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UNIVERSITI BRUNEI DARUSSALAM

Regression modelling using I-priors

NUS Department of Statistics & Data Science Seminar

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Regression analysis

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

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

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:

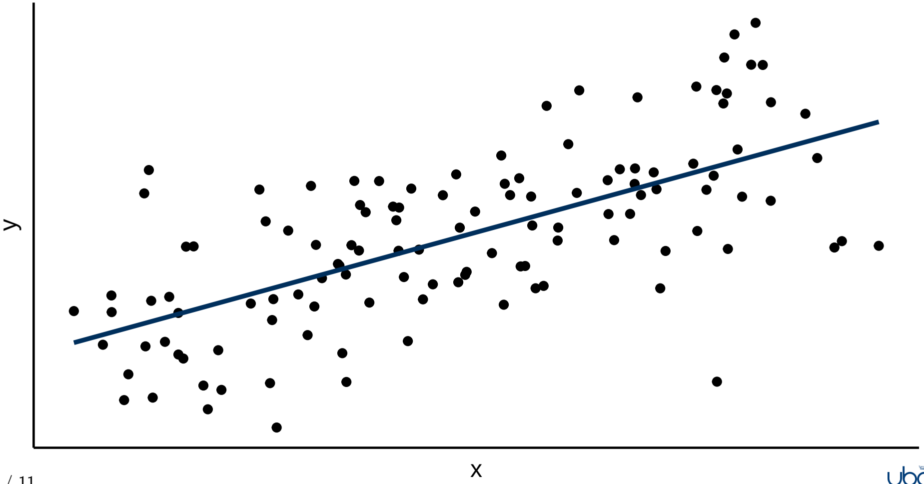
1. Ordinary linear regression when f is parameterised linearly.
2. Varying intercepts/slopes model when $\mathcal{X}$ is grouped.
3. Smoothing models when f is a smooth function.
4. Functional regression when $\mathcal{X}$ is functional.

Goal

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

Ordinary linear regression

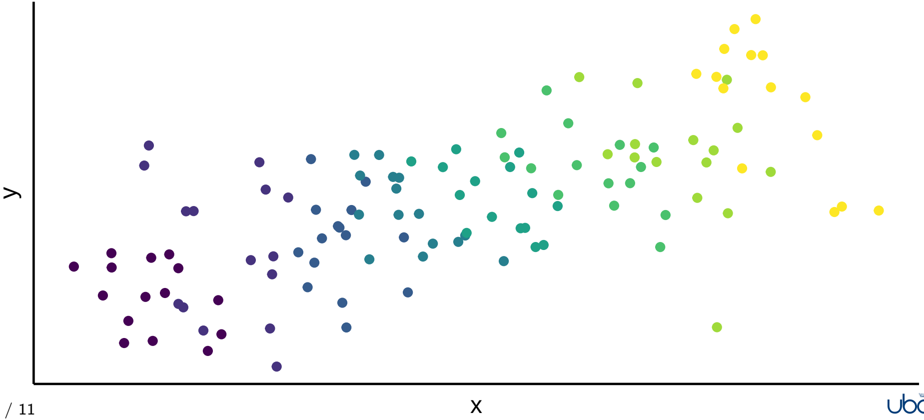
Suppose $f(x_i) = x_i^\top \beta$ for $i = 1, \ldots, n$, where $x_i, \beta \in \mathbb{R}^p$.



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:

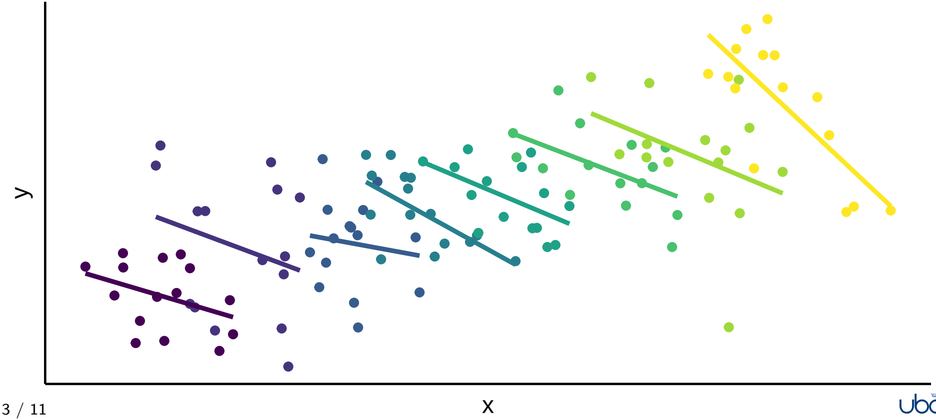
$$f(x_{kj}, j) = f_1(x_{kj}) + f_2(j) + f_{12}(x_{kj}, j).$$



Varying intercepts/slopes model

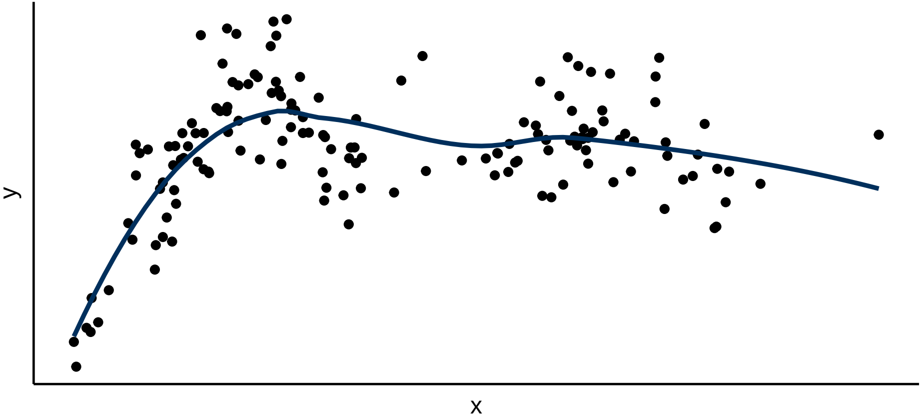
Suppose each unit $i = 1, \ldots, n$ relates to the kth observation in group $j \in \{1, \ldots, m\}$. Model the function f additively:

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



Smoothing models

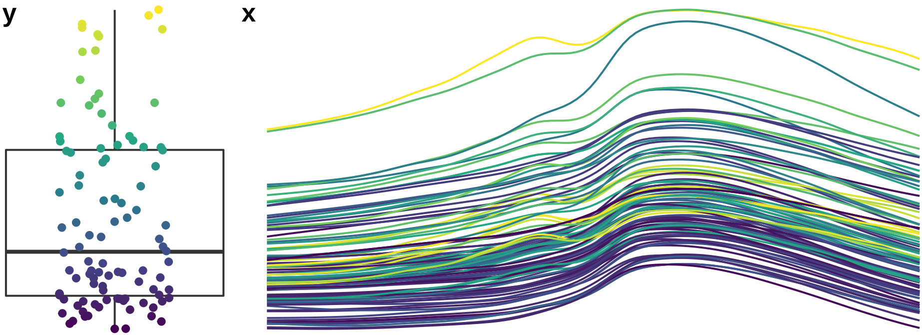
Suppose $f \in \mathcal{F}$ where $\mathcal{F}$ is a space of "smoothing functions" (models like LOESS, kernel regression, smoothing splines, etc.).



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)

With f_0 a prior guess, the entropy maximising prior distribution for f, subject to constraints, is

$$f(x) = f_0(x) + \sum_{i=1}^{n} h(x, x_i) w_i$$
$$(w_1, \dots, w_n)^\top \sim \mathrm{N}_n(0, \Psi) \tag{2}$$

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

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

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

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

Lemma 2

The posterior distribution for f is Gaussian with mean and covariance kernel

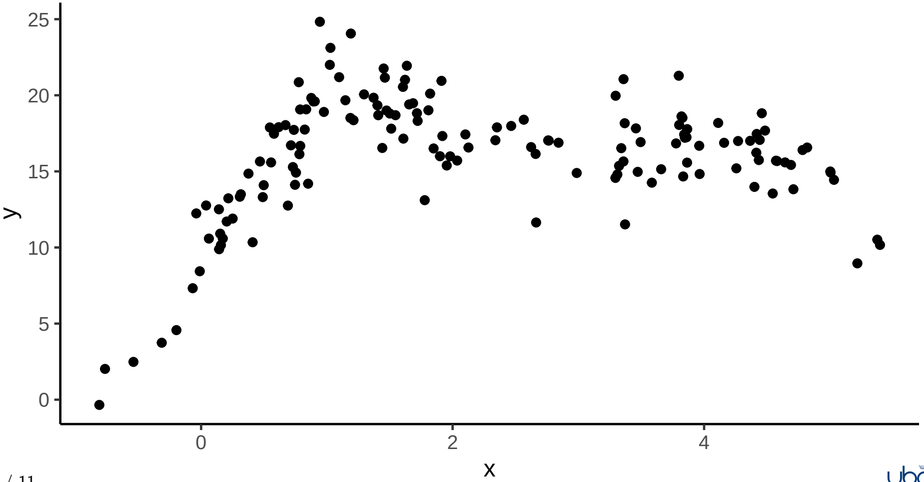
$$\mathrm{E}\big(f(x) \mid \mathbf{y}\big) = f_0(x) + \sum_{i=1}^n h(x, x_i)\hat{w}_i$$

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

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

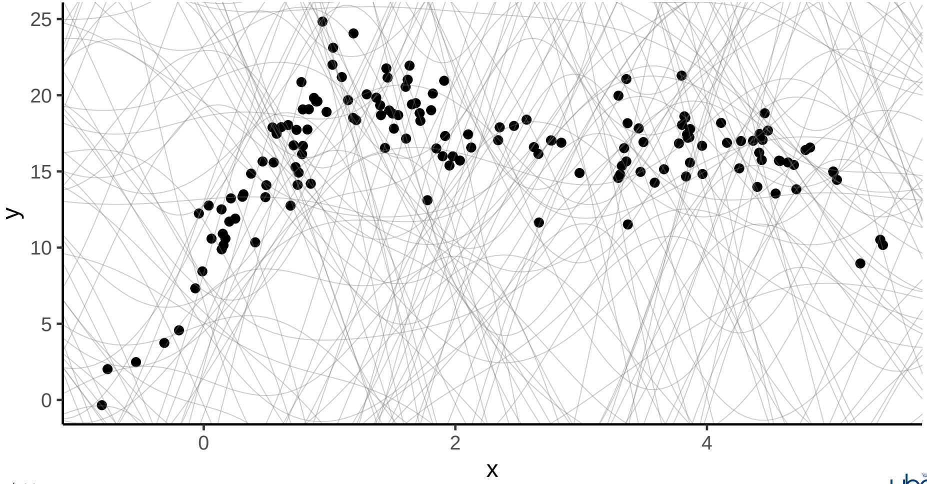
Illustration

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



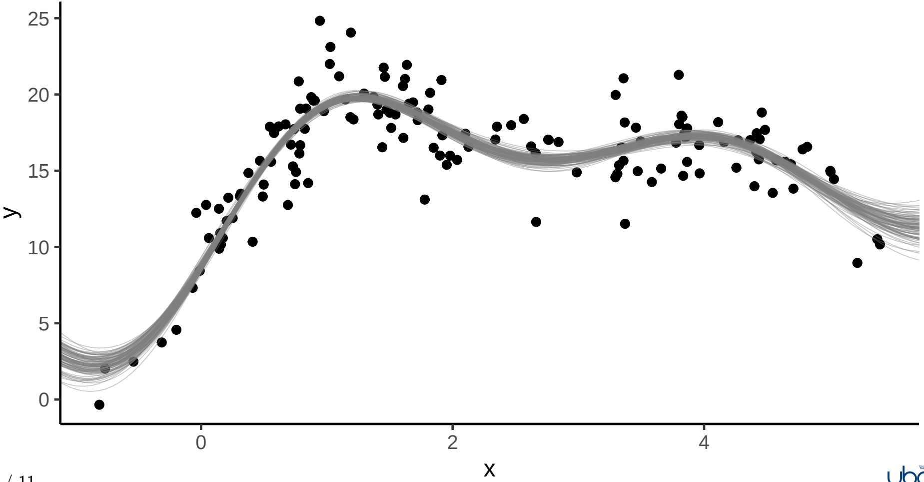
Illustration

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



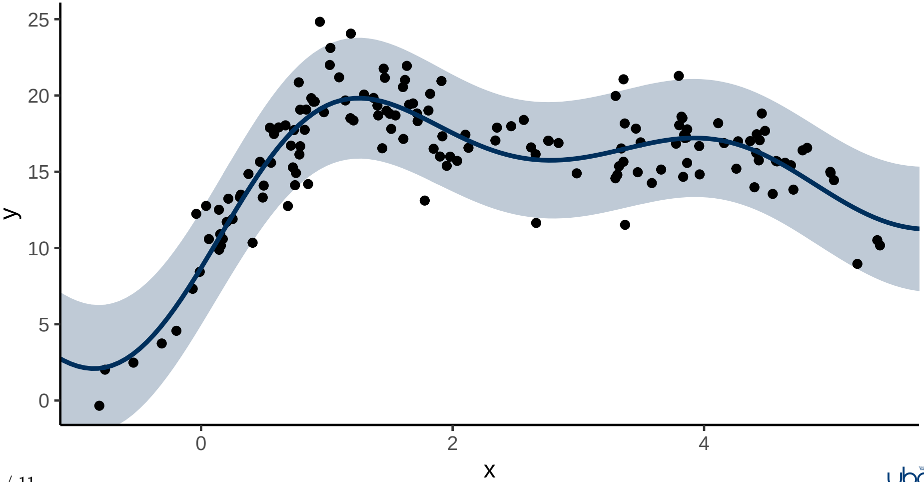
Illustration

Sample paths from the posterior of f:



Illustration

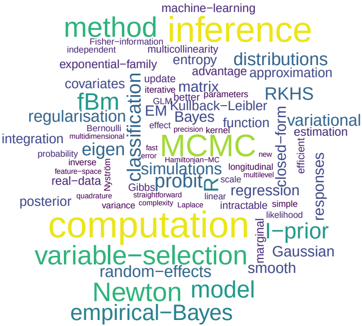
Posterior mean estimate for $y = f(x)$ and its 95% credibility interval.



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 (Rasmussen & Williams, 2006)

State of the art

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