Nonlinear functional regression: a functional RKHS approach

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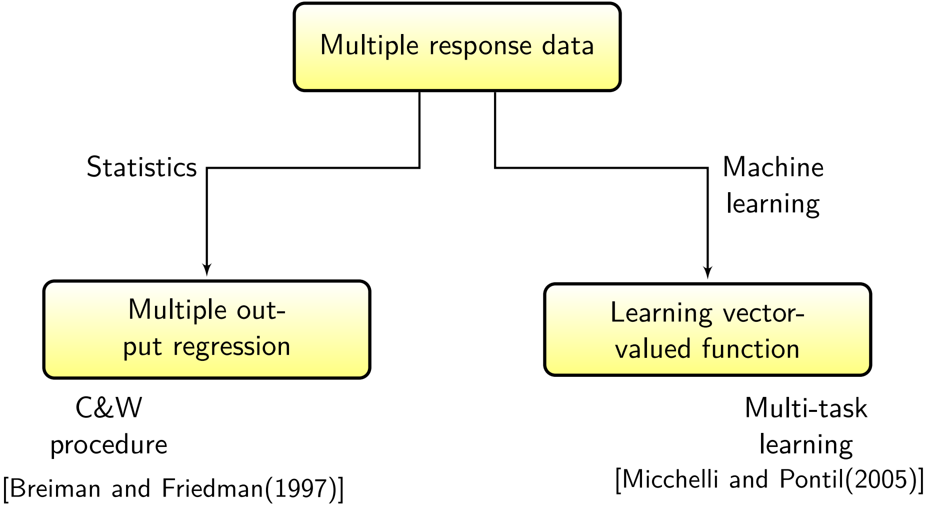
Outline

Regression

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

Predictor $\longmapsto$	Response	Model
$\mathbb{R}^d$	$\mathbb{R}$	Multiple Regression, GLM
$\mathbb{R}^d$	$\mathbb{R}^d$	Multivariate Regression
$\mathbf{L}^2$	$\mathbb{R}$	Generalized Functional Linear Model
$\mathbb{R}^d$	$\mathbf{L}^2$	Functional Response Model
$\mathbf{L}^2$	$\mathbf{L}^2$	Functional Regression Model

Multiple response data



Functional Data Analysis (FDA) - FAQ -

- **What is functional data analysis ? goals ?**
  The study of curves, shapes or other high-dimensional objects. [Ramsay and Silverman(2002), Ramsay and Silverman(2005)]
- **What is functional data ?**
  Represent a number of discrete observations about an individual in the form of a function or curve.
- **Where to find such data ?**
  Meteorology / Finance / Biology / Chemometrics / Speech analyis / Brain imaging
- **How to treat these data ?**
  3 schools: English - French - Stochastic
- **Multivariate data or Functional data ?**
  No answer ??? !!!

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Summary of Motivations

- Nonlinear functional methods
- High dimensional data
- Correlation between data
- Time information - sequential tools -

Functional kernel

$(x_i(s), y_i(t))_{i=1}^n \in \mathcal{G}_x \times \mathcal{G}_y$ where $\mathcal{G}_x : \Omega_x \longrightarrow \mathbb{R}$ and $\mathcal{G}_y : \Omega_y \longrightarrow \mathbb{R}$

Definition

An $\mathcal{L}(\mathcal{G}_y)$-valued kernel $K_\mathcal{F}(w, z)$ on $\mathcal{G}_x$ is a function $K_\mathcal{F}(.,.) : \mathcal{G}_x \times \mathcal{G}_x \longrightarrow \mathcal{L}(\mathcal{G}_y)$;

- *$K_\mathcal{F}$ is Hermitian if $K_\mathcal{F}(w, z) = K_\mathcal{F}(z, w)^*$,*
- *it is nonnegative on $\mathcal{G}_x$ if for any $\{(w_i, u_i)_{i=1,\ldots,r}\} \in \mathcal{G}_x \times \mathcal{G}_y$*

$$\sum_{i,j} \langle K_\mathcal{F}(w_i, w_j) u_i, u_j \rangle_{\mathcal{G}_y} \geq 0$$

Functional RKHS (1/4)

Definition

A Hilbert space $\mathcal{F}$ of functions from $\mathcal{G}_x$ to $\mathcal{G}_y$ is called a reproducing kernel Hilbert space if there is a nonnegative $\mathcal{L}(\mathcal{G}_y)$-valued kernel $K_{\mathcal{F}}(w, z)$ on $\mathcal{G}_x$ such that:

- *the function $z \longmapsto K_{\mathcal{F}}(w, z)g$ belongs to $\mathcal{F}$ for every choice of $w \in \mathcal{G}_x$ and $g \in \mathcal{G}_y$*
- *for every $f \in \mathcal{F}, \langle f, K_{\mathcal{F}}(w, .)g\rangle_{\mathcal{F}} = \langle f(w), g\rangle_{\mathcal{G}_y}$*

(reproducing property)

Functional RKHS (2/4)

Theorem

If a Hilbert space $\mathcal{F}$ of functions on $\mathcal{G}_y$ admits a reproducing kernel, then the reproducing kernel $K_{\mathcal{F}}(w,z)$ is uniquely determined by the Hilbert space $\mathcal{F}$.

Proof:

$$\langle K'(w',.)h, K(w,.)g\rangle_{\mathcal{F}} = \langle K'(w',w)h, g\rangle_{\mathcal{G}} \tag{1}$$

$$\begin{aligned} \langle K'(w',.)h, K(w,.)g\rangle_{\mathcal{F}} &= \langle K(w,.)g, K'(w',.)h\rangle_{\mathcal{F}} \\ &= \langle K(w,w')g, h\rangle_{\mathcal{G}} \\ &= \langle g, K(w,w')^{*}h\rangle_{\mathcal{G}} \\ &= \langle g, K(w',w)h\rangle_{\mathcal{G}} \end{aligned} \tag{2}$$

(1) and $(2) \Longrightarrow K_{\mathcal{F}}(w,z) \equiv K'_{\mathcal{F}}(w,z)$ □

Functional RKHS (3/4)

Theorem

A $\mathcal{L}(\mathcal{G}_y)$-valued kernel $K_{\mathcal{F}}(w,z)$ on $\mathcal{G}_x$ is the reproducing kernel of some Hilbert space $\mathcal{F}$, if and only if it is positive definite.

Proof: Function-valued RKHS ⇒ positive operator-valued kernel

$$\sum_{i,j=1}^{n} \langle K_{\mathcal{F}}(w_i,w_j),u_j\rangle_{\mathcal{G}_y}$$
$$= \sum_{i,j=1}^{n} \langle K_{\mathcal{F}}(w_i,.)u_i, K_{\mathcal{F}}(w_j,.)u_j\rangle_{\mathcal{F}}$$
$$= \langle \sum_{i=1}^{n} K_{\mathcal{F}}(w_i,.)u_i, \sum_{i=1}^{n} K_{\mathcal{F}}(w_i,.)u_i\rangle_{\mathcal{F}}$$
$$= \| \sum_{i=1}^{n} K_{\mathcal{F}}(w_i,.)u_i\|^2_{\mathcal{F}} \geq 0 \qquad \square$$

Functional RKHS (4/4)

Proof: Function-valued RKHS $\Leftarrow$ positive operator-valued kernel

- $\mathcal{F}_0, \ \forall f \in \mathcal{F}_0, \ f(.) = \sum_{i=1}^{n} K_{\mathcal{F}}(w_i, .)\alpha_i$
- $\langle f(.), g(.)\rangle_{\mathcal{F}_0} = \sum_{i,j=1}^{n} \langle K_{\mathcal{F}}(w_i, z_j)\alpha_i, \beta_j\rangle_{\mathcal{G}_y}$
- $(\mathcal{F}_0, \langle ., .\rangle_{\mathcal{F}_0})$ is a pre-Hilbert space
- $\mathcal{F}$ the completion of $\mathcal{F}_0$ space via Cauchy sequences

Functional kernel construction

- $\mathcal{L}(\mathcal{G})$-valued kernel

$$\begin{array}{rccc} K_{\mathcal{F}}: & \mathcal{G}\times\mathcal{G} & \longrightarrow & \mathcal{L}(\mathcal{G}) \\ & x,y & \longmapsto & T^{h(x,y)} \end{array}$$

- Operator

$$\begin{array}{rccc} T^{h}: & \mathcal{G} & \longrightarrow & \mathcal{G} \\ & x & \longmapsto & T_x^h \quad ; \quad T_x^h(t) = h(t)x(t) \end{array}$$

- characterestic function

$$\begin{array}{rccc} K_{\mathcal{F}}: & \mathcal{G}\times\mathcal{G} & \longrightarrow & \mathcal{G} \\ & x,y & \longmapsto & h(x,y) = \exp(c.(x-y)^2) \end{array}$$

Representer theorem (1/2)

Theorem

The solution of the minimization problem

$$\min_{f \in \mathcal{F}} \sum_{i=1}^{n} \|y_i - f(x_i)\|^2_{\mathcal{G}_y} + \lambda \|f\|^2_{\mathcal{F}}$$

is achieved by a function of the form

$$f^*(.) = \sum_{i=1}^{n} K_{\mathcal{F}}(x_i, .)\beta_i$$

Representer theorem (2/2)

Proof:

$$D_h J_\lambda(f) = \lim_{\tau \longrightarrow 0} \frac{J_\lambda(f+\tau h) - J_\lambda(f)}{\tau} = \langle J_\lambda^{'}(f), h \rangle$$

i. $G(f) = \|f\|_{\mathcal{F}}^2$

$$\lim_{\tau \longrightarrow 0} \frac{\|f+\tau h\|_{\mathcal{F}}^2 - \|f\|_{\mathcal{F}}^2}{\tau} = 2\langle f, h \rangle \qquad \Longrightarrow \qquad G^{'}(f) = 2f$$

ii. $H_i(f) = \|y_i - f(x_i)\|_{\mathcal{G}}^2$

$$\lim_{\tau \longrightarrow 0} \frac{\|y_i - f(x_i) - \tau h(x_i)\|_{\mathcal{G}}^2 - \|y_i - f(x_i\|_{\mathcal{G}}^2}{\tau}$$
$$= -2\langle y_i - f(x_i), h(x_i)\rangle_{\mathcal{G}} = -2\langle K_{\mathcal{F}}(x_i,.)(y_i - f(x_i)), h\rangle_{\mathcal{F}}$$
$$= -2\langle K_{\mathcal{F}}(x_i,.)\alpha_i, h\rangle_{\mathcal{F}} \qquad \Longrightarrow \qquad H_i^{'}(f) = 2K_{\mathcal{F}}(x_i,.)\alpha_i$$

(i), (ii), and $J_\lambda^{'}(f^*) = 0 \Longrightarrow f^*(.) = \frac{1}{\lambda}\sum_{i=1}^{n} K_{\mathcal{F}}(x_i,.)\alpha_i$ □

Regression function estimation (1/2)

$$\min_{f \in \mathcal{F}} \sum_{i=1}^{n} \|y_i - f(x_i)\|_{\mathcal{G}_y}^2 + \lambda \|f\|_{\mathcal{F}}^2$$

using the representer theorem

$$\Longleftrightarrow \quad \min_{\beta_i} \sum_{i=1}^{n} \|y_i - \sum_{j=1}^{n} K_{\mathcal{F}}(x_i, x_j)\beta_j\|_{\mathcal{G}_y}^2 + \lambda \|\sum_{j=1}^{n} K_{\mathcal{F}}(., x_j)\beta_j\|_{\mathcal{F}}^2$$

using the reproducing property

$$\Longleftrightarrow \quad \min_{\beta_i} \sum_{i=1}^{n} \|y_i - \sum_{j=1}^{n} K_{\mathcal{F}}(x_i, x_j)\beta_j\|_{\mathcal{G}_y}^2 + \lambda \sum_{i,j}^{n} \langle K_{\mathcal{F}}(x_i, x_j)\beta_i, \beta_j \rangle_{\mathcal{G}_y}$$

Regression function estimation (2/2)

$$\min_{\beta_i} \sum_{i=1}^{n} \|y_i - \sum_{j=1}^{n} K_{\mathcal{F}}(x_i, x_j)\beta_j\|^2_{\mathcal{G}_y} + \lambda \sum_{i,j}^{n} \langle K_{\mathcal{F}}(x_i, x_j)\beta_i, \beta_j\rangle_{\mathcal{G}_y}$$

Multiplication operator

$$\iff \quad \min_{\beta_i} \sum_{i=1}^{n} \|y_i - \sum_{j=1}^{n} c_{ij}\beta_j\|^2_{\mathcal{G}_y} + \lambda \sum_{i,j}^{n} \langle c_{ij}\beta_i, \beta_j\rangle_{\mathcal{G}}$$

Discrete points

$$\iff \quad \min_{\beta_i} \sum_{i=1}^{n} \sum_{l=1}^{p} \left(y_i(t_i^l) - \sum_{j=1}^{n} c_{ij}(t_{ij}^l)\beta_j(t_j^l) \right)^2 + \lambda \sum_{i,j}^{n} \sum_{l}^{p} c_{ij}(t_{ij}^l)\beta_i(t_i^l)\beta_j(t_j^l)$$

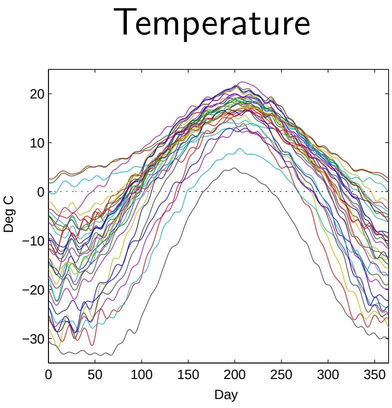
Matrix formulation

$$\iff \quad \min_{\beta} trace((Y - C\beta)(Y - C\beta)^T) + \lambda\, trace(C\beta\beta^T)$$

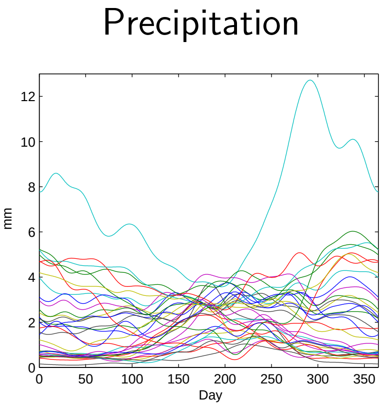
Matrix derivative

$$\implies \quad (C + \lambda I)\beta = Y$$

Meteorological data

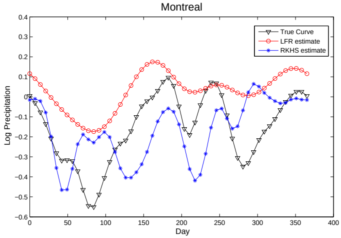


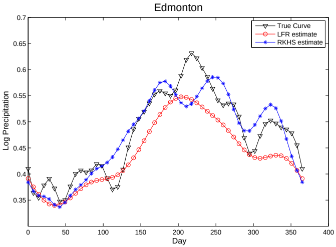
(a)

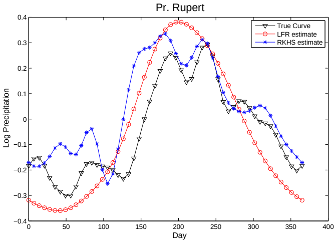


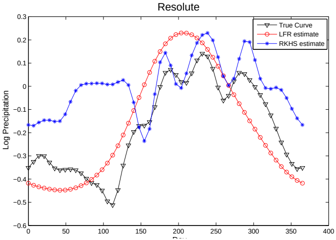
(b)

Prediction results









Conclusion

- Nonlinear functional regression
- RKHS - operator sapces
- Multiple functional regression
- Operator-valued kernels
- Regularization path algorithm

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