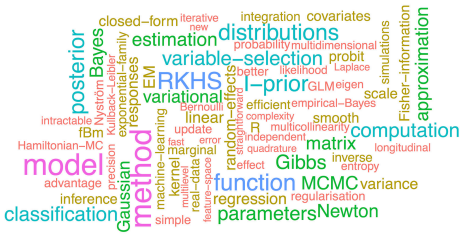
Haziq Jamil &
Wicher Bergsma

Department of Statistics
London School of Economics and
Political Science

http://phd.haziqj.ml

Binary and Multinomial Regression using Fisher Information Covariance Kernels (I-priors)



Introduction

Consider the regression model for $i = 1, \dots, n$:

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

where $y_i \in \mathbb{R}$, $x \in \mathcal{X}$, $f \in \mathcal{F}$ and $\alpha \in \mathbb{R}$ is an intercept. Let $\mathcal{F}$ be a reproducing kernel Hilbert space (RKHS) with kernel $h_\lambda : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. The Fisher information for f evaluated at x and x' is

$$\mathcal{I}\big(f(x), f(x')\big) = \sum_{k=1}^{n}\sum_{l=1}^{n} \Psi_{k,l} h_\lambda(x, x_k) h_\lambda(x', x_l). \tag{2}$$

The I-prior

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

$$\mathbf{f} = \big(f(x_1), \dots, f(x_n)\big)^\top \sim \mathrm{N}_n\big(\mathbf{f}_0, \mathcal{I}[f]\big).$$

Equivalently, $f(x) = f_0(x) + \sum_{i=1}^n h_\lambda(x, x_i) w_i$, with

$$(w_1, \dots, w_n)^\top \sim \mathrm{N}_n(0, \Psi).$$

Of interest are

- the posterior distribution for the regression function

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

- the posterior predictive distribution for new data points

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

Model parameters (error precision Ψ, RKHS scale parameters λ, and any other kernel parameters) may need to be estimated.

A Unified Regression Framework

- Multiple linear regression (linear RKHS)
- Smoothing models (fBm RKHS)
- Multilevel regression (ANOVA RKHS: linear & Pearson)

$$f(x_i^{(j)}) = f_1(j) + f_2(x_i^{(j)}) + f_{12}(x_i^{(j)}, j)$$

- Longitudinal modelling (ANOVA RKHS: fBm & Pearson)

$$f(x_i, t_i) = f_1(t_i) + f_2(x_i) + f_{12}(x_i, t_i)$$

- Functional covariates ($\mathcal{X}$ a Hilbert-Sobolev space)

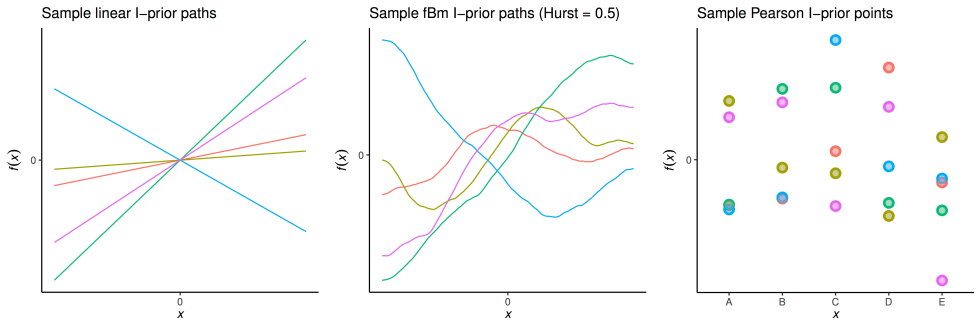


Figure 1: (L-R) Sample paths from the linear, fractional Brownian motion (fBm), and Pearson RKHS. The (reproducing) kernels corresponding to each RKHS are: $h_\lambda(x, x') = \lambda\langle x, x'\rangle_{\mathcal{X}}$ (linear), $h_\lambda(x, x') = -\frac{\lambda}{2}(\|x - x'\|_{\mathcal{X}}^{2\gamma} - \|x\|_{\mathcal{X}}^{2\gamma} - \|x'\|_{\mathcal{X}}^{2\gamma})$ (fBm), and $h_\lambda(x, x') = \lambda(\delta_{xx'}/\mathrm{P}[X = x] - 1)$ (Pearson).

Categorical Responses

When each $y_i \in \{1, \dots, m\}$, normality assumptions are violated. Model instead $y_i = \arg\max_k y_{ik}^*$, where

$$\begin{aligned} y_{ij}^* &= \alpha_j + f_j(x_i) + \epsilon_{ij} \\ (\epsilon_{i1}, \dots, \epsilon_{im})^\top &\sim \mathrm{N}_m(0, \Sigma) \end{aligned} \tag{3}$$

with $\mathrm{Cov}(\epsilon_{ij}, \epsilon_{kj}) = 0$, for all $i \neq k$, $j = 1, \dots, m$. In other words, $\Psi = I_n$ in (1). The I-prior is

$$\begin{aligned} \mathbf{f}_j = \big(f_j(x_1), \dots, f_j(x_n)\big)^\top &\sim \mathrm{N}_n\big(\mathbf{f}_{0j}, \Sigma_{jj}^{-1} \cdot \mathcal{I}[f]\big) \\ \mathrm{Cov}(\mathbf{f}_j, \mathbf{f}_k) &= \Sigma_{jk}^{-1} \cdot \mathcal{I}[f]. \end{aligned}$$

Class probabilities p_{ij} are obtained using a *conically truncated m-variate normal* density

$$p_{ij} = \int_{\{y_{ij}^* > y_{ik}^* \,|\, k \neq j\}} \mathrm{N}_m\big(\mathbf{y}_i^* \,|\, f(x_i), \Sigma\big)\,\mathrm{d}\mathbf{y}_i^* =: g_j^{-1}\big(f(x_i)\big).$$

where we had defined $f(x_i) = \big(f_1(x_i), \dots, f_m(x_i)\big)^\top$. Now, the marginal, on which the posterior depends,

$$p(\mathbf{y}) = \int \prod_{i,j} \Big\{g_j^{-1}\big(f(x_i)\big)\Big\}^{[y_i = j]} \cdot \mathrm{N}_{nm}\big(\mathbf{f} \,|\, \mathbf{f}_0, \Sigma \otimes \mathcal{I}[f]\big)\,\mathrm{d}\mathbf{f},$$

cannot be found in closed form. By working in a fully Bayesian setting, we append model parameters and employ a *variational approximation*.

Spatio-Temporal Modelling of BTB[a]

Determine the existence of spatial segregation of the different spoligotypes of bovine tuberculosis (BTB) in Cornwall, UK, and whether the spatial distribution had changed over time.

1. Constant model (constant RKHS)

$$p_{ij} = g_j^{-1}\big(\alpha_k\big)_{k=1}^m$$

2. Spatial segregation (fBm RKHS)

$$p_{ij} = g_j^{-1}\big(\alpha_k + f_{1k}(x_i)\big)_{k=1}^m$$

3. Spatio-temporal segregation (ANOVA RKHS)

$$p_{ij} = g_j^{-1}\big(\alpha_k + f_{1k}(x_i) + f_{2k}(t_i) + f_{12k}(x_i, t_i)\big)_{k=1}^m$$

Evidence Lower Bound (ELBO) values for the three models are -1197.4, -665.3, and -656.2 respectively.

Detecting Cardiac Arrhythmia[b]

Predict whether or not patients suffer from a cardiac disease based on various patient profiles such as age, height, weight and a myriad of electrocardiogram (ECG) readings ($p = 271, n = 451$).

Table 1: Mean out-of-sample misclassification rates and standard errors for 100 runs of various training (s) and test ($451 - s$) sizes for the cardiac arrhythmia binary classification task.

	Misclassification rate (%)		
Method	$s = 50$	$s = 100$	$s = 200$
I-probit (linear)	34.5 (0.4)	31.4 (0.4)	29.7 (0.4)
I-probit (fBm)	34.7 (0.6)	27.3 (0.3)	24.5 (0.3)
GP (Gaussian)	37.3 (0.4)	33.8 (0.4)	29.3 (0.4)
L-1 logistic	34.9 (0.4)	30.5 (0.3)	26.1 (0.3)
SVM (linear)	36.2 (0.5)	35.6 (0.4)	35.2 (0.4)
SVM (Gaussian)	48.4 (0.5)	47.2 (0.5)	46.9 (0.4)
RF	31.7 (0.4)	26.7 (0.3)	22.4 (0.3)
k-NN	40.6 (0.3)	38.9 (0.3)	35.8 (0.4)

Conclusions

- Simple estimation of various categorical models:
  - Choice models (with or without IIA);
  - Random-effects models;
  - Binary and multiclass classification.
- Inference is straightforward (e.g. model comparison or (transformed) credibility intervals).
- Often gives better predictions.

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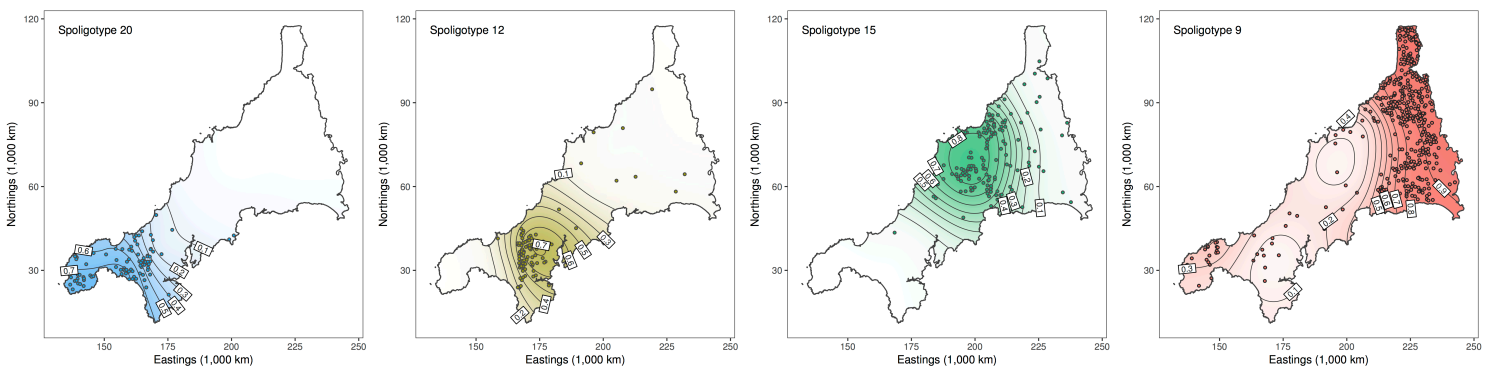

Figure 2: Predicted probability surfaces for BTB contraction in Cornwall for the four largest spoligotypes of the bacterium *Mycobacterium bovis* over the entire time period 1989–2002 using Model 2.

Data sources: [a]Peter Diggle, Pingping Zheng, and Peter Durr. Nonparametric estimation of spatial segregation in a multivariate point process: bovine tuberculosis in Cornwall, UK. *J. Royal Stat. Soc. Series C (Appl. Statist.)*, 54(3):645–658, 2005. [b]Timothy I Cannings and Richard J Samworth. Random projection ensemble classification. *J. Royal Stat. Soc. Series B (Stat. Methodol.)*, 79(4):959–1035, 2017.