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Regression modelling using I-priors

NUS Department of Statistics & Data Science Seminar

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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:

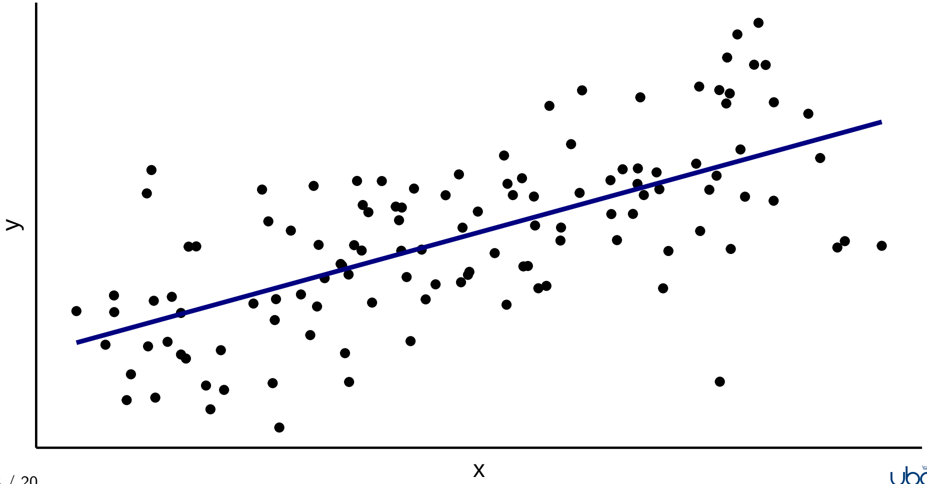
1. Ordinary linear regression when f is parameterised linearly.
2. Varying intercepts/slopes model when $\mathcal{X}$ is grouped.
3. Smoothing models when f is a smooth function.
4. Functional regression when $\mathcal{X}$ is functional.

Goal

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

Ordinary linear regression

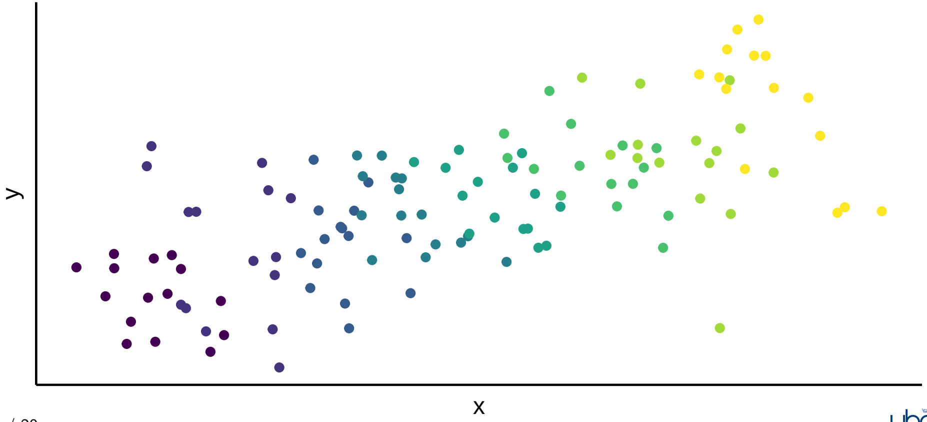
Suppose $f(x_i) = x_i^\top \beta$ for $i = 1, \dots, n$, where $x_i, \beta \in \mathbb{R}^p$.



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:

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



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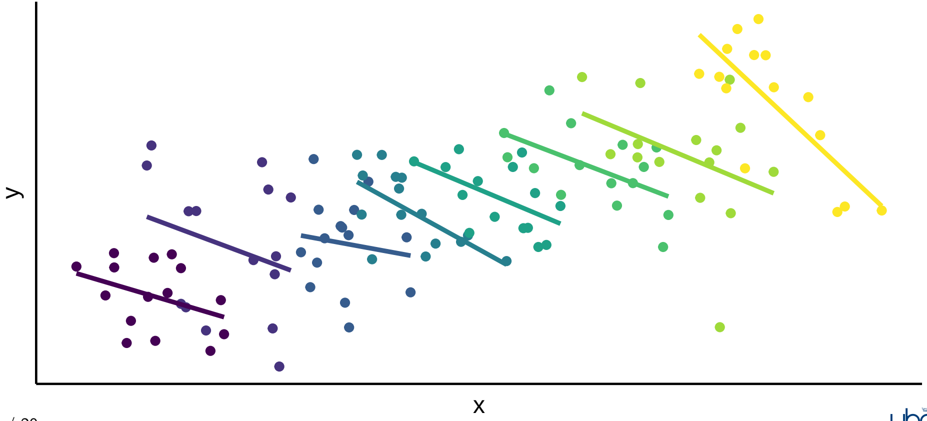
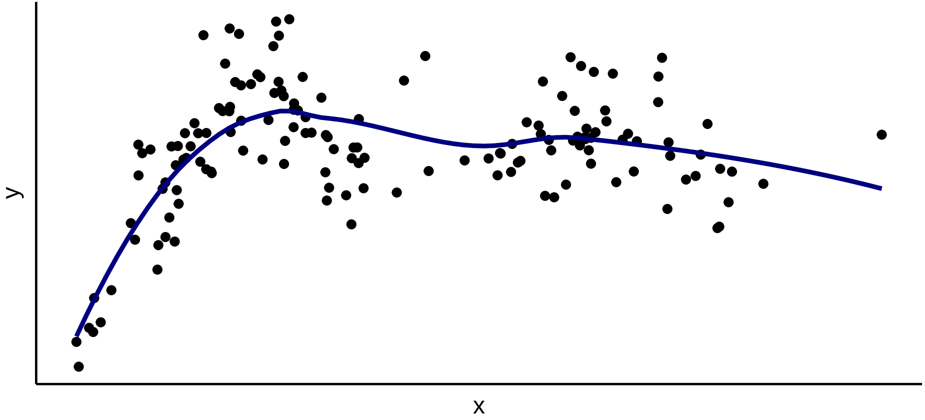
$$f(x_{kj}, j) = \underbrace{x_{kj}^\top \beta_1}_{f_1} + \underbrace{\beta_{0j}}_{f_2} + \underbrace{x_{kj}^\top \beta_{1j}}_{f_{12}}$$



Smoothing models

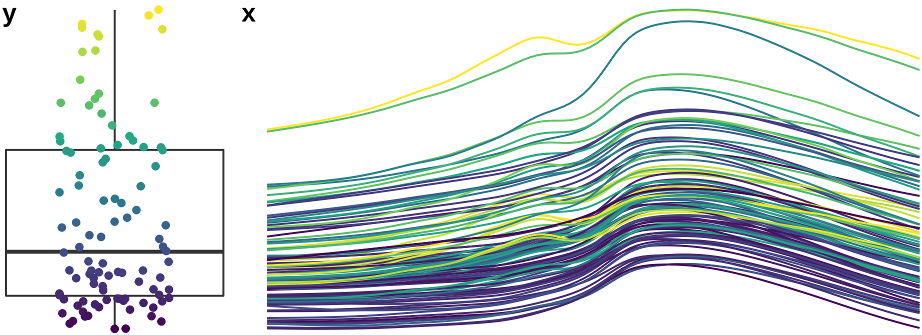
Suppose $f \in \mathcal{F}$ where $\mathcal{F}$ is a space of "smoothing functions" (models like LOESS, kernel regression, smoothing splines, etc.).



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,

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

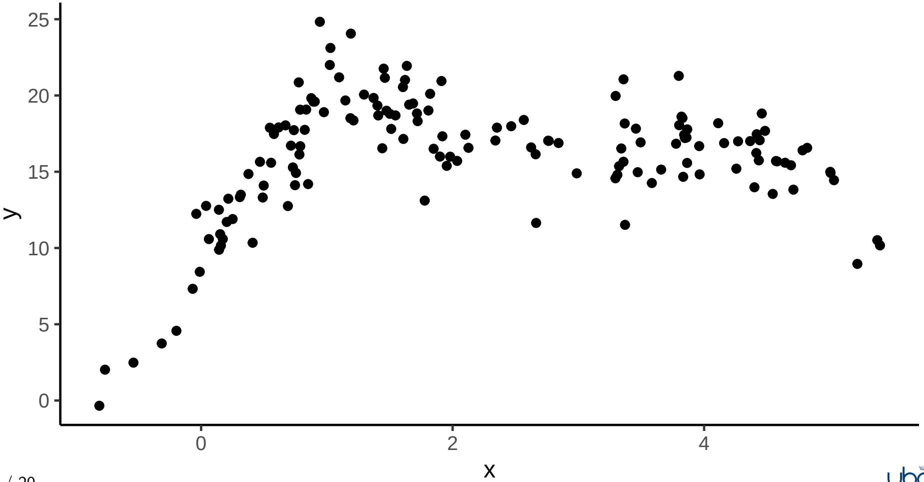
2. Posterior predictive distribution (given a new data point x_{new})

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

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

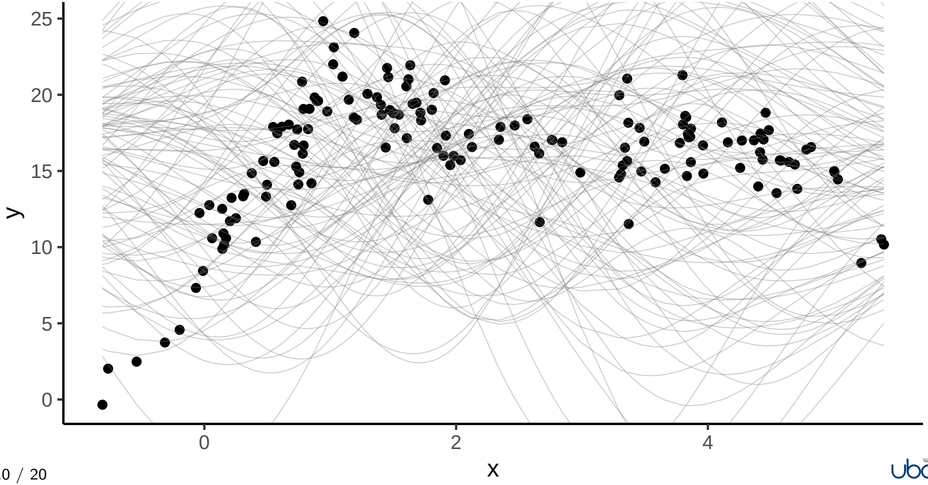
Introduction (cont.)

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



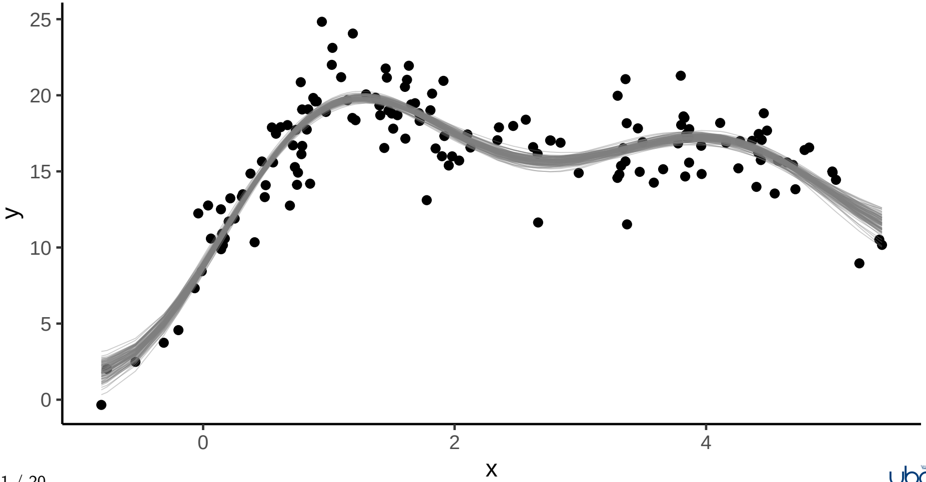
Introduction (cont.)

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



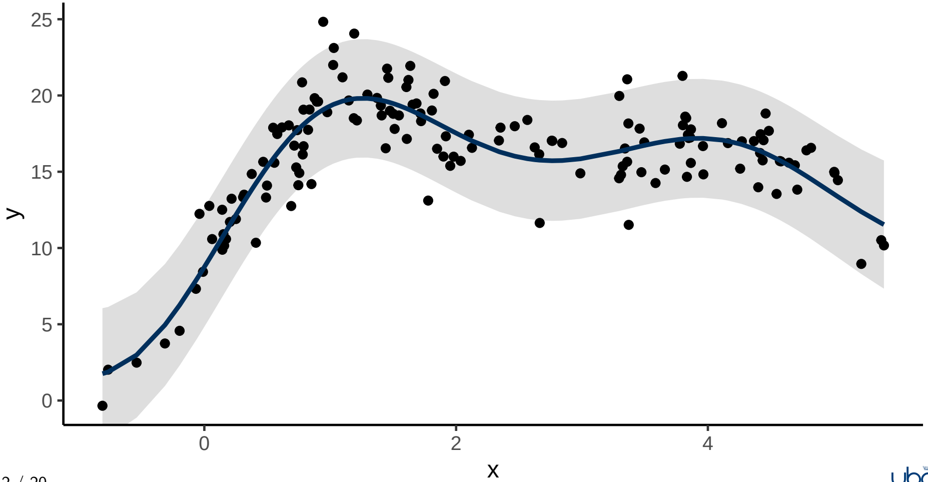
Introduction (cont.)

Sample paths from the posterior of f:



Introduction (cont.)

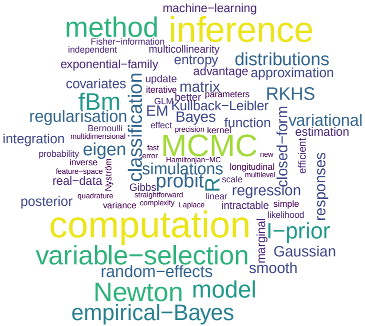
Posterior mean estimate for $y = f(x)$ and its 95% credibility interval.



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

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

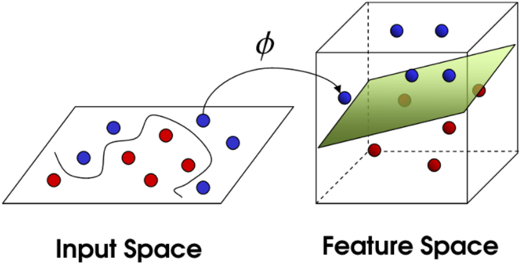
In particular, $\forall x, x' \in \mathcal{F}$, $h(x, x') = \langle h(\cdot, x), h(\cdot, x') \rangle_{\mathcal{F}}$.

Reproducing kernel Hilbert spaces (cont.)

- In ML literature, Mercer's Theorem states

$$h(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{V}} \quad \Leftrightarrow \quad h \text{ is semi p.d.}$$

  where $\phi : \mathcal{X} \to \mathcal{V}$ is a mapping from $\mathcal{X}$ to the *feature space* $\mathcal{V}$.
- In many ML models, need not specify ϕ explicitly; computation is made simpler by the use of kernels.



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.

Corollary 5

Any $f \in \mathcal{F}$ can be approximated arbitrarily well by functions of the form

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

for some constants $w_1, \ldots, w_n \in \mathbb{R}$, because $\mathcal{F}$ is the completion of the vector space $\tilde{\mathcal{F}} = \operatorname{span}\{h(\cdot, x) \mid x \in \mathcal{X}\}$ equipped with the squared norm $\|\tilde{f}\|^2 = \sum_{i,j=1}^{n} w_i w_j h(x_i, x_j)$.

Examples of RKHSs

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.

Further research

Hello