

# Regression modelling using I-priors

NUS Department of Statistics & Data Science Seminar

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### **Overview**

Introduction

#### Introduction

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

#### Estimation

Parameters of the model

#### Examples

Further research



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

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

$$(\epsilon_1, \dots, \epsilon_n)^{\top} \sim N_n(0, \Psi^{-1})$$
(1)

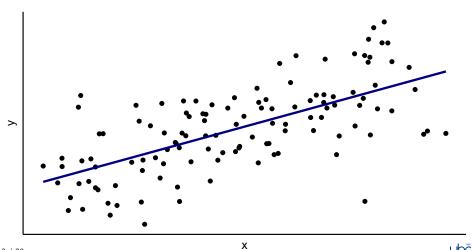
where each  $y_i \in \mathbb{R}$ ,  $x_i \in \mathcal{X}$  (some set of covariates), and f is a regression function. This forms the basis for a multitude of statistical models:

- 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  $\{(y_i, x_i)\}_{i=1}^n$ .

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



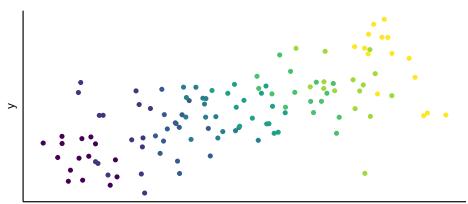
Introduction

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# 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:

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

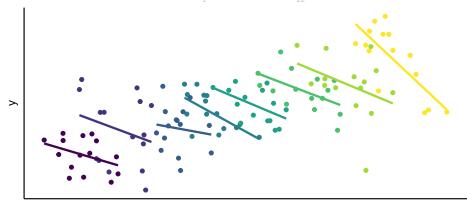


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# Varying intercepts/slopes model

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

$$f(x_{kj},j) = \underbrace{x_{kj}^{\top} \beta_{1}}_{f_{1}} + \underbrace{\beta_{0j}}_{f_{2}} + \underbrace{x_{kj}^{\top} \beta_{1j}}_{f_{12}}$$



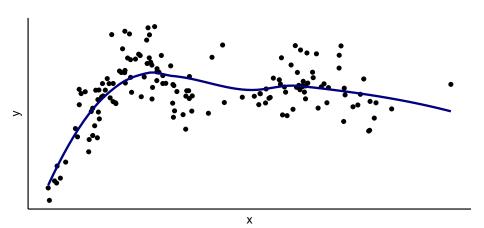
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# **Smoothing models**

Introduction

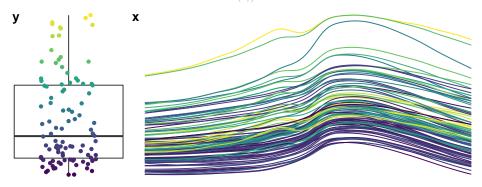
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Suppose  $f \in \mathcal{F}$  where  $\mathcal{F}$  is a space of "smoothing functions" (models like LOESS, kernel regression, smoothing splines, etc.).



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

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



# 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

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

$$(w_1, \dots, w_n)^{\top} \sim N_n(0, \Psi)$$
(2)

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

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

which happens to be **Fisher information** between two linear forms of f.

# The I-prior (cont.)

#### Interpretation:

Introduction

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

 $1. \ \ Posterior \ distribution \ for \ the \ regression \ function,$ 

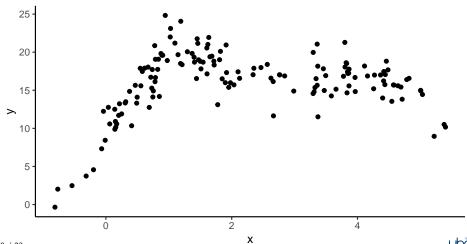
$$p(f|y) = \frac{p(y|f)p(f)}{\int p(y|f)p(f) df}.$$

2. Posterior predictive distribution (given a new data point  $x_{new}$ )

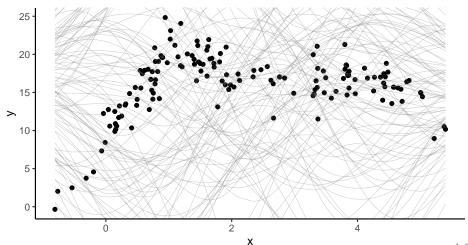
$$p(y_{new} \mid \mathbf{y}) = \int p(y_{new} \mid f_{new}) p(f_{new} \mid \mathbf{y}) \, \mathrm{d}f_{new},$$

where  $f_{new} = f(x_{new})$ .

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



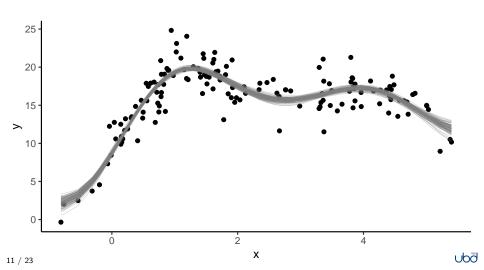
Choose  $h(x, x') = e^{-\frac{\|x - x'\|^2}{2s^2}}$  (Gaussian kernel). Sample paths from I-prior:



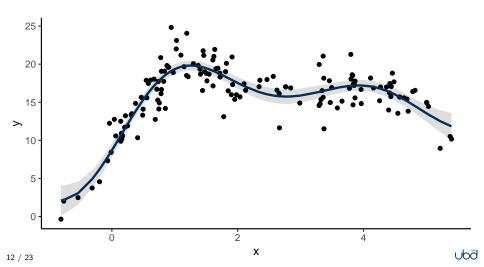
Introduction

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Sample paths from the posterior of f:



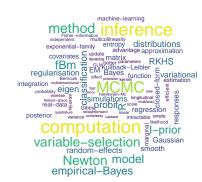
Posterior mean estimate for y = f(x) and its 95% credibility interval.



# 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)

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

Gaussian process regression



### State of the art

Introduction

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Professor Wicher Bergsma London School of Economics and Political Science

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- 3. Jamil, H., & Bergsma, W. (2019). iprior: An R Package for Regression Modelling using I-priors. arXiv:1912.01376 [stat]
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Regression using I-priors
Reproducing kernel Hilbert spaces
The Fisher information
The I-prior

Estimation

Examples

Further research

# 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.  $\langle f, h(\cdot, x) \rangle_{\mathcal{F}} = f(x), \forall f \in \mathcal{F}.$

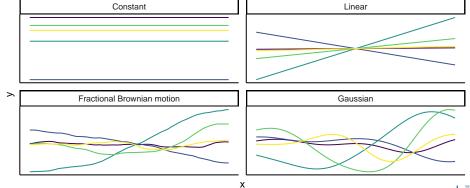
In particular,  $\forall x, x' \in \mathcal{F}$ ,  $h(x, x') = \langle h(\cdot, x), h(\cdot, x') \rangle_{\mathcal{F}}$ .

# 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  $h_k$ ,  $k=1,\ldots,p$ . The ANOVA kernel over the set  $\mathcal{X}=\mathcal{X}_1\times\cdots\times\mathcal{X}_p$  defining the ANOVA RKHS  $\mathcal{F}$  is

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

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

Introduction

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

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

### Lemma 6 (Fisher information for regression function)

The Fisher information for f is

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

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

Examples

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  $f_q = \langle f, g \rangle_{\mathcal{F}}, \ \forall g \in \mathcal{F} \ \text{as} \ \mathcal{I}_{f_q} = \langle \mathcal{I}_f, g \otimes g \rangle_{\mathcal{F} \otimes \mathcal{F}}.$ 

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:

$$\mathcal{I}_{f}(x, x') = \left\langle \mathcal{I}_{f}, h(\cdot, x) \otimes h(\cdot, x') \right\rangle_{\mathcal{F} \otimes \mathcal{F}}$$

$$= \left\langle \sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{ij} h(\cdot, x_{i}) \otimes h(\cdot, j), h(\cdot, x) \otimes h(\cdot, x') \right\rangle_{\mathcal{F} \otimes \mathcal{F}}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{ij} \left\langle h(\cdot, x), h(\cdot, x_{i}) \right\rangle_{\mathcal{F}} \left\langle h(\cdot, x'), h(\cdot, x_{j}) \right\rangle_{\mathcal{F}}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{ij} h(x, x_{i}) h(x', x_{j}) =: k(x, x')$$

(3)

Introduction

### Lemma 7

Introduction

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  $w_i$ s) equipped with the squared norm

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

where  $\psi_{ii}^-$  is the (i,j)th entry of  $\Psi^{-1}$ .

- 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  $\nu$  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

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

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

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

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

Regression using I-priors

Estimation
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**Examples** 

Further research

#### Further assumptions

Introduction

- 1. The error variance  $\Psi$  is known up to a low-dimensional parameter, e.g.  $\Psi = \psi I_n$ ,  $\psi > 0$ .
- 2. Each RKHS  $\mathcal{F}$  of function is defined by the kernel  $h = \lambda \tilde{h}$ , where  $\tilde{h}$  is a positive semidefinite kernel and  $\lambda \in \mathbb{R}$  is a scale parameter.



Regression using I-priors

Estimation

Examples

Further research

Regression using I-priors

Estimation

Examples

Further research

### **Further research**

Hello



### References

- Bergsma, W. (2019). Regression with I-priors. *Journal of Econometrics and Statistics*. https://doi.org/10.1016/j.ecosta.2019.10.002
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