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Regression Modelling with Priors using Fisher Information Covariance Kernels (I-priors)

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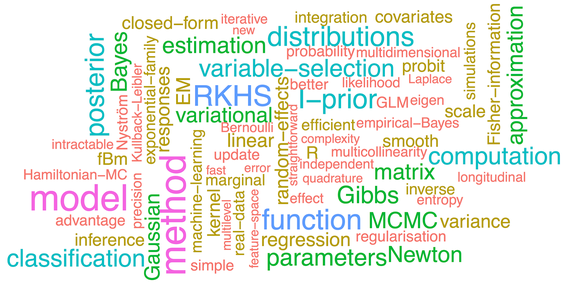

Introduction

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

$$y_i = f(x_i) + \epsilon_i$$
$$(\epsilon_1, \dots, \epsilon_n)^\top \sim \mathrm{N}_n(0, \Psi^{-1}) \qquad (1)$$

where $y_i \in \mathbb{R}$, $x \in \mathcal{X}$, and $f \in \mathcal{F}$. 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

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

The I-prior

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

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

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

Estimation

Model parameters (error precision Ψ, RKHS scale parameters λ, and any others) may be estimated via

- Maximum marginal likelihood, a.k.a. empirical Bayes;
- Expectation-maximisation (EM) algorithm; or
- Markov chain Monte Carlo (MCMC) methods.

Under the normal model (1), the posterior for y, given some x and model parameters, is normal with mean

$$\hat{y}(x) = f_0(x) + \mathbf{h}_\lambda^\top(x)\Psi H_\lambda\big(H_\lambda \Psi H_\lambda + \Psi^{-1}\big)^{-1}\big(y - f_0(x)\big)$$

and variance (3)

$$\hat{\sigma}^2(x) = \mathbf{h}_\lambda^\top(x)\big(H_\lambda \Psi H_\lambda + \Psi^{-1}\big)^{-1}\mathbf{h}_\lambda(x) + \nu_x^{-1},$$

where ν_x is some covariance term.

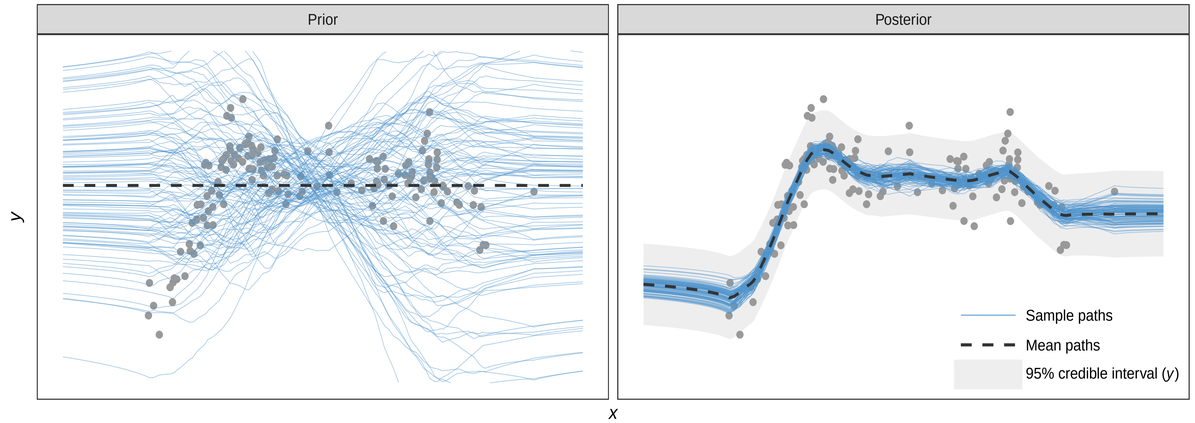

Figure 1: Sample paths from the fractional Brownian motion RKHS under an I-prior (left) and the posterior (right). There is somewhat controlled behaviour at the boundaries (compared to Gaussian process priors, say). Fewer information in this region pulls the function estimate towards the prior mean. The 95% credibility interval for posterior estimates of y are shaded grey.

Computational Hurdle

Computational complexity is dominated by the $n \times n$ matrix inversion in (3), which is $O(n^3)$. Suppose that $H_\lambda \Psi H_\lambda = QQ^\top$, with Q an $n \times q$ matrix, is a valid low-rank decomposition. Then

$$\big(H_\lambda \Psi H_\lambda + \Psi^{-1}\big)^{-1} = \Psi - \Psi Q\big(I_q + Q^\top \Psi Q\big)^{-1} Q^\top \Psi$$

is a much cheaper $O(nq^2)$ operation, especially if $q \ll n$. The Nyström method for low-rank matrix approximations is explored.

I-prior advantages

- Unifies methodology for various regressions models, including:
  - Multidimensional smoothing.
  - Random effects/multilevel models.
  - Longitudinal models.
  - Functional linear/smooth regression.
- Straightforward estimation and inference.
- Often gives better prediction for new data.

Categorical Responses

Suppose now that each $y_i \in \{1, \dots, m\}$ and that

$$y_i \sim \mathrm{Cat}(p_{i1}, \dots, p_{im})$$

with probability mass function

$$p(y_i) = \prod_{j=1}^{m} p_{ij}^{y_{ij}}, \qquad y_{ij} = [y_i = j],$$

satisfying $p_{ij} > 0$, $\sum_j p_{ij} = 1$ for $j \in \{1, \dots, m\}$. In the spirit of generalised linear models, take

$$\mathrm{E}[y_{ij}] = p_{ij} = g^{-1}\big(f_j(x_i)\big)$$

with some link function $g : [0, 1] \to \mathbb{R}$ and an I-prior on f_j.

Now, the marginal (on which the posterior depends),

$$p(\mathbf{y}) = \int \prod_{i=1}^{n} \prod_{j=1}^{m} \left[\left\{ g^{-1}\big(f_j(x_i)\big) \right\}^{[y_i = j]} \cdot \mathrm{N}_n(\mathbf{f}_{0j}, \mathcal{I}[f_j])\,\mathrm{d}\mathbf{f}_j \right],$$

cannot be found in closed form.

Variational Approximation

An approximation $q(\mathbf{f})$ to the true posterior density $p(\mathbf{f}|\mathbf{y})$ is considered, with q chosen to minimise the Kullback-Leibler divergence (under certain restrictions):

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

By working in a fully Bayesian setting, we append model parameters to $\mathbf{f}$ and employ the variational method. The result is an iterative algorithm similar to the EM.

As this variational-EM works harmoniously with exponential family distributions, the ***probit*** link is preferred.

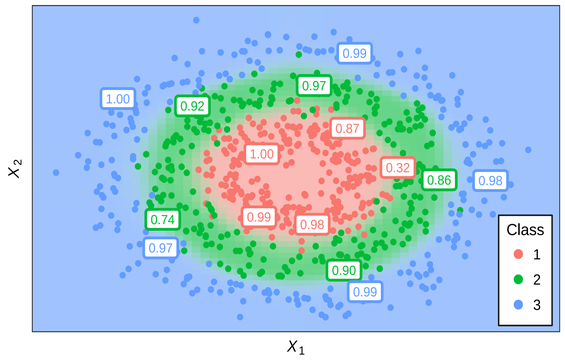

Figure 2: A toy example of three-class classification using I-priors and the fBm-0.5 kernel over a two-dimensional predictor. Points indicate realisations, while background colours denote predicted classes. Several predicted probabilities for new data are shown too.

Variable Selection for Linear Models

Model selection can easily be done by comparing likelihoods (empirical Bayes factors). However, with p variables to select, the 2^p comparisons could prove intractable with large p.

For linear models of the form

$$(y_1, \dots, y_n)^\top \sim \mathrm{N}_n\left(\beta_0 \mathbf{1}_n + \sum_{j=1}^{p} \beta_j X_j, \Psi^{-1}\right),$$

the prior

$$(\beta_1, \dots, \beta_p)^\top \sim \mathrm{N}_p(0, \Lambda X^\top \Psi X \Lambda)$$

is an equivalent I-prior representation of (1) in the feature space of β under the linear kernel.

Gibbs-based methods are used in order to estimate *posterior model probabilities*

$$p(M|\mathbf{y}) \propto \int p(\mathbf{y}|M, \theta) p(\theta|M) p(M)\,\mathrm{d}\theta$$

where M is the model index and θ are model parameters.

Table 1: Simulation results (proportion of false choices) for experiments in selecting 100 pairwise-correlated variables using I-priors under differing SNR. Our method outperforms methods such as greedy selection, g-priors, and regularisation (ridge and Lasso).

	Signal-to-noise Ratio (SNR)				
False choices	**90%**	**75%**	**50%**	**25%**	**10%**
0-2	0.92	0.92	0.92	0.78	0.52
3-5	0.08	0.08	0.08	0.20	0.28
>5	0.01	0.00	0.01	0.02	0.20

Conclusions

- I-priors provide simple fitting of various regression models for prediction and inference.
- The merits of I-priors extend markedly to the binary and multinomial response case.
- Evidence suggests an I-prior advantage for linear variable selection under multicollinearity.

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