INLA Introduction

King Abdullah University of Science and Technology

جامعة الملك عبدالله
للعلوم والتقنية

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Outline

BayesComp group at KAUST

Bayesian inference

Data $\boldsymbol{y}$ (with covariates $\boldsymbol{Z}$), depend on $\boldsymbol{X}$ and $\boldsymbol{\theta}$ such that, $E[Y] = h(\boldsymbol{A}(\boldsymbol{Z})\boldsymbol{X})$.

Bayes' theorem:

$$\begin{aligned} q(\boldsymbol{X}, \boldsymbol{\theta}) &\propto L(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) p(\boldsymbol{X}, \boldsymbol{\theta}) \\ \text{Posterior} &\propto \text{Likelihood} \times \text{Prior} \end{aligned}$$

Computational aspects

- Analytical methods - conjugacy (pre-computer era)
- Approximate methods - Laplace (can be inaccurate)
- Exact methods - MCMC (very slow for complex models or large data)

Now, due to computing resources approximate methods are gaining popularity - INLA, VB, EP etc.

INLA - 2009 [Rue et al., 2009]

2021+ [Van Niekerk et al., 2023]

HPC [Gaedke-Merzhäuser et al., 2023]

Model definition - GAMM

Suppose we have response data $\boldsymbol{y}_{n\times 1}$ (conditionally independent) with density function $\pi(y|\boldsymbol{X},\boldsymbol{\theta})$ and link function $h(.)$, that is linked to some covariates $\boldsymbol{Z}$ through linear predictors

$$\boldsymbol{\eta}_n = \beta_0 + \boldsymbol{Z}_\beta\boldsymbol{\beta} + \sum f^k(\boldsymbol{Z}_f) = \boldsymbol{A}\boldsymbol{X}$$

The inferential aim is to estimate the latent field $\boldsymbol{X}_m = \{\beta_0, \boldsymbol{\beta}, \boldsymbol{f}\}$, and $\boldsymbol{\theta}$.

GAMM $\rightarrow$ LGM

Assume

$$\boldsymbol{X}|\boldsymbol{\theta} \sim N(\mathbf{0}, \boldsymbol{Q}(\boldsymbol{\theta})^{-1})$$

where $\boldsymbol{Q}(\boldsymbol{\theta})$ is a sparse matrix ($\boldsymbol{X}$ is a GMRF).

$p(\boldsymbol{X}, \boldsymbol{\theta}) = p(\boldsymbol{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})$ and $p(\boldsymbol{\theta})$ can be non-Gaussian.

Why is INLA so accurate and so fast?

- LGM structure
- Sparse precision matrix
- Specialized matrix algebra for sparse matrices
- NEW: VB (low-rank) correction [van Niekerk and Rue, 2024]

Use precision matrix instead of covariance matrix $\rightarrow$ natural occurrence

How common are sparse $\boldsymbol{Q}(\boldsymbol{\theta})$?

Consider an AR(1) model..

AR(1) example

AR(1) example

Posterior approximations by INLA

$$
\begin{aligned}
\pi(\boldsymbol{X}, \boldsymbol{\theta}, \boldsymbol{y}) &= \pi(\boldsymbol{\theta})\pi(\boldsymbol{X}|\boldsymbol{\theta}) \prod_{i=1}^{n} \pi(y_i|(\boldsymbol{A}\boldsymbol{X})_i, \boldsymbol{\theta}) \\
\tilde{\pi}(\boldsymbol{\theta}|\boldsymbol{y}) &\propto \left. \frac{\pi(\boldsymbol{X}, \boldsymbol{\theta}, \boldsymbol{y})}{\pi_G(\boldsymbol{X}|\boldsymbol{\theta}, \boldsymbol{y})} \right|_{\boldsymbol{X}=\boldsymbol{\mu}(\boldsymbol{\theta})} \\
\tilde{\pi}(\theta_j|\boldsymbol{y}) &= \int \tilde{\pi}(\boldsymbol{\theta}|\boldsymbol{y}) d\boldsymbol{\theta}_{-j} \\
\tilde{\pi}(\boldsymbol{X}_j|\boldsymbol{y}) &= \int \tilde{\pi}(\boldsymbol{X}_j|\boldsymbol{\theta}, \boldsymbol{y}) \tilde{\pi}(\boldsymbol{\theta}|\boldsymbol{y}) d\boldsymbol{\theta},
\end{aligned}
$$

$\tilde{\pi}(\boldsymbol{X}_j|\boldsymbol{\theta}, \boldsymbol{y})$ depends on the approximation used, for Gaussian it is straightforward for the Laplace approximation we do another Gaussian approximation to $\tilde{\pi}(\boldsymbol{X}_{-j}|\boldsymbol{\theta}, \boldsymbol{y})$.

Modern INLA

The Gaussian approximation $\pi_G(\boldsymbol{X}|\boldsymbol{\theta},\boldsymbol{y})$ to $\pi(\boldsymbol{X}|\boldsymbol{\theta},\boldsymbol{y})$ is calculated from a second order expansion of the likelihood around the mode of $\pi(\boldsymbol{X}|\boldsymbol{\theta},\boldsymbol{y})$, $\boldsymbol{\mu}(\boldsymbol{\theta})$ as follows

$$
\begin{aligned}
\log\left(\pi(\boldsymbol{X}|\boldsymbol{\theta},\boldsymbol{y})\right) &\propto -\frac{1}{2}\boldsymbol{X}^\top\boldsymbol{Q}(\boldsymbol{\theta})\boldsymbol{X} + \sum_{i=1}^{n}\left(b_i(\boldsymbol{A}\boldsymbol{X})_i - \frac{1}{2}c_i(\boldsymbol{A}\boldsymbol{X})_i^2\right) \\
&= -\frac{1}{2}\boldsymbol{X}^\top\left(\boldsymbol{Q}(\boldsymbol{\theta}) + \boldsymbol{A}^\top\boldsymbol{D}\boldsymbol{A}\right)\boldsymbol{X} - \boldsymbol{b}^\top\boldsymbol{A}\boldsymbol{X}
\end{aligned}
$$

where $\boldsymbol{b}$ is an n-dimensional vector with entries $\{b_i\}$ and $\boldsymbol{D}$ is a diagonal matrix with n entries $\{c_i\}$. Note that both $\boldsymbol{b}$ and $\boldsymbol{D}$ depend on $\boldsymbol{\theta}$, so the Gaussian approximation is for a fixed $\boldsymbol{\theta}$.

Modern INLA

The process is iterated to find $\boldsymbol{b}$ and $\boldsymbol{D}$ that gives the Gaussian approximation at the mode, $\boldsymbol{\mu}(\boldsymbol{\theta})$, so that

$$\boldsymbol{X}|\boldsymbol{\theta},\boldsymbol{y} \sim N\left(\boldsymbol{\mu}(\boldsymbol{\theta}), \boldsymbol{Q}_{\boldsymbol{X}}^{-1}(\boldsymbol{\theta})\right).$$

The graph of the Gaussian approximation consists of two components,

1. $\mathcal{G}_p$: the graph obtained from the prior of the latent field through $\boldsymbol{Q}(\boldsymbol{\theta})$
2. $\mathcal{G}_d$: the graph obtained from the data based on the non-zero entries of $\boldsymbol{A}^\top\boldsymbol{A}$

Modern INLA

Next, the marginal conditional posteriors of the elements of $\boldsymbol{X}$ is calculated from the joint Gaussian approximation as

$$\boldsymbol{X}_j|\boldsymbol{\theta},\boldsymbol{y} \sim N\left((\boldsymbol{\mu}(\boldsymbol{\theta}))_j\,, \left(\boldsymbol{Q}_{\boldsymbol{X}}^{-1}(\boldsymbol{\theta})\right)_{jj}\right).$$

and the marginals

$$\tilde{\pi}(\boldsymbol{X}_j|\boldsymbol{y}) = \int \pi_G(\boldsymbol{X}_j|\boldsymbol{\theta},\boldsymbol{y})\tilde{\pi}(\boldsymbol{\theta}|\boldsymbol{y})d\boldsymbol{\theta} \approx \sum_{k=1}^{K} \pi_G(\boldsymbol{X}_j|\boldsymbol{\theta}_k,\boldsymbol{y})\tilde{\pi}(\boldsymbol{\theta}_k|\boldsymbol{y})\delta_k.$$

Conditional posterior of η_i

In order to calculate $\tilde{\pi}(\eta_i|\boldsymbol{y})$, we first calculate $\tilde{\pi}(\eta_i|\boldsymbol{\theta},\boldsymbol{y})$. We postulate a Gaussian density for $\eta_i|\boldsymbol{\theta},\boldsymbol{y}$ such that $\tilde{\pi}(\eta_i|\boldsymbol{\theta},\boldsymbol{y}) = \pi_G(\eta_i|\boldsymbol{\theta},\boldsymbol{y})$, with mean

$$E(\boldsymbol{\eta}|\boldsymbol{\theta},\boldsymbol{y}) = \boldsymbol{A}E(\boldsymbol{X}|\boldsymbol{\theta},\boldsymbol{y}) = \boldsymbol{A}\boldsymbol{\mu}(\boldsymbol{\theta})$$

and covariance matrix

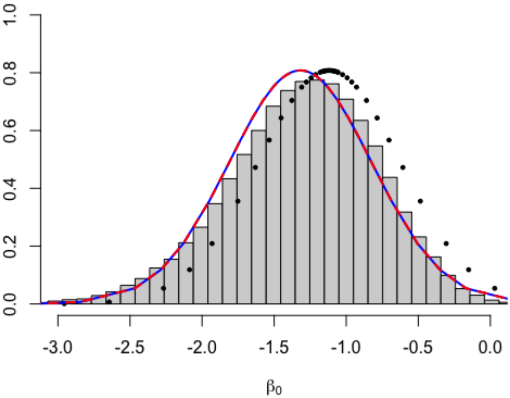
$$\text{Cov}(\boldsymbol{\eta}|\boldsymbol{\theta},\boldsymbol{y}) = \boldsymbol{A}\text{Cov}(\boldsymbol{X}|\boldsymbol{\theta},\boldsymbol{y})\boldsymbol{A}^\top,$$

VB corrected marginal posterior of η_i

$$
\begin{aligned}
\eta_j|\boldsymbol{\theta},\boldsymbol{y} &\sim N(\mu_j(\boldsymbol{\theta}),\sigma_j^2(\boldsymbol{\theta}))\\
\mu_j(\boldsymbol{\theta}) &= (\boldsymbol{A}\boldsymbol{\mu}^*(\boldsymbol{\theta}))_j\\
\tilde{\pi}(\eta_j|\boldsymbol{y}) &\approx \sum_{k=1}^{K}\pi_G(\eta_j|\boldsymbol{\theta}_k,\boldsymbol{y})\tilde{\pi}(\boldsymbol{\theta}_k|\boldsymbol{y})\delta_k.
\end{aligned}
$$

Example (small data)

$$Y_i|\beta_0 = -1, \beta_1 = -0.5 \quad \sim \quad \text{Poisson}(\exp(\beta_0 + \beta_1 X_i))$$



Example (large data)

$$Y_i|\beta_0 = -1, \beta_1 = -0.5 \quad \sim \quad \text{Poisson}(\exp(\beta_0 + \beta_1 X_i))$$

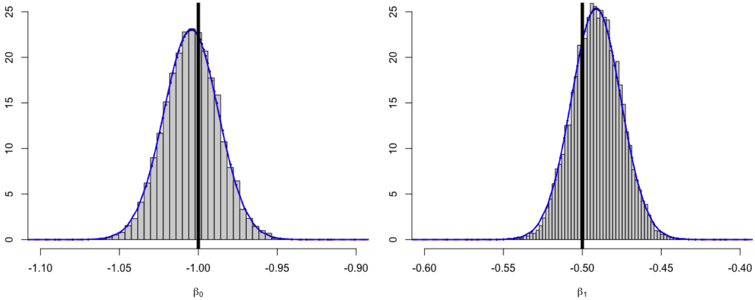


Figure: Marginal posterior of β_0 (center) and β_1 (right) from the Laplace method (points), VBC (solid line) and INLA (broken line) approximations

Tokyo example

The Tokyo dataset in the R INLA library contains information on the number of times the daily rainfall measurements in Tokyo was more than $1mm$ on a specific day t for two consecutive years. In order to model the annual rainfall pattern, a stochastic spline model with fixed precision is used to smooth the data.

$$
\begin{aligned}
y_i|\mathcal{X} &\sim Bin\left(n_i, p_i = \frac{\exp(\alpha_i)}{1+\exp(\alpha_i)}\right) \\
(\alpha_{i+1} - 2\alpha_i + \alpha_{i-1})|\tau &\overset{\text{iid}}{\sim} N(0, \tau^{-1}),
\end{aligned}
$$

where $i = 1, 2, ..., 366$ on a torus, and $n_{60} = 1$ else $n_i = 2$.

Results

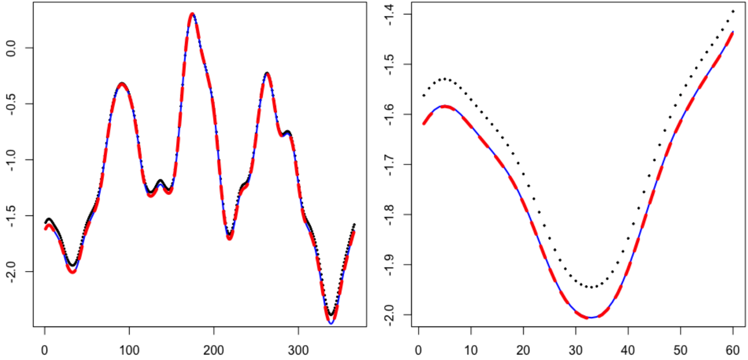
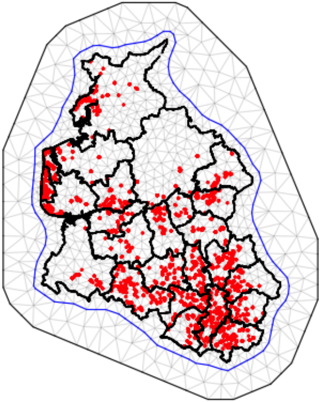


Figure: Posterior mean of α (left) (zoomed for the first two months (right)) from the Laplace method (points), VBC (solid line) and INLA (broken line)

Spatial survival example

Consider the R dataset `Leuk` that features the survival times of 1043 patients with acute myeloid leukemia (AML) in Northwest England between 1982 to 1998.



Cox spatial model

$$h(t, \boldsymbol{s}) = h_0(t) \exp(\beta \boldsymbol{X} + \boldsymbol{u}(\boldsymbol{s})),$$

with

$$\eta_i(s) = \beta_0 + \beta_1 \text{Age}_i + \beta_2 \text{WBC}_i + \beta_3 \text{TPI}_i + u(s).$$

which implies a latent field of size $m = 39158$.

Results

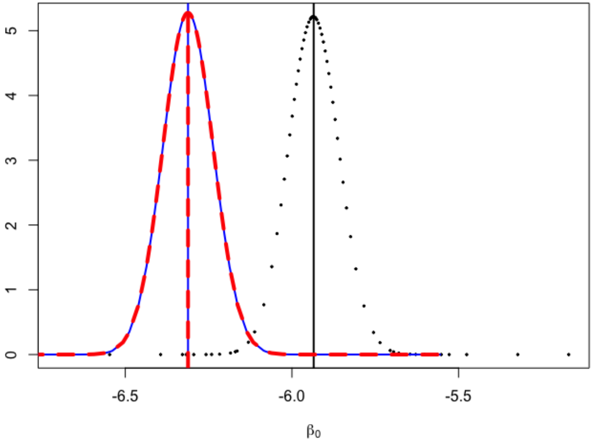


Figure: Marginal posteriors from the Laplace method (points), VBC (solid line) and INLA (broken line)

Results

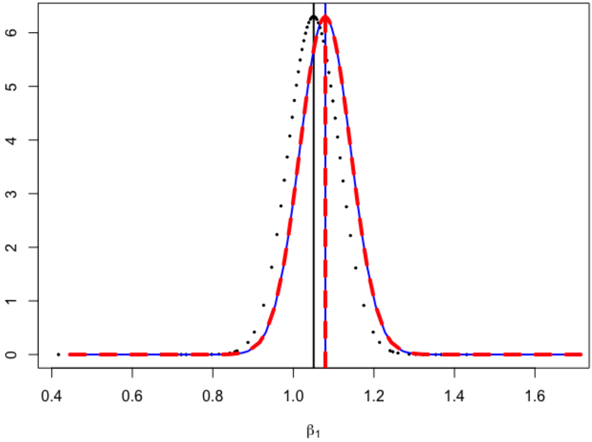


Figure: Marginal posteriors from the Laplace method (points), VBC (solid line) and INLA (broken line)

Results

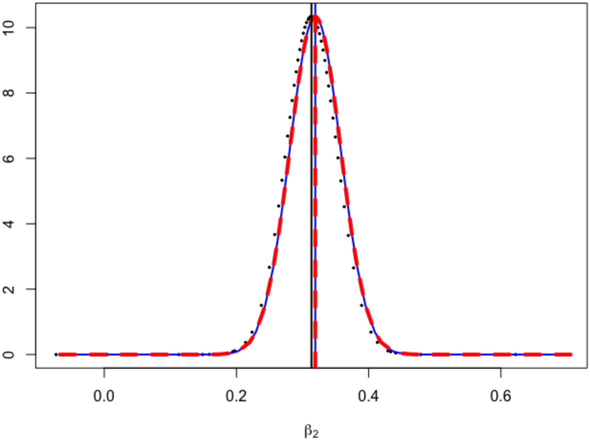


Figure: Marginal posteriors from the Laplace method (points), VBC (solid line) and INLA (broken line)

Cox proportional hazards model

We simulate survival data for n patients using the following very simple Cox proportional hazards model

$$h_i(t) = h_0(t)\exp(\beta x_i) = 1.2t^{0.2}\exp\left(0.1x_i\right), \quad 1 = 1, 2, \ldots, n,$$

where x is a scaled and centered continuous covariate, and the baseline hazard, $h_0(t)$ is estimated using a scaled random walk order one model with 50 bins. We also consider four different values of n which are $n = 10^2$, to 10^5.

Cox proportional hazards model

n	Augmented size	classic INLA (s)	modern INLA (s)
10^2	1 327	1.6	0.1
10^3	12 657	1.3	0.4
10^4	131 807	10.2	2.3
10^5	1 302 413	113.3	22.5

Table: Results from simulation of Cox proportional hazards model

cs-fMRI model

Functional magnetic resonance imaging (fMRI) is a noninvasive neuro-imaging technique used to localize regions of specific brain activity during certain tasks.
For T timepoints and N vertices per hemisphere resulting in data $\boldsymbol{y}_{TN\times 1}$ with the latent Gaussian model as follows:

$$
\begin{aligned}
\boldsymbol{y}|\beta, \boldsymbol{b}, \boldsymbol{\theta} &\sim N(\boldsymbol{\mu}_y, \boldsymbol{V}), \quad \boldsymbol{\mu}_y = \sum_{k=0}^{K} \boldsymbol{X}_k \beta_k + \sum_{j=1}^{J} \boldsymbol{Z}_j \boldsymbol{b}_j \\
\beta_k &= \boldsymbol{\Psi}_k \boldsymbol{w}_k \quad \text{(SPDE prior on } \beta_k\text{)} \\
\boldsymbol{w}_k|\boldsymbol{\theta} &\sim N(\boldsymbol{0}, \boldsymbol{Q}^{-1}_{\tau_k,\kappa_k}) \\
\boldsymbol{b}_j &\sim N(\boldsymbol{0}, \delta \boldsymbol{I}) \quad \text{(Diffuse priors for } \boldsymbol{b}_j\text{)} \\
\boldsymbol{\theta} &\sim \pi(\boldsymbol{\theta}),
\end{aligned}
$$

where we have K task signals and J nuisance signals.

cs-fMRI model

The data consists of a 3.5-min fMRI for each subject, consisting of 284 volumes, where each subject performs 5 different motor tasks interceded with a 3 second visual cue. Each hemisphere of the brain contained 32492 surface vertices. From these, 5000 are resampled to use for the analysis. This results in a response data vector $\boldsymbol{y}$ of size **2 523 624**, with an SPDE model defined on a mesh with 8795 triangles.

The inference based on the modern formulation of INLA was computed in 148 seconds.

cs-fMRI model

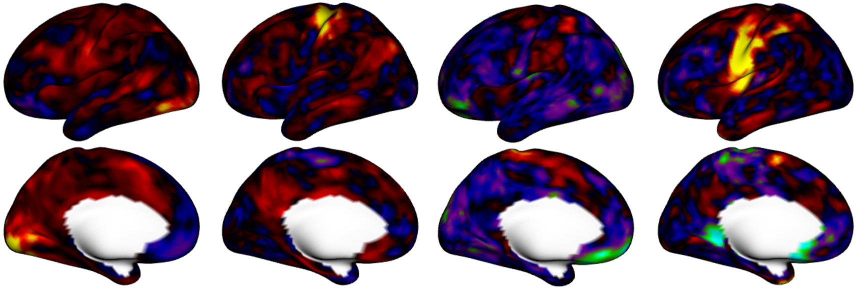


Figure: Activation areas for the different tasks in the left hemisphere - visual cue, right hand motor, right foot motor, tongue motor task (from left to right)

Further details

`www.r-inla.org`

New default setting in INLA (VB) (previously inla.mode = "experimental")

- INLA can fit many different statistical models and complex models can be built using multiple "building blocks"/random effects.
- Remove the linear predictors from the latent field $\rightarrow$ accurate posterior inference with VB correction (I - VB - LA)
- New applications that aren't feasible with INLA 1.0

- Gaedke-Merzhäuser, L., van Niekerk, J., Schenk, O., and Rue, H. (2023).
  Parallelized integrated nested Laplace approximations for fast Bayesian inference.
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  A new avenue for Bayesian inference with INLA.
  Computational Statistics & Data Analysis, 181:107692.

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  Journal of Machine Learning Research, 25(62):1–25.

Thank you • شكرا

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