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Regression modelling using I-priors

NUS Department of Statistics & Data Science Seminar

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Abstract

Regression analysis is undoubtedly an important tool to understand the relationship between one or more explanatory and independent variables of interest. The problem of estimating a generic regression function in a model with normal errors is considered. For this purpose, a novel objective prior for the regression function is proposed, defined as the distribution maximizing entropy (subject to a suitable constraint) based on the Fisher information on the regression function. This prior is called the I-prior. The regression function is then estimated by its posterior mean under the I-prior, and accompanying hyperparameters are estimated via maximum marginal likelihood. Estimation of I-prior models is simple and inference straightforward, while predictive performances are comparative, and often better, to similar leading state-of-the-art models–as will be illustrated by several data examples. Further plans for research in this area are also presented, including variable selection for interaction effects and extending the I-prior methodology to non-Gaussian errors. Please visit the project website for further details: `https://phd.haziqj.ml/`

Plan

- Introduction
- Some basic functional analysis (?)
- The I-prior
- Estimation
- Inference
- Examples
- Further work (variable selection, interaction effects, non-gaussian errors)

Introduction

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. This forms the basis for a multitude of statistical models:

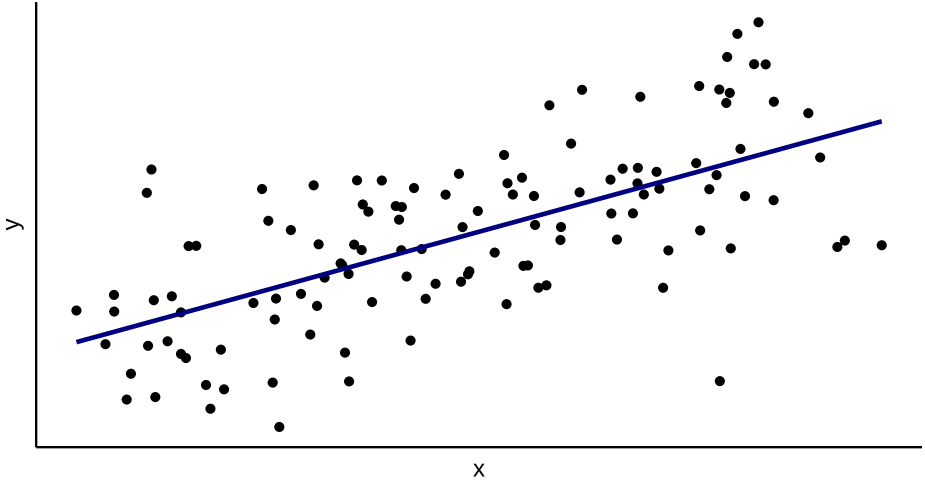
1. Ordinary linear regression when f is parameterised linearly.
2. Varying intercepts/slopes model when $\mathcal{X}$ is grouped.
3. Smoothing models when f is a smooth function.
4. Functional regression when $\mathcal{X}$ is functional.

Goal

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

Ordinary linear regression

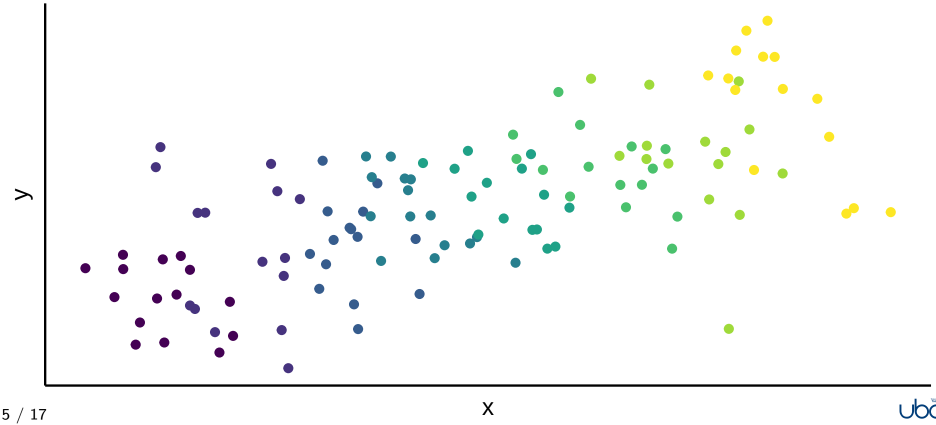
Suppose $f(x_i) = x_i^\top \beta$ for $i = 1, \ldots, n$, where $x_i, \beta \in \mathbb{R}^p$.



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:

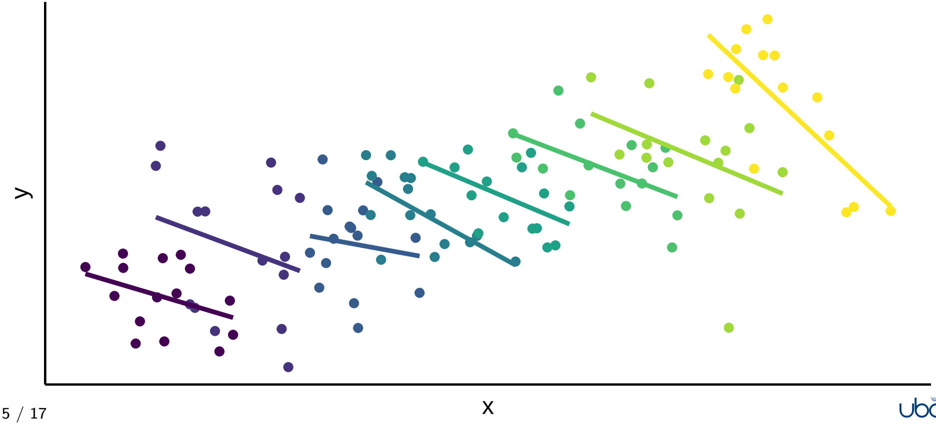
$$f(x_{kj}, j) = f_1(x_{kj}) + f_2(j) + f_{12}(x_{kj}, j).$$



Varying intercepts/slopes model

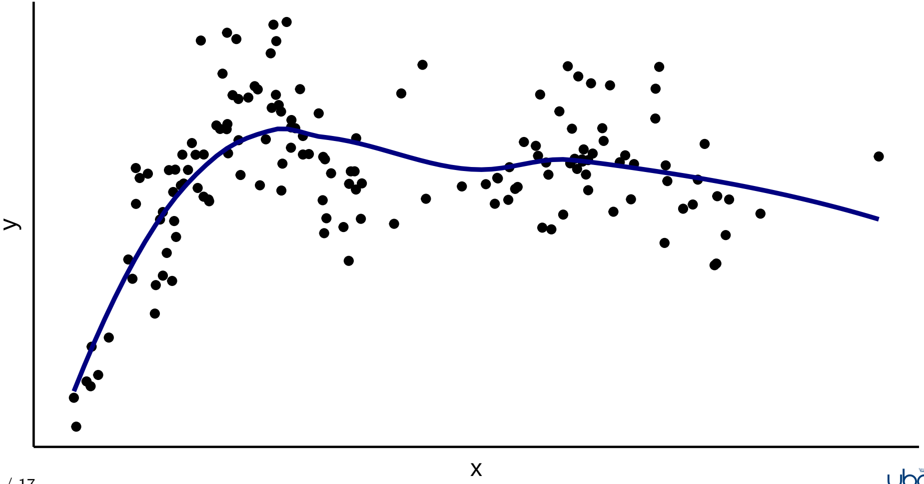
Suppose each unit $i = 1, \dots, n$ relates to the kth observation in group $j \in \{1, \dots, m\}$. Model the function f additively:

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



Smoothing models

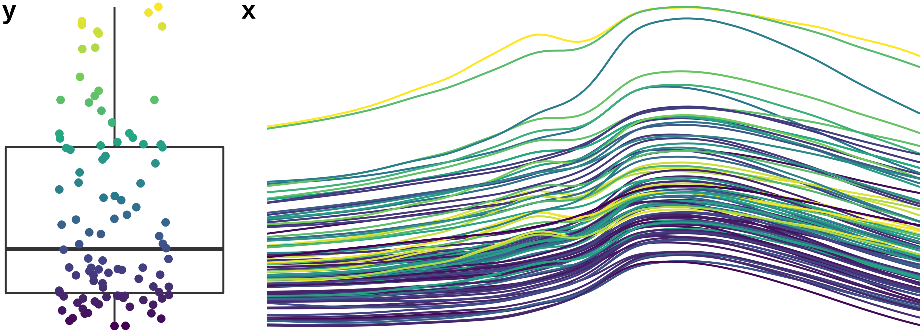
Suppose $f \in \mathcal{F}$ where $\mathcal{F}$ is a space of "smoothing functions" (models like LOESS, kernel regression, smoothing splines, etc.).



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

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

Therefore, the covariance kernel of $\mathbf{f} = \big(f(x_1), \dots, f(x_n)\big)^\top$ is determined by the function

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

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).

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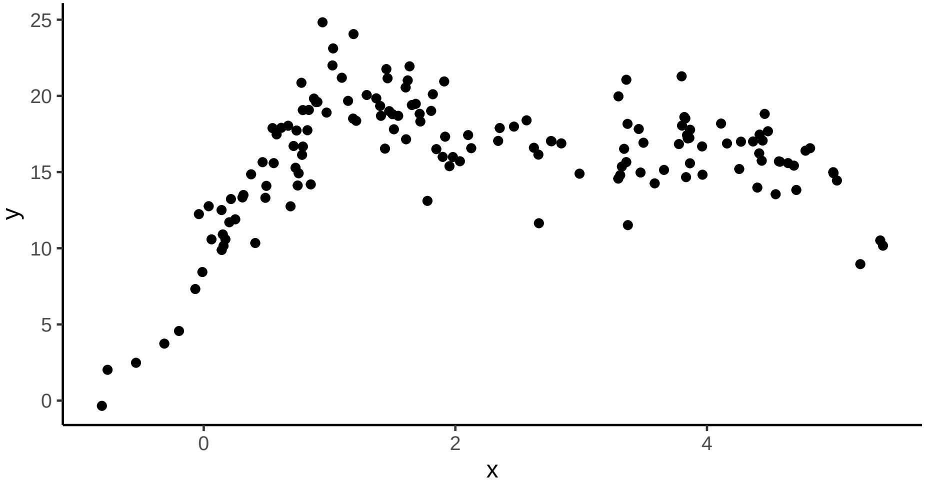
Of interest then are

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

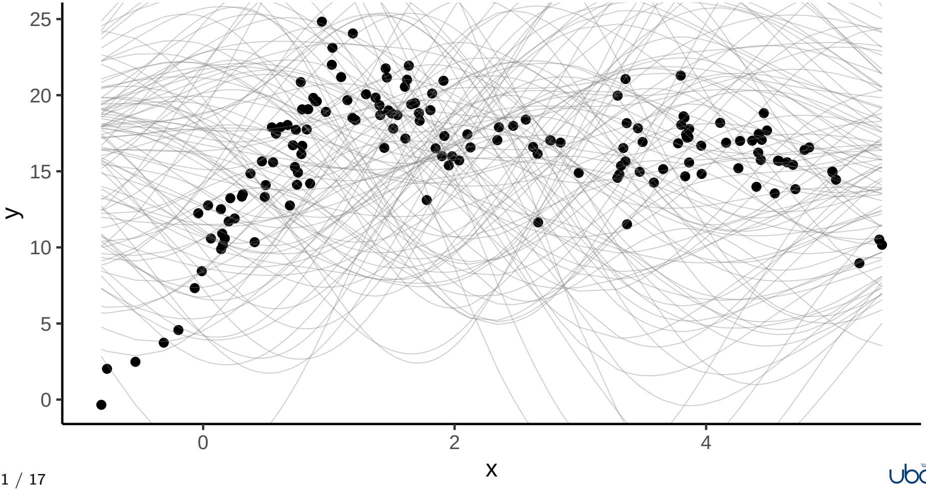
Introduction (cont.)

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



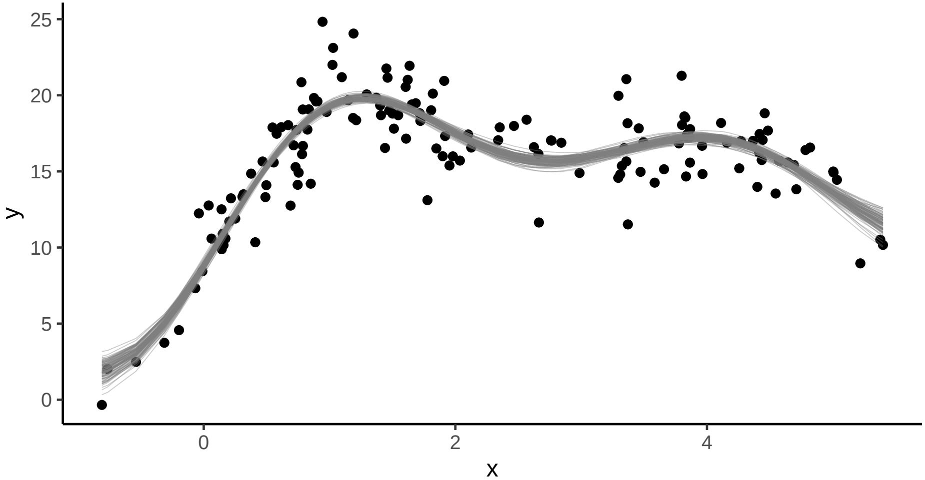
Introduction (cont.)

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



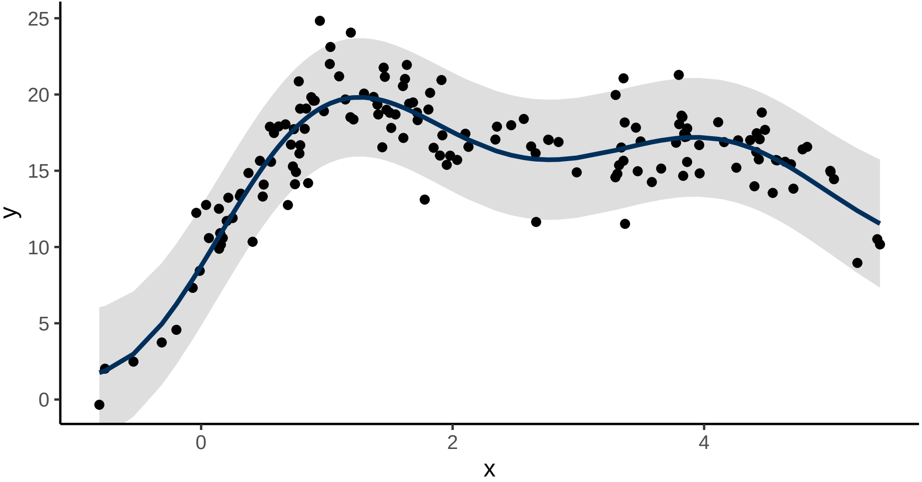
Introduction (cont.)

Sample paths from the posterior of f:



Introduction (cont.)

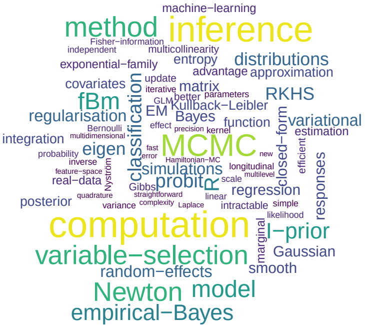
Posterior mean estimate for $y = f(x)$ and its 95% credibility interval.



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)

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

- Gaussian process regression

Introduction

Regression using I-priors

Reproducing kernel Hilbert spaces

Estimation

Examples

Further research

The Fisher information

Suppose further that $f \in \mathcal{F}$ where $\mathcal{F}$ is a reproducing kernel Hilbert space (RKHS) with reproducing kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. Then (1) can be expressed as

$$\begin{gathered} y_i = \big\langle f, h(\cdot, x_i) \big\rangle_{\mathcal{F}} + \epsilon_i \\ (\epsilon_1, \dots, \epsilon_n)^\top \sim \mathrm{N}(\mathbf{0}, \mathbf{\Psi}^{-1}) \end{gathered} \tag{3}$$

The Fisher information for f is given by

$$\mathcal{I}_f = \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} h(\cdot, x_i) \otimes h(\cdot, x_j)$$

It's helpful to think of $\mathcal{I}_f$ as a bilinear form $\mathcal{I}_f : \mathcal{F} \times \mathcal{F} \to \mathbb{R}$ defined by

$$\mathcal{I}_f = -\operatorname{E} \nabla^2 L(f|y)$$

so between two linear functionals of f....

where each $y_i \in \mathbb{R}$,, and $f \in \mathcal{F}$ a reproducing kernel Hilbert space (RKHS) with kernel $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. The I-prior (Bergsma, 2019) for the regression function f is the random function defined

$$\begin{gathered} f(x_i) = f_0(x_i) + \sum_{k=1}^{n} h(x_i, x_k) w_k \\ (w_1, \dots, w_n)^\top \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Psi}) \end{gathered} \tag{4}$$

where f_0 is some prior mean for the regression function.

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Hello