2}\cos(2\pi t) + 1.2\sqrt{2}\cos(4\pi t) - 0.5\sqrt{2}\cos(8\pi t) \\ &\quad + \sum_{k>4} \frac{\sqrt{2}}{(2k-1)^3}\cos(2k\pi t), \\ \beta_2(t) &= 0.45\sqrt{2}\cos(2\pi t) + 0.6\sqrt{2}\cos(4\pi t) - 3\sqrt{2}\sin(6\pi t) \\ &\quad + 1.2\sqrt{2}\sin(8\pi t) + \sum_{k>4} \frac{(-1)^k\sqrt{2}}{(2k)^3}\sin(2k\pi t).\end{aligned}$$

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- $$\begin{array}{lrrrrrrr} \mathbf{b}_{1,(m)} = & .9, & 0, & 1.2, & 0, & 0, & 0, & \ldots \\ \mathbf{b}_{2,(m)} = & .45, & 0, & .6, & 0, & 0, & \text{-}3, & \ldots \end{array}$$

Sliced inverse regression

- Data: $(X_1, Y_1), \cdots, (X_n, Y_n)$, fully observed.
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- Compute the PC scores $\widehat{\eta}_{ij} = \widehat{\omega}_j^{-1/2} \langle \widehat{\psi}_j, X_i - \bar{X} \rangle$
- Let $S_1, \cdots, S_H$ be a partition of the the range of Y. Let

$$
\begin{aligned}
n_h &= \sum_{i=1}^{n} I(Y_i \in S_h), \ \widehat{p}_h = \frac{n_h}{n} \\
\bar{\boldsymbol{\eta}}_{h,(m)} &= \frac{1}{n_h} \sum_{i=1}^{n} \widehat{\boldsymbol{\eta}}_{i,(m)} I(Y_i \in S_h) \\
\widehat{\Gamma}_{IR,(m)} &= \sum_{h=1}^{H} \widehat{p}_h \bar{\boldsymbol{\eta}}_{h,(m)} \bar{\boldsymbol{\eta}}_{h,(m)}^T
\end{aligned}
$$

- $\widehat{\Gamma}_{IR,(m)}$ estimates $\Gamma_{IR,(m)}$.
- Let $\widehat{\mathbf{b}}_{1,(m)}, \cdots, \widehat{\mathbf{b}}_{K,(m)}$ be the leading eigenvectors of $\widehat{\Gamma}_{IR,(m)}$.

  $\mathrm{span}(\widehat{\mathbf{b}}_{1,(m)}, \cdots, \widehat{\mathbf{b}}_{K,(m)})$ estimates $\mathrm{span}(\mathbf{b}_{1,(m)}, \cdots, \mathbf{b}_{K,(m)})$.
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- If X is infinite-dimensional, then in general m must increase to ∞ with n in establishing consistency [Ferré and Yao 2003].
- Prerequisite: Need to know K.

Deciding the dimension of EDR space

- To determine K, we sequentially test $H_0 : K \leq K_0$ vs. $H_a : K > K_0$ for $K_0 = 0, 1, \ldots$, and conclude $K = K_0$ the first time we fail to reject H_0.

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- Reject H_0 for large values of $\mathscr{T}_{K_0,(m)}$.

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Theorem

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$$\mathscr{T}_{K_0,(m)} \xrightarrow{d} \mathscr{X} \text{ as } n \to \infty.$$

- *If $K_{(m)} < K_0$, then $\mathscr{T}_{K_0,(m)}$ is asymptotically stochastically bounded by $\mathscr{X}$; namely,*

$$\limsup_{n\to\infty} \mathbb{P}(\mathscr{T}_{K_0,(m)} > x) \leq \mathbb{P}(\mathscr{X} > x) \text{ for all } x.$$

Example, continued

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- $$\begin{aligned}\mathbf{b}_{1,(m)} &= .9, \quad 0, \quad 1.2, \quad 0, \quad 0, \quad 0, \quad \ldots \\ \mathbf{b}_{2,(m)} &= .45, \quad 0, \quad .6, \quad 0, \quad 0, \quad \text{-}3, \quad \ldots\end{aligned}$$

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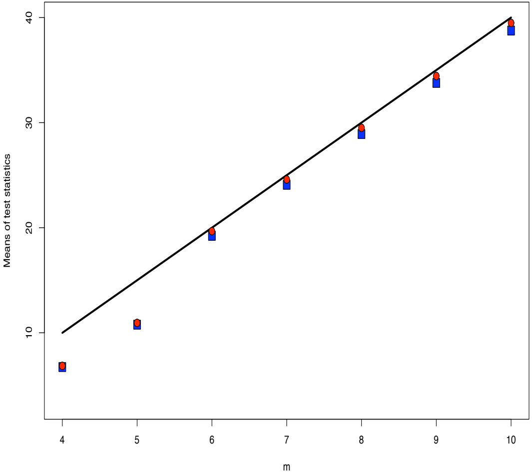
Let $K_0 = 2$ and $n = 500$. Compute $\mathbb{E}(\mathscr{T}_{K_0,(m)})$ and $\mathbb{E}(\mathscr{T}^*_{K_0,(m)})$.



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- Ideally, case (i) holds and the χ^2 test has the correct size asymptotically.

- For a number of reasons case (ii) may be true, for which the χ^2 test will be conservative.

Proposition

Let Z be a $p \times q$ random matrix and we write $Z = [\ Z_1 \mid Z_2\ ]$ where Z_1 and Z_2 have sizes $p \times r$ and $p \times (q - r)$, respectively, for some $0 < r < \min(p, q)$. Assume that Z_1 and Z_2 are independent, and Z_2 contains i.i.d. Normal $(0, 1)$ entries. Then $\sum_{j=r+1}^{p} \lambda_j(ZZ^T)$ is stochastically bounded by χ^2 with $(p - r)(q - r)$ degrees of freedom.

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The case where Z is a matrix of i.i.d. Normal$(0,1)$ entries can be viewed as the special case, $r = 0$. For that the bound is exact since $\sum_{j=1}^{p} \lambda_j(ZZ^T)$ equals the sum of squares of all of the entries of Z and is therefore distributed as χ^2 with pq degrees of freedom.

Proof

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$$\begin{aligned} &\sum_{j=r+1}^{p} \lambda_j(ZZ^T) \\ = \; &\min_{\Phi} \Big\{ \mathrm{tr}(\Phi^T ZZ^T \Phi), \; \Phi \text{ is a } p \times (p-r) \\ &\qquad\qquad \text{matrix with orthonormal columns} \Big\} \end{aligned}$$

Construct Φ by Gram-Schmidt procedure on the columns of Z.

Adjusted test

- For the non-Gaussian case, we need to eliminate nuisance parameters in the limit.
  - Let $\widehat{P}$ be the matrix whose columns are the eigenvectors that correspond to the $m - K_0$ smallest eigenvalues of $\widehat{V}$.
  - $\widehat{\tau}_h := \frac{1}{(m-K_0)n_h} \mathrm{tr}\{\widehat{P}\widehat{P}^T \sum_{i=1}^{n} (\widehat{\boldsymbol{\eta}}_{i,(m)} - \bar{\boldsymbol{\eta}}_{h,(m)}) \times (\widehat{\boldsymbol{\eta}}_{i,(m)} - \bar{\boldsymbol{\eta}}_{h,(m)})^T I(Y_i \in S_h)\}$
  - $\widehat{\Lambda} := \mathrm{diag}(\widehat{\tau}_1^{1/2}, \cdots, \widehat{\tau}_H^{1/2})$
  - $\widehat{\mathscr{J}} := I - (\widehat{p}_1^{1/2}, \cdots, \widehat{p}_H^{1/2})^T (\widehat{p}_1^{1/2}, \cdots, \widehat{p}_H^{1/2})$
  - $\widehat{G} = \mathrm{diag}\{\widehat{p}_1^{1/2}, \cdots, \widehat{p}_H^{1/2}\}$
  - $\widehat{M} = [\bar{\boldsymbol{\eta}}_{1,(m)}, \cdots, \bar{\boldsymbol{\eta}}_{H,(m)}]_{m \times H}$
- $\widehat{W}_{(m)} = \widehat{M}\widehat{G}\widehat{\mathscr{J}}\widehat{\Lambda}(\widehat{\Lambda}\widehat{\mathscr{J}}\widehat{\Lambda})^{-}(\widehat{M}\widehat{G}\widehat{\mathscr{J}}\widehat{\Lambda}(\widehat{\Lambda}\widehat{\mathscr{J}}\widehat{\Lambda})^{-})^T$

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Theorem

Suppose X has an elliptically contoured distribution. Assume that the true dimension $K \le K_0$ and let $H > K_0 + 1$ and $m \ge K_0 + 1$. If $K_{(m)} = K_0$ then $\mathscr{T}^*_{K_0,(m)} \xrightarrow{d} \chi^2_{(m-K_0)(H-K_0-1)}$ as $n \to \infty$.

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  When the sample size is fixed, the power of the tests will decrease with m. Intuitively, when m is large the information contained in the individual components becomes diluted. This is also true for the "small n, large p" situation of multivariate data.
- If m is chosen appropriately and the level α is fixed for all of the tests, then the probability of correct identification of K tends to $1 - \alpha$ as $n \to \infty$. The choice of H is less important.

Adaptive Neyman test for the normal mean

Let $\mathbf{X} \sim N(\boldsymbol{\theta}, I_n)$ be an n-dimensional normal random vector. We wish to test $H_0 : \boldsymbol{\theta} = 0$ versus $H_a : \boldsymbol{\theta} \neq 0$.

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- Fan (1996) and Fan and Lin (1998) considered the test statistic

$$T_N = \max_{1 \leq m \leq N} \frac{1}{\sqrt{2m}} \sum_{j=1}^{m} (X_j^2 - 1).$$

"Adaptive Neyman" procedure

For $N > K_0$ define

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Theorem

Suppose X is a Gaussian process. Assume that $K \le K_0$ and let $H > K_0 + 1$. Let χ_i^2, $i \ge 1$, be i.i.d. χ^2 random variables with $H - K_0 - 1$ degrees of freedom and define

$$\mathscr{X}_{(m)} = \sum_{i=1}^{m-K_0} \chi_i, \quad m \ge K_0 + 1.$$

Then, for all positive integers $N > K_0$, the collection of test statistics $\mathscr{T}_{K_0,(m)}, m = K_0 + 1, \cdots, N$, are jointly stochastically bounded by $\mathscr{X}_{(m)}, m = K_0 + 1, \cdots, N$, as n tends to ∞.

Simulations

- $$X(t) = \sum_{k=1}^{\infty} \omega_{2k-1}^{1/2} \eta_{2k-1} \sqrt{2} \cos(2k\pi t) + \sum_{k=1}^{\infty} \omega_{2k}^{1/2} \eta_{2k} \sqrt{2} \sin(2k\pi t),$$

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- For the adaptive Neyman test, we choose $N = K_0 + 30$ ($N \sim 30$ to 35).
- We let $\alpha = .05$.

Simulations

	$n = 200$	$n = 500$
χ^2 test ($m = 5$)	0.040	0.047
Adj. χ^2 ($m = 5$)	0.068	0.068
χ^2 test ($m = 7$)	0.358	0.913
Adj. χ^2 ($m = 7$)	0.410	0.899
χ^2 test ($m = 30$)	0.085	0.566
Adj. χ^2 ($m = 30$)	0.170	0.616
Adaptive Neyman	0.229	0.885

Table: Empirical frequencies of finding the correct model

Tecator data

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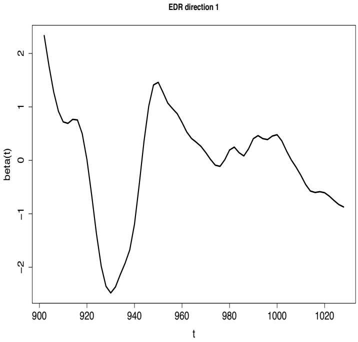
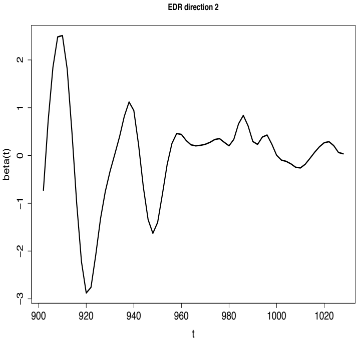
- All of our tests identified EDR dimension $K = 3$.





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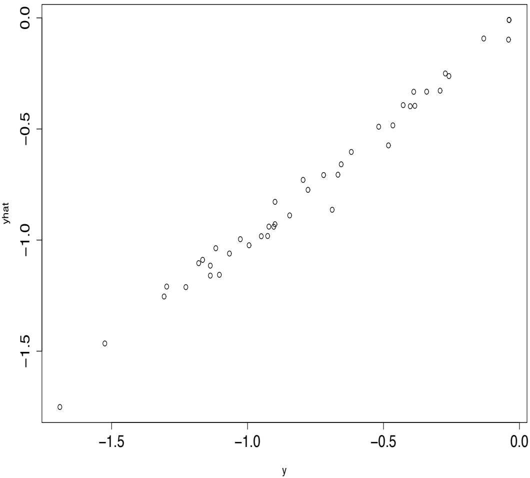

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Concluding remarks

- In this talk we deal with the problem of deciding the dimension of the EDR space in a functional-data setting.
- We assume that the predictor is a random function residing in a Hilbert space and has an elliptically contoured distribution, and develop inference procedures based on rigorous statistical tests to determine the dimension of the EDR space.
- While we focus on infinite-dimensional functional data, all of our results hold without modification for finite-dimensional data, including the "small n, large p" setting for which dimension reduction issues are especially important.

Concluding remarks

- Our procedures are defined by focusing on the information contained in sample principal component scores of the functional data. At the heart of our methodology is an asymptotic representation of the sum of small eigenvalues of the sliced-inverse-regression sample covariance matrix.

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- Our procedures are defined by focusing on the information contained in sample principal component scores of the functional data. At the heart of our methodology is an asymptotic representation of the sum of small eigenvalues of the sliced-inverse-regression sample covariance matrix.

- In this work we focus on densely recorded functional data, for which standard nonparametric regression techniques can be applied to preprocess the data. A large proportion of commonly seen functional data fall in this category. Many authors have considered principal component analysis for sparsely observed functional data, e.g., data obtained from longitudinal studies. Extending those approaches to the context of this paper requires further research.