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Regression modelling using I-priors

NUS Department of Statistics & Data Science Seminar

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Overview

Introduction
- Regression analysis
- I-priors

Regression using I-priors
- Reproducing kernel Hilbert spaces
- The Fisher information
- The I-prior

Estimation
- Model hyperparameters
- Estimation methods
- Computational bottleneck

Data examples
- Longitudinal analysis
- Predicting fat content

Conclusions & further work

Regression analysis

For $i = 1, \dots, n$, consider the regression model

$$\begin{aligned} y_i &= f(x_i) + \epsilon_i \\ (\epsilon_1, \dots, \epsilon_n)^\top &\sim \mathrm{N}_n(0, \Psi^{-1}) \end{aligned} \tag{1}$$

where each $y_i \in \mathbb{R}$, $x_i \in \mathcal{X}$ (some set of covariates), and f is a regression function.

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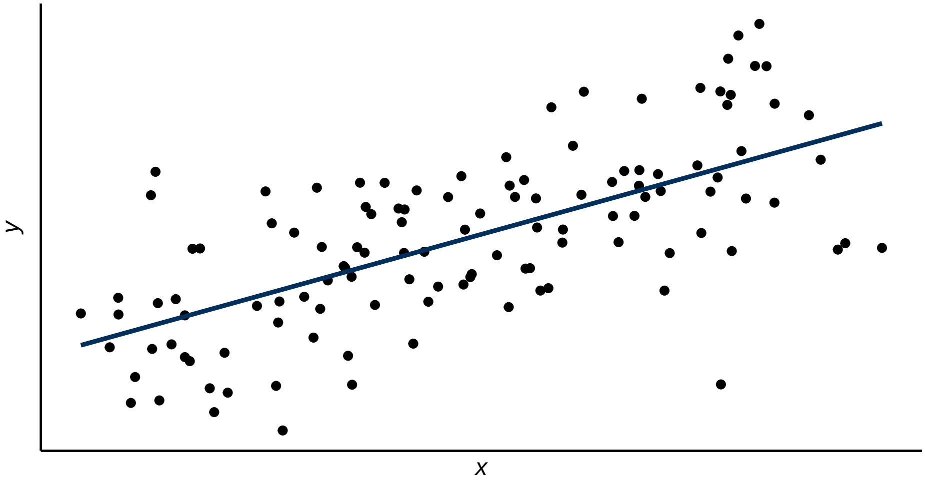
Goal

To estimate the regression function f given the observations $\{(y_i, x_i)\}_{i=1}^n$.

1. Ordinary linear regression

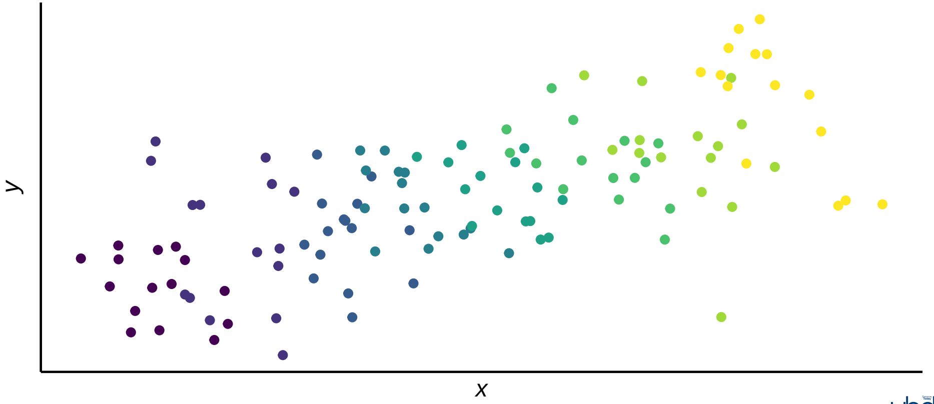
Suppose $f(x_i) = x_i^\top \beta$ for $i = 1, \dots, n$, where $x_i, \beta \in \mathbb{R}^p$.



2. Varying intercepts/slopes model

Suppose each unit $i = 1, \dots, n$ relates to the kth observation in group $j \in \{1, \dots, m\}$. Model the function f additively:

$$f(x_{kj}, j) = f_1(x_{kj}) + f_2(j) + f_{12}(x_{kj}, j).$$



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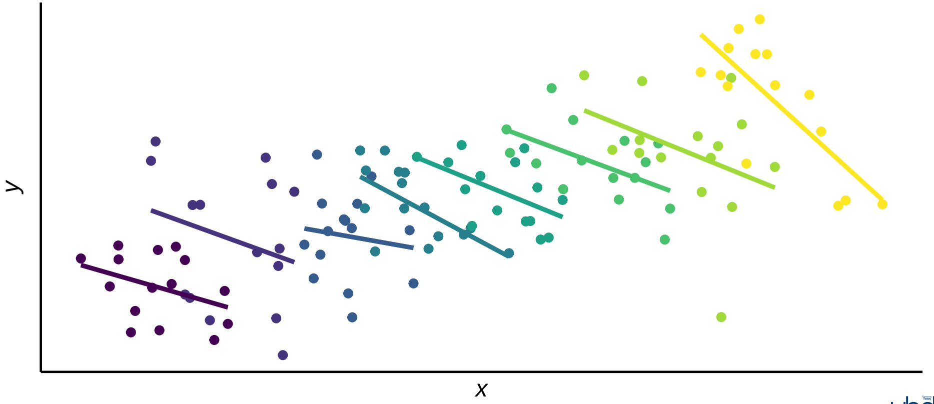
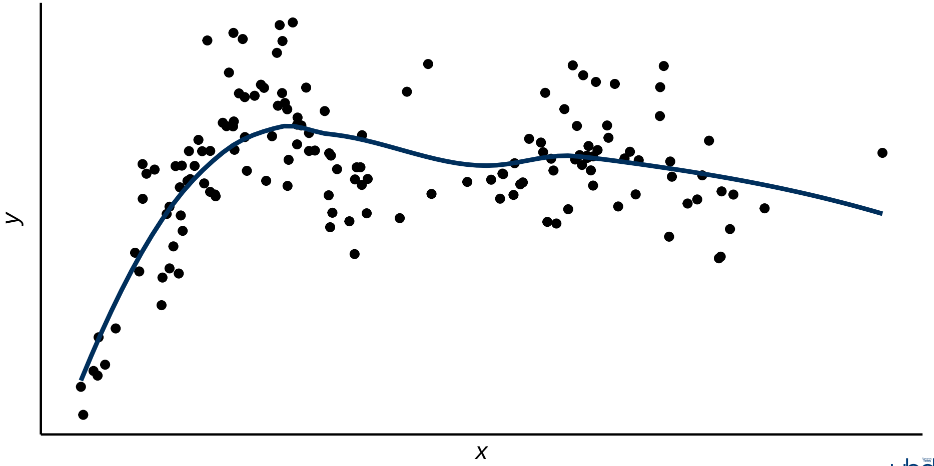
$$f(x_{kj}, j) = \underbrace{x_{kj}^\top \beta_1}_{f_1} + \underbrace{\beta_{0j}}_{f_2} + \underbrace{x_{kj}^\top \beta_{1j}}_{f_{12}}$$



3. Smoothing models

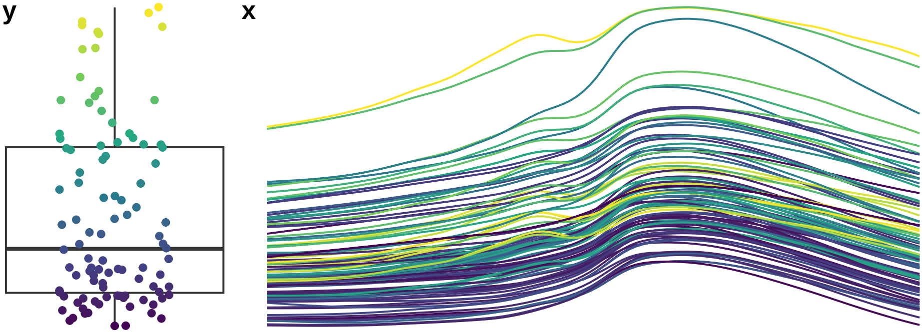
Suppose $f \in \mathcal{F}$ where $\mathcal{F}$ is a space of "smoothing functions" (models like LOESS, kernel regression, smoothing splines, etc.).



4. Functional regression

Suppose the input set $\mathcal{X}$ is functional. The (linear) regression aims to estimate a coefficient function $\beta : \mathcal{T} \to \mathbb{R}$

$$y_i = \underbrace{\int_{\mathcal{T}} x_i(t)\beta(t)\,\mathrm{d}t}_{f(x_i)} + \epsilon_i$$



The I-prior

For the normal model stated in (1), we assume that f lies in some RKHS of functions $\mathcal{F}$, with reproducing kernel h over $\mathcal{X}$.

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Definition 1 (I-prior)

With $f_0 \in \mathcal{F}$ a prior guess, the entropy maximising prior distribution for f, subject to constraints, is

$$f(x) = f_0(x) + \sum_{i=1}^{n} h(x, x_i) w_i \tag{2}$$

$$(w_1, \ldots, w_n)^\top \sim \mathrm{N}_n(0, \Psi)$$

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Therefore, the covariance kernel of $f(x)$ is determined by the function

$$k(x, x') = \sum_{i=1}^n \sum_{j=1}^n \Psi_{ij} h(x, x_i) h(x', x_j), \tag{3}$$

which happens to be the *Fisher information* between evaluations of f.

The I-prior (cont.)

Interpretation:

> The more information about f, the larger its prior variance, and hence the smaller the influence of the prior mean f_0 (and vice versa).

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Of interest then are

1. Posterior distribution for the regression function,

$$p(f \mid y) = \frac{p(y \mid f)p(f)}{\int p(y \mid f)p(f)\,\mathrm{d}f}.$$

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$$p(f \mid y) = \frac{p(y \mid f)p(f)}{\int p(y \mid f)p(f)\,\mathrm{d}f}.$$

2. Posterior predictive distribution (given a new data point x_*)

$$p(y_* \mid y) = \int p(y_* \mid f_*)p(f_* \mid y)\,\mathrm{d}f_*,$$

where $f_* = f(x_*)$.

Posterior regression function

Denote by

- $\mathbf{y} = (y_1, \dots, y_n)^\top$
- $\mathbf{f} = \big(f(x_1), \dots, f(x_n)\big)^\top$
- $\mathbf{f}_0 = \big(f_0(x_1), \dots, f_0(x_n)\big)^\top$
- $\mathbf{H} = \big(h(x_i, x_j)\big)_{i,j=1}^n \in \mathbb{R}^{n \times n}$

(1) + an I-prior on f implies

$$\mathbf{y} \mid \mathbf{f} \sim \mathrm{N}_n(\mathbf{f}, \mathbf{\Psi}^{-1})$$
$$\mathbf{f} \sim \mathrm{N}_n(\mathbf{f}_0, \mathbf{H\Psi H})$$

Thus, $\mathbf{y} \sim \mathrm{N}_n(\mathbf{f}_0, \mathbf{V}_y := \mathbf{H\Psi H} + \mathbf{\Psi}^{-1})$.

Lemma 2

The posterior distribution for f is Gaussian with mean and covariance

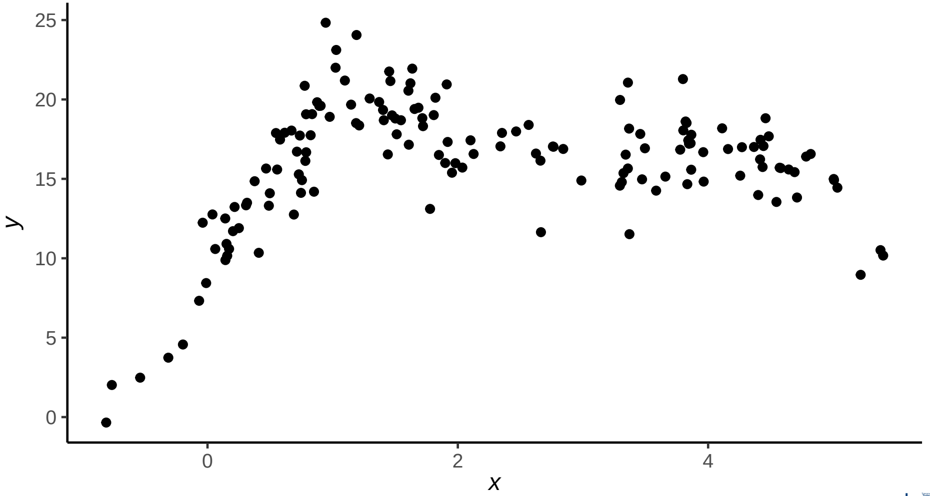
$$\mathrm{E}\big(f(x) \mid \mathbf{y}\big) = f_0(x) + \sum_{i=1}^n h(x, x_i)\hat{w}_i \tag{4}$$

$$\mathrm{Cov}\big(f(x), f(x') \mid \mathbf{y}\big) = \sum_{i=1}^n \sum_{j=1}^n \big(\mathbf{V}_y^{-1}\big)_{ij} h(x, x_i) h(x', x_j) \tag{5}$$

where $\hat{w}_1, \dots, \hat{w}_n$ are given by $\hat{\mathbf{w}} := \mathrm{E}\big(\mathbf{w} \mid \mathbf{y}\big) = \mathbf{\Psi H V}_y^{-1}(\mathbf{y} - \mathbf{f}_0)$.

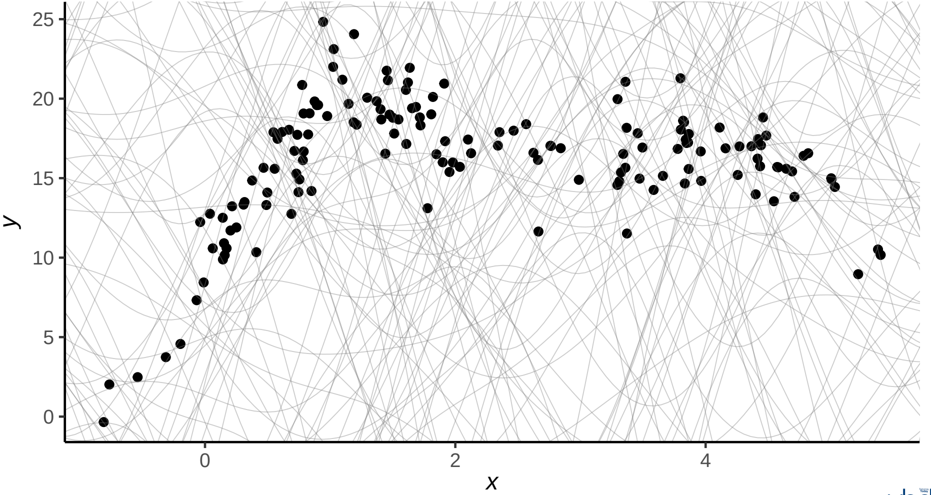
Illustration

Observations $\{(y_i, x_i) \mid y_i, x_i \in \mathbb{R}\ \forall i = 1, \ldots, n\}$.



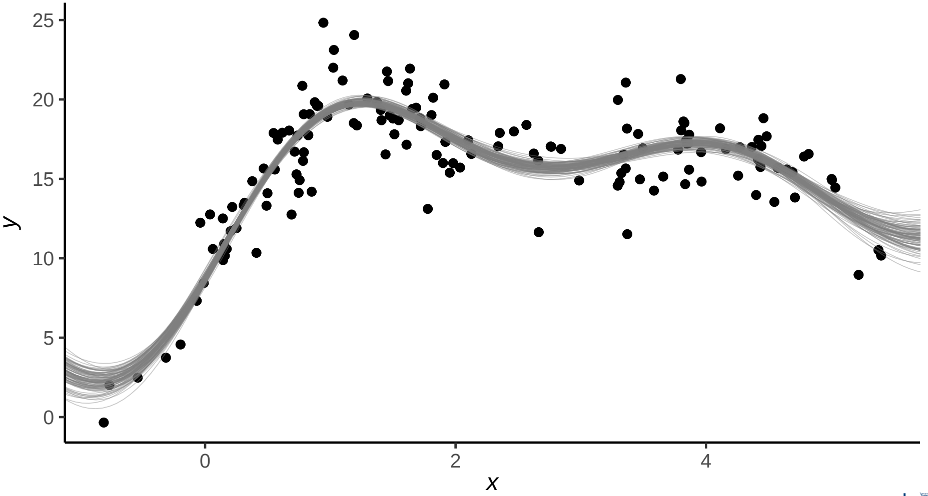
Illustration

Choose $h(x, x') = e^{-\frac{\|x-x'\|^2}{2}}$ (Gaussian kernel). Sample paths from I-prior:



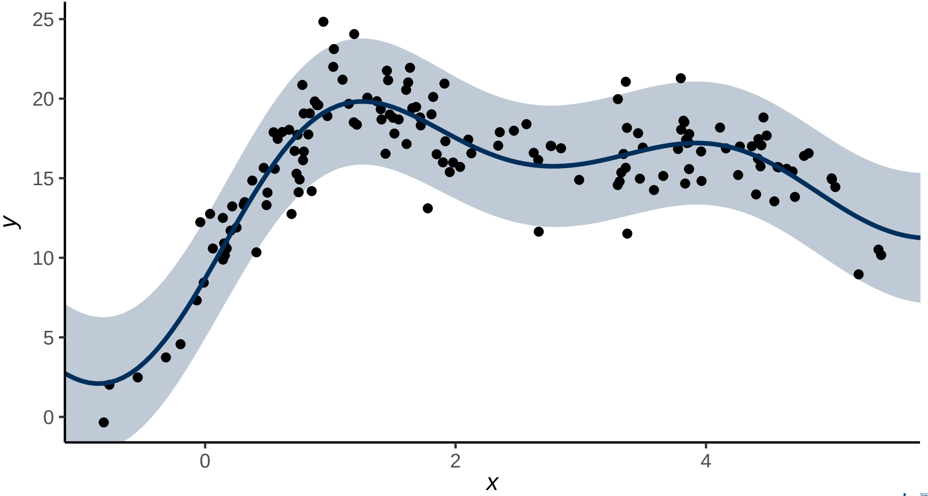
Illustration

Sample paths from the posterior of f:



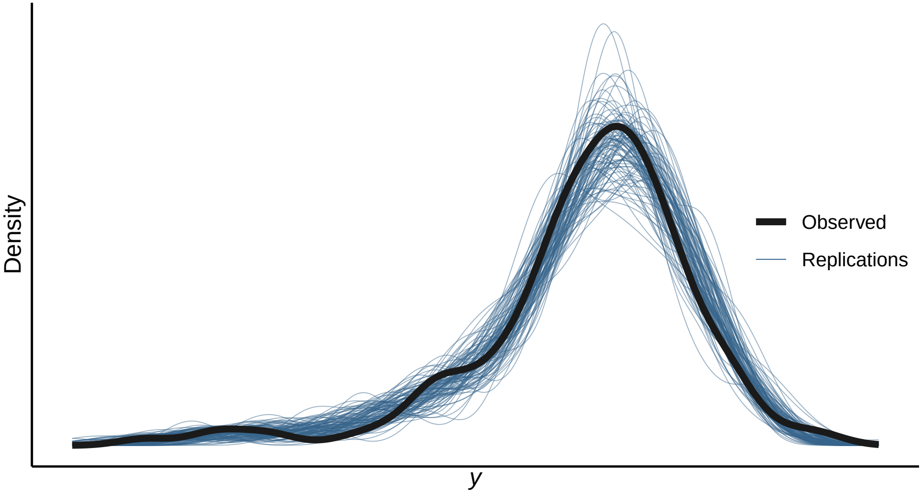
Illustration

Posterior mean estimate for $y = f(x)$ and its 95% credibility interval:



Illustration

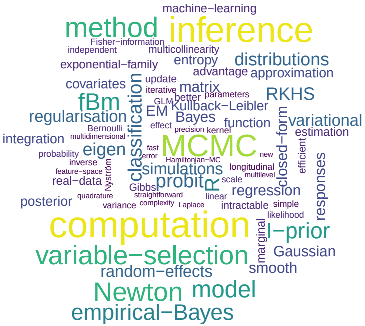
Other Bayesian stuff e.g. posterior predictive checks for $\{y_1, \ldots, y_n\}$:



Why I-priors?

Highlights

- An objective, data-driven prior. No user input required.
- The I-prior is proper; posterior estimates are thus *admissible*.
- Intuitive regression approach–model purpose is effected by kernel choices.



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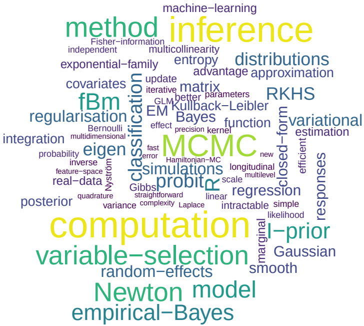

Competitors:

- Tikhonov regulariser (e.g. cubic spline smoother)

$$\hat{f} = \arg\min_f \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \int f''(x)^2 \, \mathrm{d}x$$

- Gaussian process regression (Rasmussen & Williams, 2006)

State of the art

Professor Wicher Bergsma
London School of Economics and Political Science

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Introduction

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Reproducing kernel Hilbert spaces
The Fisher information
The I-prior

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Reproducing kernel Hilbert spaces

Assumption: $f \in \mathcal{F}$ *where* $\mathcal{F}$ *is an RKHS with kernel* h *over* $\mathcal{X}$.

Definition 3 (Hilbert spaces)

A *Hilbert space* $\mathcal{F}$ is a vector space equipped with a positive definite inner product $\langle \cdot, \cdot \rangle_{\mathcal{F}} : \mathcal{F} \times \mathcal{F} \to \mathbb{R}$.

Definition 4 (Reproducing kernels)

A symmetric, bivariate function $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a *kernel*, and it is a *reproducing kernel* of $\mathcal{F}$ if h satisfies

i. $\forall x \in \mathcal{X}$, $h(\cdot, x) \in \mathcal{F}$;
ii. $\forall x \in \mathcal{X}$ and $\forall f \in \mathcal{F}$, $\langle f, h(\cdot, x) \rangle_{\mathcal{F}} = f(x)$.

In particular, $\forall x, x' \in \mathcal{F}$, $h(x, x') = \langle h(\cdot, x), h(\cdot, x') \rangle_{\mathcal{F}}$.

Reproducing kernel Hilbert spaces (cont.)

Theorem 5 (Moore-Aronszajn, etc.)

There is a bijection between

i. the set of positive definite functions; and
ii. the set of RKHSs.

Reproducing kernel Hilbert spaces (cont.)

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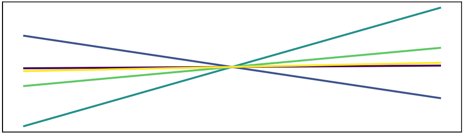
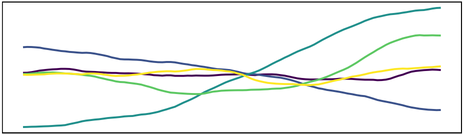
$h(x, x') = 1$ (constant)

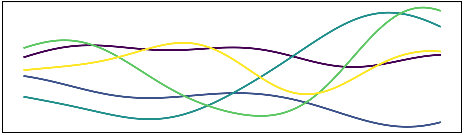
$h(x, x') = \langle x, x' \rangle_{\mathcal{X}}$ (linear)



$h(x, x') = -\frac{1}{2}(\|x - x'\|_{\mathcal{X}}^{2\gamma} - \|x\|_{\mathcal{X}}^{2\gamma} - \|x'\|_{\mathcal{X}}^{2\gamma})$ (fBm)



$h(x, x') = \exp\left(-\frac{\|x-x'\|_{\mathcal{X}}^{2\gamma}}{2s^2}\right)$ (Gaussian)



Building more complex RKHSs

We can build complex RKHSs by adding and multiplying kernels:

- $\mathcal{F} = \mathcal{F}_1 \oplus \mathcal{F}_2$ is an RKHS defined by $h = h_1 + h_2$.
- $\mathcal{F} = \mathcal{F}_1 \otimes \mathcal{F}_2$ is an RKHS defined by $h = h_1 h_2$.

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Example 6 (ANOVA RKHS)

Consider RKHSs $\mathcal{F}_k$ with kernel h_k, $k = 1, \dots, p$. The ANOVA kernel over the set $\mathcal{X} = \mathcal{X}_1 \times \cdots \times \mathcal{X}_p$ defining the ANOVA RKHS $\mathcal{F}$ is

$$h(x, x') = \prod_{k=1}^{p} \big(1 + h_k(x, x')\big).$$

For $p = 2$ let $\mathcal{F}_k$ be linear RKHS of functions over $\mathbb{R}$. Then $f \in \mathcal{F}$ where $\mathcal{F} = \mathcal{F}_\emptyset \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \mathcal{F}_1 \otimes \mathcal{F}_2$ are of the form

$$f(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2.$$

The Fisher information

For the normal model (1), the log-likelihood of f is given by

$$\ell(f|y) = \text{const.} - \frac{1}{2}\sum_{i=1}^n\sum_{j=1}^n \psi_{ij}\big(y_i - \langle f, h(\cdot, x_i)\rangle_{\mathcal{F}}\big)\big(y_j - \langle f, h(\cdot, x_j)\rangle_{\mathcal{F}}\big)$$

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Variational calculus leads us to the following result:

Lemma 7 (Fisher information for regression function)

The Fisher information for f is

$$\mathcal{I}_f = -\operatorname{E}\nabla^2 \ell(f|y) = \sum_{i=1}^n\sum_{j=1}^n \psi_{ij} h(\cdot, x_i) \otimes h(\cdot, x_j)$$

where '$\otimes$' is the tensor product of two vectors in $\mathcal{F}$.

The Fisher information (cont.)

It's helpful to think of $\mathcal{I}_f$ as a bilinear form $\mathcal{I}_f : \mathcal{F} \times \mathcal{F} \to \mathbb{R}$, making it possible to compute the Fisher information on linear functionals $f_g = \langle f, g \rangle_{\mathcal{F}}, \forall g \in \mathcal{F}$ as $\mathcal{I}_{f_g} = \langle \mathcal{I}_f, g \otimes g \rangle_{\mathcal{F} \otimes \mathcal{F}}$.

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In particular, between two points $f_x := f(x)$ and $f_{x'} := f(x')$ we have:

$$
\begin{aligned}
\mathcal{I}_f(x, x') &= \big\langle \mathcal{I}_f, h(\cdot, x) \otimes h(\cdot, x') \big\rangle_{\mathcal{F} \otimes \mathcal{F}} \\
&= \left\langle \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} h(\cdot, x_i) \otimes h(\cdot,_j) \ , \ h(\cdot, x) \otimes h(\cdot, x') \right\rangle_{\mathcal{F} \otimes \mathcal{F}} \\
&= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} \left\langle h(\cdot, x), h(\cdot, x_i) \right\rangle_\mathcal{F} \left\langle h(\cdot, x'), h(\cdot, x_j) \right\rangle_\mathcal{F}
\end{aligned}
$$

$$
\boxed{= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} h(x, x_i) h(x', x_j) =: k(x, x')} \qquad \text{(from 3)}
$$

The I-prior

Lemma 8

The kernel (3) induces a finite-dimensional RKHS $\mathcal{F}_n < \mathcal{F}$, consisting of functions of the form $\tilde{f}(x) = \sum_{i=1}^n h(x, x_i) w_i$ (for some real-valued w_is) equipped with the squared norm

$$\|\tilde{f}\|^2_{\mathcal{F}_n} = \sum_{i,j=1}^n \psi^-_{ij} w_i w_j,$$

where ψ^-_{ij} is the (i,j)th entry of Ψ^{-1}.

- Let $\mathcal{R}$ be the orthogonal complement of $\mathcal{F}_n$ in $\mathcal{F}$. Then $\mathcal{F} = \mathcal{F}_n \oplus \mathcal{R}$, and any $f \in \mathcal{F}$ can be uniquely decomposed as $f = \tilde{f} + r$, with $\tilde{f} \in \mathcal{F}_n$ and $r \in \mathcal{R}$.
- The Fisher information for g is zero iff $g \in \mathcal{R}$. The data only allows us to estimate $f \in \mathcal{F}$ by considering functions in $\tilde{f} \in \mathcal{F}_n$.

The I-prior (cont.)

Theorem 9 (I-prior)

Let ν be a volume measure induced by the norm above, and let

$$\tilde{p} = \arg\max_p \left\{ -\int_{\mathcal{F}_n} p(f) \log p(f) \, \nu(\mathrm{d}f) \right\}$$

subject to the constraint

$$\mathrm{E}_{f \sim p} \|f - f_0\|^2_{\mathcal{F}_n} = \text{constant}, \qquad f_0 \in \mathcal{F}.$$

Then $\tilde{p}$ is the Gaussian with mean f_0 and covariance function $k(x, x')$.

Equivalently, under the I-prior, f can be written in the form

$$f(x) = f_0(x) + \sum_{i=1}^n h(x, x_i) w_i, \qquad (w_1, \ldots, w_n)^\top \sim \mathrm{N}(0, \Psi)$$

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Model hyperparameters

$$
\begin{aligned}
y_i &= f_0(x_i) + \sum_{j=1}^n h_\lambda(x_i, x_j) w_j + \epsilon_i \\
(\epsilon_1, \dots, \epsilon_n)^\top &\sim \mathrm{N}_n(0, \boldsymbol{\Psi}^{-1}) \\
(w_1, \dots, w_n)^\top &\sim \mathrm{N}_n(0, \boldsymbol{\Psi})
\end{aligned}
\tag{6}
$$

A number of hyperparameters remain undetermined.

Model hyperparameters

$$\begin{gathered} y_i = f_0(x_i) + \sum_{j=1}^n h_\lambda(x_i, x_j) w_j + \epsilon_i \\ (\epsilon_1, \dots, \epsilon_n)^\top \sim \mathrm{N}_n(0, \boldsymbol{\Psi}^{-1}) \\ (w_1, \dots, w_n)^\top \sim \mathrm{N}_n(0, \boldsymbol{\Psi}) \end{gathered} \tag{6}$$

A number of hyperparameters remain undetermined. Further assumptions:

1. The error variance $\boldsymbol{\Psi}$ is known up to a low-dimensional parameter, e.g. $\boldsymbol{\Psi} = \psi \mathbf{I}_n$, $\psi > 0$ (iid errors).

[1] This necessitates the use of reproducing kernel Krein spaces, as the kernels may no longer be positive definite.

Model hyperparameters

$$\begin{aligned} y_i &= f_0(x_i) + \sum_{j=1}^n h_\lambda(x_i, x_j) w_j + \epsilon_i \\ (\epsilon_1, \dots, \epsilon_n)^\top &\sim \mathrm{N}_n(0, \boldsymbol{\Psi}^{-1}) \\ (w_1, \dots, w_n)^\top &\sim \mathrm{N}_n(0, \boldsymbol{\Psi}) \end{aligned} \tag{6}$$

A number of hyperparameters remain undetermined. Further assumptions:

1. The error variance $\boldsymbol{\Psi}$ is known up to a low-dimensional parameter, e.g. $\boldsymbol{\Psi} = \psi \mathbf{I}_n$, $\psi > 0$ (iid errors).
2. Each RKHS $\mathcal{F}$ is defined by the kernel $h_\lambda = \lambda \tilde{h}$, where $\lambda \in \mathbb{R}$ is a scale[1] parameter.

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3. Certain kernels also require tuning, e.g. the Hurst coefficient of the fBm or the lengthscale of the Gaussian. For now, assume fixed.

---

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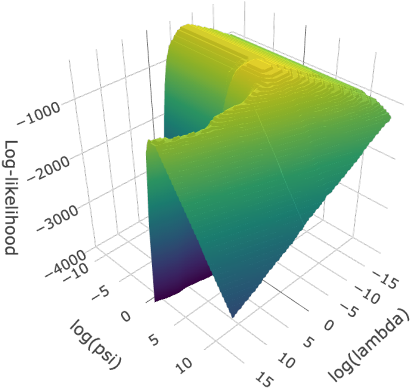
Direct optimisation of (marginal) log-likelihood

The marginal log-likelihood of $(\lambda, \boldsymbol{\Psi})$ is

$$\ell(\lambda, \boldsymbol{\Psi} \mid \mathbf{y}) = \text{const.} - \frac{1}{2}\log|\mathbf{V}_y| - \frac{1}{2}(\mathbf{y} - \mathbf{f}_0)^\top \mathbf{V}_y^{-1}(\mathbf{y} - \mathbf{f}_0),$$



- Direct optimisation using e.g. conjugate gradients or Newton methods.
- Numerical stability issues–workaround: Cholesky or eigen decomposition.
- Prone to local optima.
- Possible to also optimise kernel hyperparameters.

EM algorithm

An alternative view of the model:

$$\begin{aligned} \mathbf{y} \mid \mathbf{w} &\sim \mathrm{N}_n(\mathbf{f}_0 + \mathbf{H}_\lambda \mathbf{w}, \boldsymbol{\Psi}^{-1}) \\ \mathbf{w} &\sim \mathrm{N}_n(\mathbf{0}, \boldsymbol{\Psi}) \end{aligned}$$

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in which the $\mathbf{w}$ are "missing". The full data log-likelihood is

$$\begin{aligned} L(\lambda, \boldsymbol{\Psi} \mid \mathbf{y}, \mathbf{w}) = \text{const.} - \frac{1}{2}(\mathbf{y} - \mathbf{f}_0)^\top \boldsymbol{\Psi} (\mathbf{y} - \mathbf{f}_0) - \frac{1}{2} \operatorname{tr}\left(\mathbf{V}_y \mathbf{w}\mathbf{w}^\top\right) \\ + (\mathbf{y} - \mathbf{f}_0)^\top \boldsymbol{\Psi} \mathbf{H}_\lambda \mathbf{w} \end{aligned}$$

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The E-step entails computing

$$Q_t(\lambda, \boldsymbol{\Psi}) = \mathrm{E}\left\{ L(\lambda, \boldsymbol{\Psi} \mid \mathbf{y}, \mathbf{w}) \,\middle|\, \mathbf{y}, \lambda^{(t)}, \boldsymbol{\Psi}^{(t)} \right\}$$

in which the following posterior quantities are needed

$$\hat{\mathbf{w}} := \mathrm{E}(\mathbf{w} \mid \mathbf{y}, \lambda, \boldsymbol{\Psi}) \quad \text{and} \quad \hat{\mathbf{W}} := \mathrm{E}(\mathbf{w}\mathbf{w}^\top \mid \mathbf{y}, \lambda, \boldsymbol{\Psi}) = \mathbf{V}_y^{-1} + \hat{\mathbf{w}}\hat{\mathbf{w}}^\top.$$

EM algorithm (cont.)

Let $\tilde{\mathbf{w}}^{(t)}$and $\tilde{\mathbf{W}}^{(t)}$ be versions of $\hat{\mathbf{w}}$ and $\hat{\mathbf{W}}$ computed using $\lambda^{(t)}$ and $\boldsymbol{\Psi}^{(t)}$. The M-step entails solving

$$\begin{aligned}
\frac{\partial Q_t}{\partial \lambda} &= -\frac{1}{2}\operatorname{tr}\left(\frac{\partial \mathbf{V}_y}{\partial \lambda}\tilde{\mathbf{W}}^{(t)}\right) + (\mathbf{y}-\mathbf{f}_0)^\top \boldsymbol{\Psi}\frac{\partial \mathbf{H}_\lambda}{\partial \lambda}\tilde{\mathbf{w}}^{(t)} &= 0 \\
\frac{\partial Q_t}{\partial \psi} &= -\frac{1}{2}\operatorname{tr}\left(\frac{\partial \mathbf{V}_y}{\partial \psi}\tilde{\mathbf{W}}^{(t)}\right) - \frac{1}{2}(\mathbf{y}-\mathbf{f}_0)^\top \left(\mathbf{y}-\mathbf{f}_0 - 2\mathbf{H}_\lambda \tilde{\mathbf{w}}^{(t)}\right) &= 0
\end{aligned}$$

- This scheme admits a closed-form solution for ψ and (sometimes) for λ too (e.g. linear addition of kernels $h_\lambda = \lambda_1 h_1 + \cdots + \lambda_p h_p$).
- Sequential updating $\lambda^{(t)} \to \boldsymbol{\Psi}^{(t+1)} \to \lambda^{(t+1)} \to \cdots$ (expectation conditional maximisation, Meng and Rubin, 1993).
- Computationally unattractive for optimising kernel hyperparameters.

Computational bottleneck

In either estimation method, V_y^{-1} is computed and takes $O(n^3)$ time.

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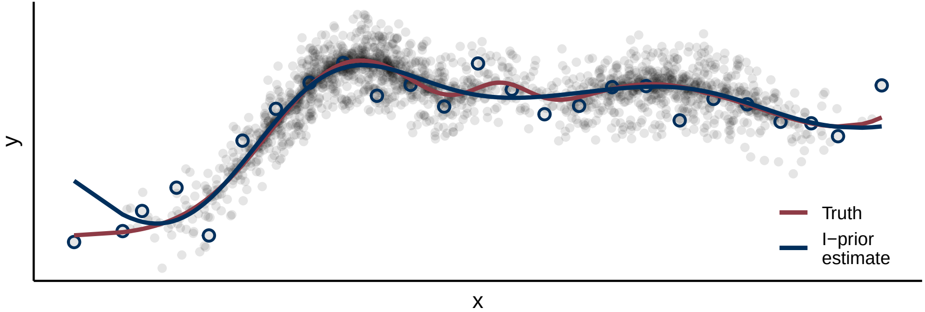


Trick: low-rank matrix approximations. Suppose $H \approx QQ^\top$, where $Q \in \mathbb{R}^{n \times m}$, $m \ll n$. Then, using the Woodbury matrix identity,

$$V_y^{-1} = (H\Psi H + \Psi^{-1})^{-1} \approx \Psi - \Psi Q\big((Q^\top \Psi Q)^{-1} + Q^\top \Psi Q\big)^{-1} Q^\top \Psi$$

is a much cheaper $O(nm^2)$ operation (Williams & Seeger, 2001).

Introduction

Regression using I-priors

Estimation

Data examples
- Longitudinal analysis
- Predicting fat content

Conclusions & further work

Longitudinal analysis of cow growth data

Aim: Discern whether there is a difference between two treatments given to cows, and whether this effect varies among individual cows.

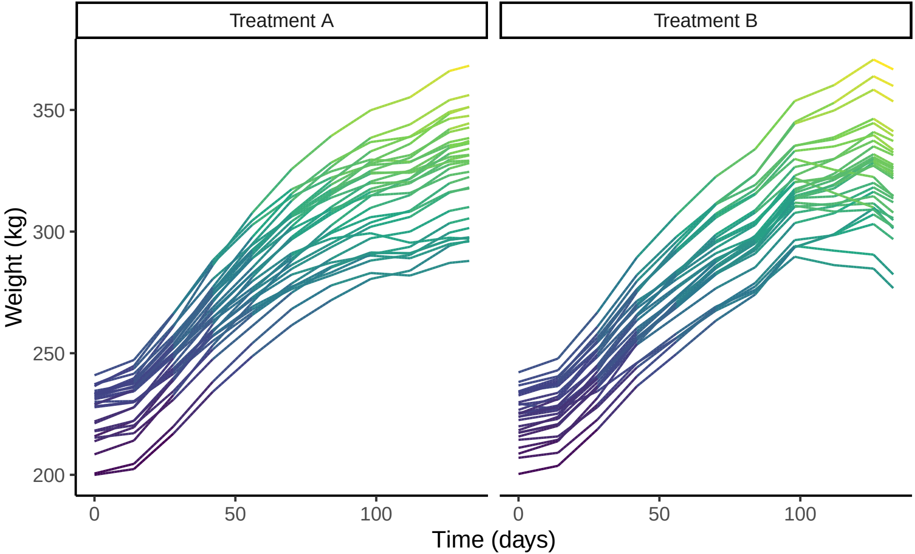
Data consists of a balanced longitudinal set of weights y_{it} for 60 cows. The herd were randomly split between two treatment groups (x_i). Model

$$y_{it} = f_{1t}(i) + f_{2t}(x_i) + f_{12t}(i, x_i) + \epsilon_{it}$$

assuming smooth effect of time, and nominal effect of cow index and treatment group.

	Explanation	Model	Log-lik.	No. of param.
1	Growth due to time only	$\emptyset$	-2792.8	2
2	Growth due to cows only	f_{1t}	-2792.2	3
3	Growth due to treatment only	f_{2t}	-2295.2	3
4	Growth due to both	$f_{1t} + f_{2t}$	-2270.9	4
5	Growth due to both with cow-treatment variation	$f_{1t} + f_{2t} + f_{12t}$	-2250.9	4

Growth curve



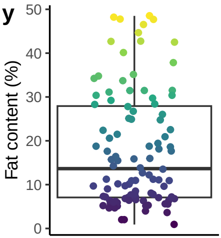
Predicting fat content in meat samples

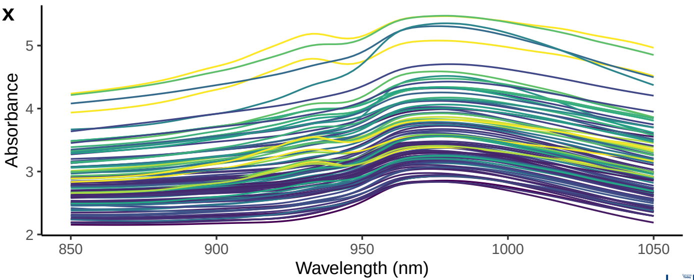
Aim: Predict fat content of meat samples from its spectrometric curves (Tecator data set).

For each meat sample i, data consist of 100 channel spectrum of absorbances $(x_i(t))$ and its corresponding fat content (y_i). Train/test split is $160 + 55$. Model

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

where x_i is the ith spectral curve.





Results

Model	RMSE Train	RMSE Test
I-prior		
Linear	2.89	2.89
Quadratic	0.72	0.97
Smooth (fBm-0.70)	0.19	0.63
Others		
Linear functional regression		2.78
Quadratic functional regression		0.80
Gaussian process regression		2.06
Neural networks		0.36
Kernel smoothing		1.49
Multivariate adaptive regression splines (MARS)		0.88
Functional additive regression (CSEFAM)		0.85

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Summary

A novel methodology for fitting a wide range of parameteric and nonparametric regression models.

- Parsimonious model specification and simple estimation.
- Inference is straightforward.
- Often yield comparable predictions to competing ML algorithms.

Further work

- Extension to non-Gaussian errors (e.g. classification or count data).
- $O(n^3)$ computational bottleneck.

End

Thank you!

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