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Regression modelling using I-priors

NUS Department of Statistics & Data Science Seminar

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Overview

Introduction

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

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

where each $y_i \in \mathbb{R}$, $x_i \in \mathcal{X}$ (some set of covariates), and f is a regression function. This forms the basis for a multitude of statistical models:

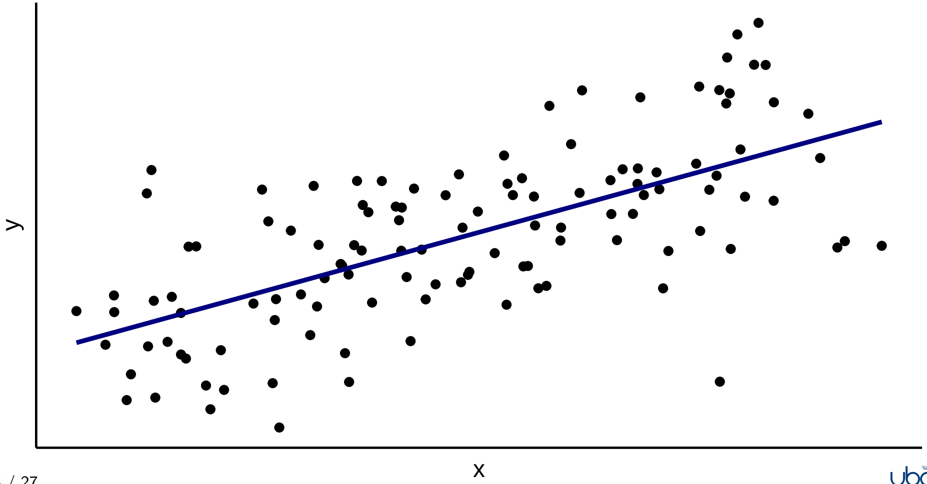
1. Ordinary linear regression when f is parameterised linearly.
2. Varying intercepts/slopes model when $\mathcal{X}$ is grouped.
3. Smoothing models when f is a smooth function.
4. Functional regression when $\mathcal{X}$ is functional.

Goal

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

Ordinary linear regression

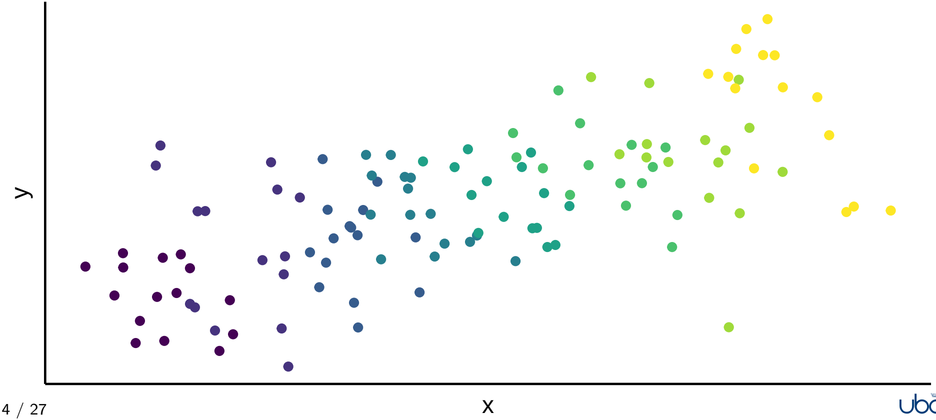
Suppose $f(x_i) = x_i^\top \beta$ for $i = 1, \dots, n$, where $x_i, \beta \in \mathbb{R}^p$.



Varying intercepts/slopes model

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

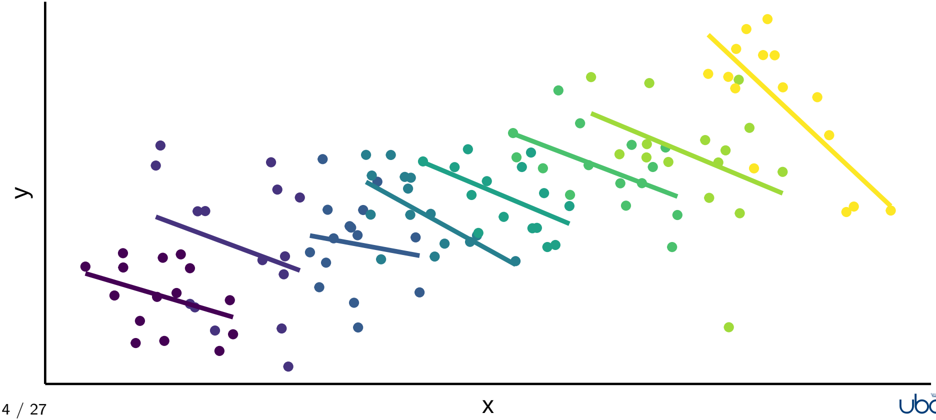
$$f(x_{kj}, j) = f_1(x_{kj}) + f_2(j) + f_{12}(x_{kj}, j).$$



Varying intercepts/slopes model

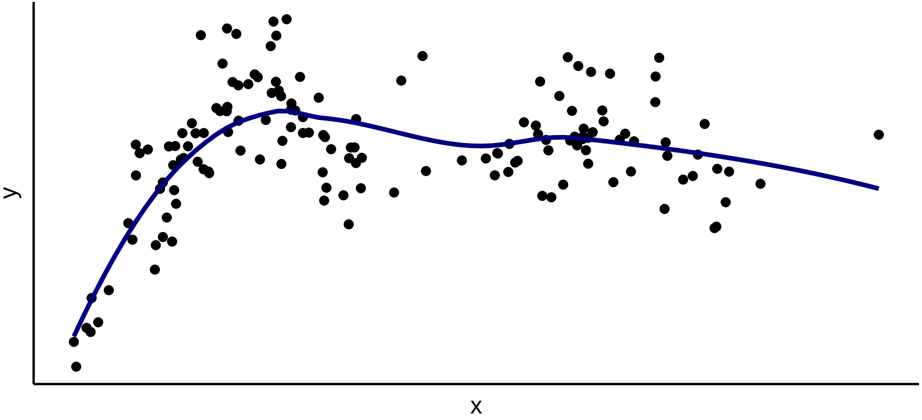
Suppose each unit $i = 1, \dots, n$ relates to the kth observation in group $j \in \{1, \dots, m\}$. Model the function f additively:

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



Smoothing models

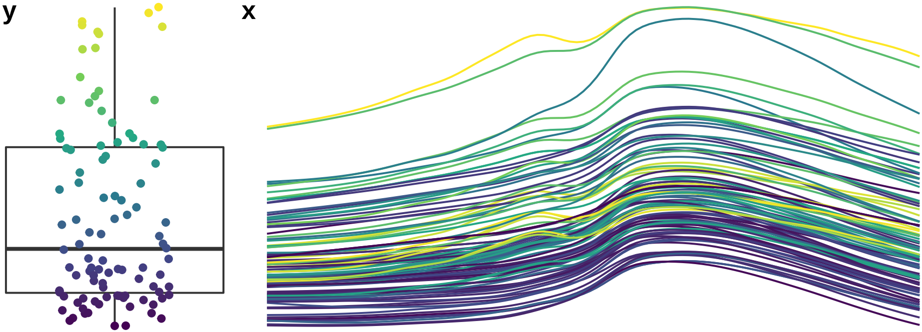
Suppose $f \in \mathcal{F}$ where $\mathcal{F}$ is a space of "smoothing functions" (models like LOESS, kernel regression, smoothing splines, etc.).



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

Definition 1 (I-prior)

The entropy maximising prior distribution for f, subject to constraints, is

$$f(x) = \sum_{i=1}^{n} h(x, x_i) w_i \\ (w_1, \dots, w_n)^\top \sim \mathrm{N}_n(0, \Psi) \tag{2}$$

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

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

which happens to be **Fisher information** between two linear forms 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 (and vice versa).

The I-prior (cont.)

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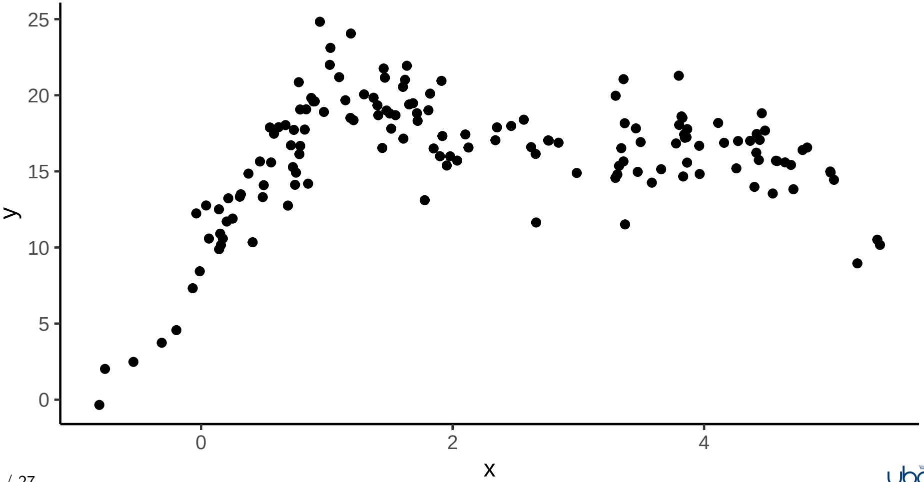
Of interest then are

1. Posterior distribution for the regression function,
$$p(f \mid y) = \frac{p(y \mid f)p(f)}{\int p(y \mid f)p(f) \, \mathrm{d} f}.$$
2. Posterior predictive distribution (given a new data point x_{new})
$$p(y_{new} \mid \mathbf{y}) = \int p(y_{new} \mid f_{new}) p(f_{new} \mid \mathbf{y}) \, \mathrm{d} f_{new},$$
where $f_{new} = f(x_{new})$.

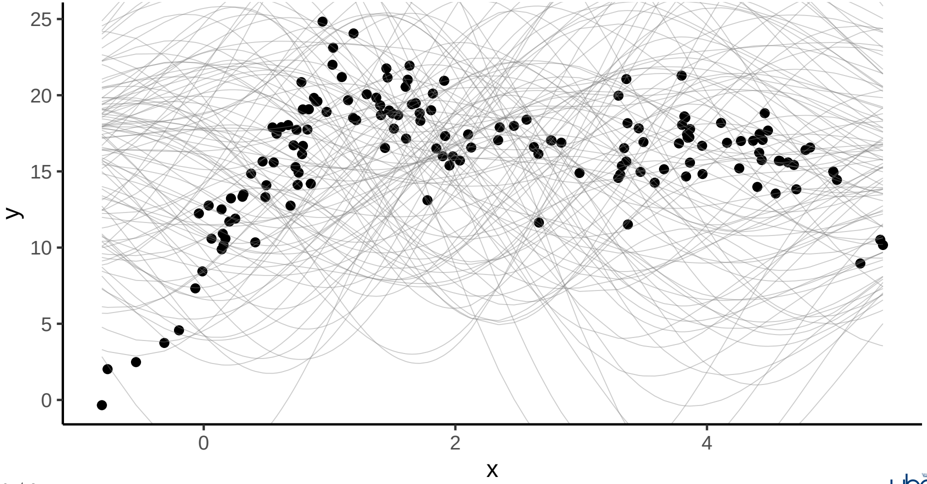
Introduction (cont.)

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



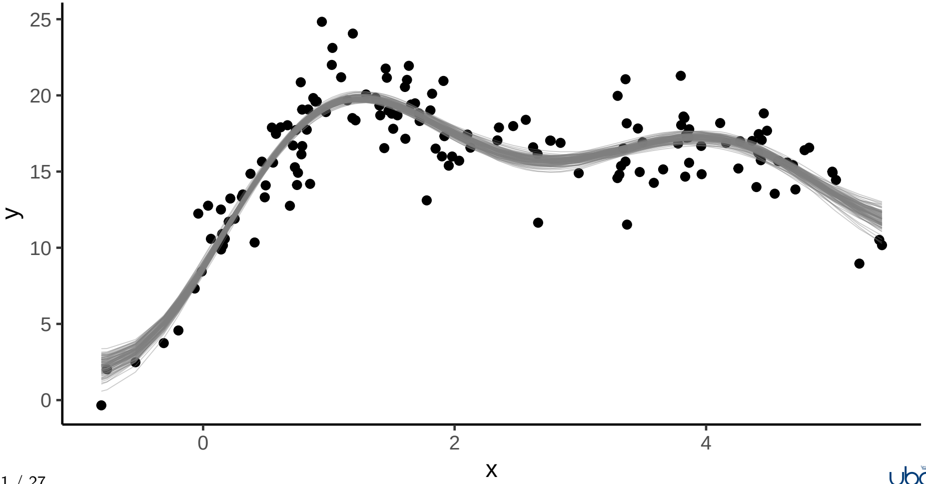
Introduction (cont.)

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



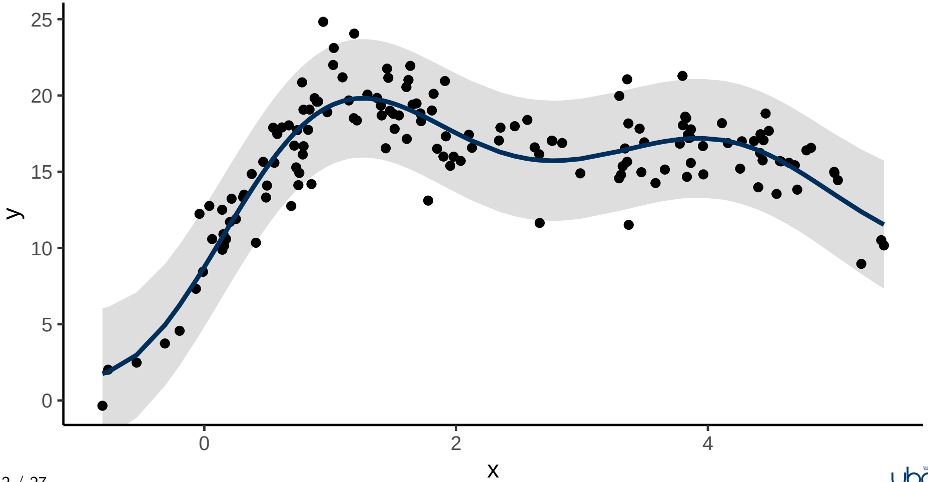
Introduction (cont.)

Sample paths from the posterior of f:



Introduction (cont.)

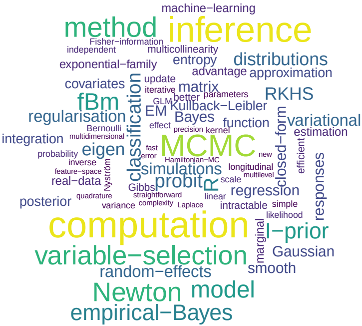
Posterior mean estimate for $y = f(x)$ and its 95% credibility interval.



Why I-priors?

Advantages

- Provides a unifying methodology for regression.
- Simple and parsimonious model specification and estimation.
- Often yield comparable (or better) predictions than competing ML algorithms.



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

State of the art

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London School of Economics and Political Science

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Reproducing kernel Hilbert spaces

Assumption: Let $f \in \mathcal{F}$ be an RKHS with kernel h over a set $\mathcal{X}$.

Definition 2 (Hilbert spaces)

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

Definition 3 (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 $\forall x \in \mathcal{X}$,

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

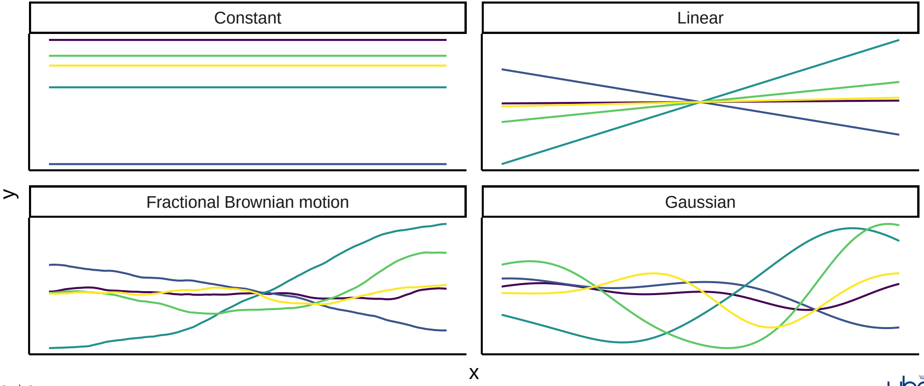
In particular, $\forall x, x' \in \mathcal{F}$, $h(x, x') = \langle h(\cdot, x), h(\cdot, x') \rangle_{\mathcal{F}}$.

Reproducing kernel Hilbert spaces (cont.)

Theorem 4

There is a bijection between

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



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 $h = h_1 h_2$.

Example 5 (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 regression model (1), the log-likelihood of f is given by

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

Lemma 6 (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 $\mathcal{I}_{f_g} = \langle \mathcal{I}_f, g \otimes g \rangle_{\mathcal{F} \otimes \mathcal{F}}$.

In particular, between two points $f_x := f(x)$ and $f_{x'} := f(x')$ [since $f_x = \langle f, h(\cdot, x) \rangle_{\mathcal{F}}$] we have:

$$\begin{aligned}
\mathcal{I}_f(x, x') &= \big\langle \mathcal{I}_f, h(\cdot, x) \otimes h(\cdot, x') \big\rangle_{\mathcal{F} \otimes \mathcal{F}} \\
&= \left\langle \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} h(\cdot, x_i) \otimes h(\cdot,_j) \ , \ h(\cdot, x) \otimes h(\cdot, x') \right\rangle_{\mathcal{F} \otimes \mathcal{F}} \\
&= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} \left\langle h(\cdot, x), h(\cdot, x_i) \right\rangle_{\mathcal{F}} \left\langle h(\cdot, x'), h(\cdot, x_j) \right\rangle_{\mathcal{F}} \\
&= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} h(x, x_i) h(x', x_j) =: k(x, x')
\end{aligned} \tag{3}$$

The I-prior

Lemma 7

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 8 (I-prior)

Let ν be a volume measure induced by the norm above. The solution to

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

subject to the constraint

$$\mathrm{E}_{f \sim p} \|f\|^2_{\mathcal{F}_n} = \text{constant}$$

is the Gaussian distribution whose covariance function is $k(x, x')$.

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

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

Posterior regression function

Lemma 9

Under the normal model (1) subject to the I-prior, the posterior distribution of $f(x)$ is given by

Parameters of the model

$$
\begin{aligned}
y_i &= f_0(x_i) + \lambda \sum_{j=1}^n h(x_i, x_j) w_j + \epsilon_i \\
(\epsilon_1, \dots, \epsilon_n)^\top &\sim \mathrm{N}_n(0, \boldsymbol{\Psi}^{-1}) \\
(w_1, \dots, w_n)^\top &\sim \mathrm{N}_n(0, \boldsymbol{\Psi})
\end{aligned}
\tag{4}
$$

Further assumptions

1. The error variance Ψ is known up to a low-dimensional parameter, e.g. $\boldsymbol{\Psi} = \psi \mathbf{I}_n$, $\psi > 0$.
2. Each RKHS $\mathcal{F}$ of function is defined by the kernel $h_\lambda = \tilde{h}$, where $\lambda \in \mathbb{R}$ is a scale[1] parameter.
3. Certain kernels also require parameters themselves, e.g. the Hurst coefficient of the fBm or the lengthscale of the Gaussian kernel.
4. A prior mean function $f_0(x)$ may be set by the user.

[1] This necessitates the use of reproducing kernel Krein spaces.

Marginal likelihood

Denote by

- $\mathbf{y} = (y_1, \dots, y_n)^\top$
- $\mathbf{f} = \big(f(x_1), \dots, f(x_n)\big)^\top$
- $\mathbf{f}_0 = \big(f_0(x_1), \dots, f_0(x_n)\big)^\top$
- $\mathbf{w} = (w_1, \dots, w_n)^\top$
- $\mathbf{H}_\lambda = \big(h_\lambda(x_i, x_j)\big)_{i,j=1}^n \in \mathbb{R}^{n \times n}$

(1) + an I-prior on f implies

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

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

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

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

- Direct optimisation using e.g. conjugate gradients or Newton methods.
- Numerical stability issues (workaround: Cholesky or eigen decomp.).
- Prone to local optima.

EM algorithm

An alternative view of the model:

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

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

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

Choose starting values $\lambda^{(0)}$ and $\boldsymbol{\Psi}^{(0)}$. The E-step entails computing

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

EM algorithm (cont.)

The following quantities are needed and are easily obtained:

$$\tilde{\mathbf{w}} := \mathrm{E}(\mathbf{w} \mid \mathbf{y}, \lambda, \boldsymbol{\Psi}) \qquad \text{and} \qquad \tilde{\mathbf{W}} := \mathrm{E}(\mathbf{w}\mathbf{w}^\top \mid \mathbf{y}, \lambda, \boldsymbol{\Psi}) = \tilde{\mathbf{V}_w} + \tilde{\mathbf{w}}\tilde{\mathbf{w}}^\top$$

Supposing $\boldsymbol{\Psi}$ but not $\mathbf{H}_\lambda$ depends on ψ; and $\mathbf{H}_\lambda$ depends on λ but not ψ, the M-step entails solving the following equations set to zero:

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

- 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).

Further research

Hello

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