

# Inference methods for extended latent Gaussian models

Waterloo SAS Student Seminar Series

Adam Howes

Imperial College London

October 2022

# Motivation

- Surveillance of the HIV epidemic in sub-Saharan Africa
- Want to estimate indicators used for monitoring and response, including:
  - Prevalence  $\rho$ : the proportion of people who are HIV positive
  - Incidence  $\lambda$ : the proportion of people newly infected
  - Treatment coverage  $\alpha$ : the proportion of PLHIV on treatment
- We would like to provide them at a local, district-level
- This is a challenging task! Data is noisy, sparse and biased

## A simple small-area model for prevalence

- Consider areas  $i = 1, \dots, n$
- Simple random sample household-survey taken in each area, with sample sizes  $m_i^{\text{HS}}$
- The number of people testing positive is  $y_i^{\text{HS}}$
- Then we can use a binomial logistic regression of the form:

$$y_i^{\text{HS}} \sim \text{Bin}(m_i^{\text{HS}}, \rho_i^{\text{HS}}),$$
$$\text{logit}(\rho_i^{\text{HS}}) \sim g(\vartheta^{\text{HS}}), \quad i = 1, \dots, n,$$

- If  $g$  is Gaussian then this is a latent Gaussian model in the sense of Rue, Martino, and Chopin (2009)
- We usually set up  $g$  as a spatial smoother, because the sample sizes in each area are too small to get reliable direct estimates
- One problem with the above model is that household surveys are expensive to run, so they only happen rarely

# Latent Gaussian models

- Three-stage Bayesian hierarchical model

$$\text{(Observations)} \quad \mathbf{y} \sim p(\mathbf{y} | \mathbf{x}),$$

$$\text{(Latent field)} \quad \mathbf{x} \sim p(\mathbf{x} | \boldsymbol{\theta}),$$

$$\text{(Hyperparameters)} \quad \boldsymbol{\theta} \sim p(\boldsymbol{\theta}),$$

where  $\mathbf{y} = (y_1, \dots, y_n)$ ,  $\mathbf{x} = (x_1, \dots, x_n)$ ,  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_m)$

- Interested in learning both  $(\boldsymbol{\theta}, \mathbf{x})$  from data  $\mathbf{y}$
- If the middle layer is Gaussian, then it's a latent Gaussian model

$$\text{(Latent field)} \quad p(\mathbf{x} | \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}(\boldsymbol{\theta}), \mathbf{Q}(\boldsymbol{\theta})^{-1}).$$

- Covers most of the models commonly used in spatiotemporal statistics
- Latent field is typically indexed by spatiotemporal location, such that  $n > m$

## Adding ANC surveillance

- Pregnant women attending antenatal care clinics are routinely tested for HIV, to avoid mother-to-child transmission
- This data source is more real-time than household surveys, but it's also more biased, because attendees are unlikely to be as representative of the population
- But perhaps this bias is consistent, in which case we can still make use of the ANC data to improve our model!

## Adding ANC surveillance

- Suppose of  $m_i^{\text{ANC}}$  women attending ANC,  $y_i^{\text{ANC}}$  are HIV positive, then we can use another binomial logistic regression:

$$\begin{aligned}y_i^{\text{ANC}} &\sim \text{Bin}(m_i^{\text{ANC}}, \rho_i^{\text{ANC}}), \\ \text{logit}(\rho_i^{\text{ANC}}) &= \text{logit}(\rho_i^{\text{HS}}) + b_i, \\ b_i &\sim \mathcal{N}(\beta_b, \sigma_b^2),\end{aligned}$$

- Similar to using  $\rho_i^{\text{ANC}}$  as a covariate in our model for household survey prevalence, but this way we allow it to vary rather than be fixed

## Adding ART coverage

- Remember that we're also interested in what proportion of PLHIV are receiving treatment
- To estimate this, we need first to know the number of PLHIV

$$H_i = N_i \rho_i^{\text{HS}}$$

- Then

$$A_i \sim \text{Bin}(N_i, \rho_i^{\text{HS}} \alpha_i),$$
$$\text{logit}(\alpha_i) \sim \mathcal{N}(\beta_\alpha, \sigma_\alpha^2),$$

# Naomi evidence synthesis model

- Combining these three modules is the basis of the Naomi evidence synthesis model
- Used by countries (which provide their own data) to produce HIV estimates in a yearly process supported by UNAIDS
- Can't run long MCMC in this setting, requires fast, accurate, approximations
- It's a complicated model, and requires something more flexible than R-INLA
- Currently using Template Model Builder TMB (Kristensen et al. 2015)



Figure 1: A supermodel



# Template Model Builder

- So what is TMB?
- R package which implements the Laplace approximation for latent variable models using automatic differentiation (via CppAD)
  - For more about AD see e.g. Griewank and Walther (2008)
  - Useful for getting the mode, Hessian
- Write an objective function  $f(\mathbf{x}, \boldsymbol{\theta})$  in C++ (“user template”)
  - We select  $f(\mathbf{x}, \boldsymbol{\theta}) = -\log p(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta})p(\mathbf{x} | \boldsymbol{\theta})p(\boldsymbol{\theta})$

# Template Model Builder

```
#include <TMB.hpp>
```

```
template <class Type>
```

```
Type objective_function<Type>::operator>()() {
```

```
  // Define data e.g.
```

```
  DATA_VECTOR(y);
```

```
  // Define parameters e.g.
```

```
  PARAMETER(mu);
```

```
  // Calculate negative log-likelihood e.g.
```

```
  nll = Type(0.0);
```

```
  nll -= dnorm(y, mu, 1, true).sum()
```

```
  return(nll);
```

```
}
```

# Template Model Builder

- Performs the Laplace approximation  $L_f(\boldsymbol{\theta}) \approx L_f^*(\boldsymbol{\theta})$  and use R to optimise this with respect to  $\boldsymbol{\theta}$  to give  $\hat{\boldsymbol{\theta}}$  (the central point in Figure 2)
  - This is done by specifying the `random` argument to be the parameters that you want to integrate out with a Laplace approximation (the latent field)
- MAP estimate of  $\mathbf{x}$  conditional on  $\hat{\boldsymbol{\theta}}$
- Standard errors calculated using the  $\delta$ -method (a Gaussian assumption)

# Integrated Nested Laplace Approximation

- Suggested reading: the paper (Rue, Martino, and Chopin 2009) or a book e.g. Blangiardo and Cameletti (2015)
- Approximate Bayesian inference for **latent Gaussian models** (LGMs), which recall are three-stage models with middle layer

$$\text{(Latent field)} \quad p(\mathbf{x} \mid \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}(\boldsymbol{\theta}), \mathbf{Q}(\boldsymbol{\theta})^{-1}).$$

- R-INLA implementation takes advantage of sparsity properties of  $\mathbf{Q}(\boldsymbol{\theta})$ , i.e. if  $\mathbf{x}$  is a Gaussian Markov random field (GMRF)

# Integrated Nested Laplace Approximation

- Gives approximate **posterior marginals**  $\{\tilde{p}(x_i | \mathbf{y})\}_{i=1}^n$  and  $\{\tilde{p}(\theta_j | \mathbf{y})\}_{j=1}^m$
- To approximate posterior marginals below requires  $\tilde{p}(\boldsymbol{\theta} | \mathbf{y})$  and  $\tilde{p}(x_i | \boldsymbol{\theta}, \mathbf{y})$

$$p(x_i | \mathbf{y}) = \int p(x_i, \boldsymbol{\theta} | \mathbf{y}) d\boldsymbol{\theta} = \int p(x_i | \boldsymbol{\theta}, \mathbf{y}) p(\boldsymbol{\theta} | \mathbf{y}) d\boldsymbol{\theta}, \quad i = 1, \dots, n, \quad (1)$$

$$p(\theta_j | \mathbf{y}) = \int p(\boldsymbol{\theta} | \mathbf{y}) d\boldsymbol{\theta}_{-j} \quad j = 1, \dots, m. \quad (2)$$

# Integrated Nested Laplace Approximation

1) First Laplace approximate hyperparameter posterior

$$\tilde{p}(\boldsymbol{\theta} | \mathbf{y}) \propto \frac{p(\mathbf{y}, \mathbf{x}, \boldsymbol{\theta})}{\tilde{p}_G(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y})} \Big|_{\mathbf{x}=\boldsymbol{\mu}^*(\boldsymbol{\theta})} \quad (3)$$

which can be marginalised to get  $\tilde{p}(\theta_j | \mathbf{y})$

- Note: this involves integrating out a Gaussian approximation to the latent field, which we denote by  $p_G(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y})$

# Integrated Nested Laplace Approximation

- 2) In both (1) and (2) we want to integrate w.r.t. (3), so choose integration points and weights  $\{\boldsymbol{\theta}^{(k)}, \Delta^{(k)}\}$
- For low  $m$  R-INLA uses a grid-strategy (illustrated in the next slide)
  - For larger  $m$  this becomes too expensive and R-INLA uses a CCD design is used
  - Other approaches, like adaptive Gaussian Hermite quadrature (AGHQ) have recently been shown to have theoretical guarantees (Bilodeau, Stringer, and Tang 2021) and may be preferable

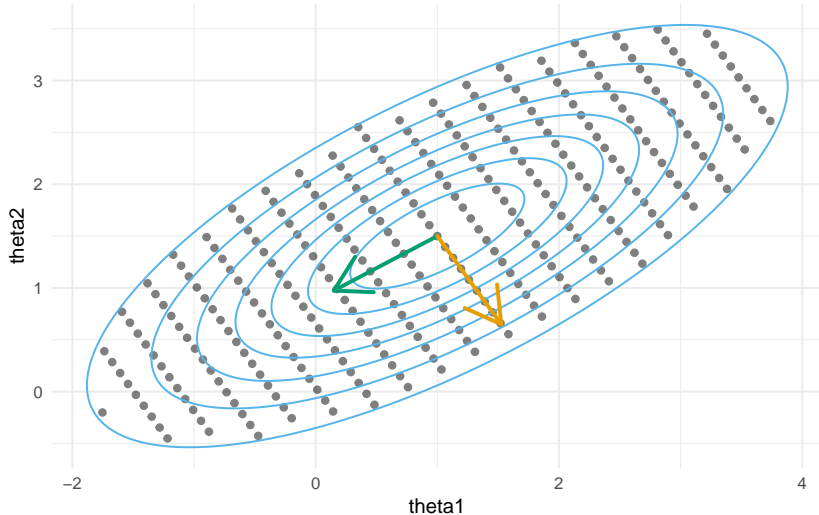


Figure 2: An illustration of the R-INLA grid method for selecting integration points using a toy bivariate Gaussian distribution for  $\theta$ . Start at the mode and work outwards along the eigenvectors until the density drops sufficiently low.



# Adaptive Gaussian Hermite Quadrature

- `aghq` R package and vignette (Stringer 2021)
- Gauss-Hermite quadrature is a way of picking nodes and weights, and is based on the theory of polynomial interpolation
- The adaptive part means that it uses the location (mode) and curvature (Hessian) of the target (posterior)
- Use  $k$  quadrature points
  - If  $k$  is odd then they include the mode
  - If  $k = 1$  then it's a Laplace approximation
  - In the vignette  $k = 3$  (for each dimension, so  $3^m$  total) is chosen quite often

# Integrated Nested Laplace Approximation

3) Choose approximation for  $\tilde{p}(x_i | \boldsymbol{\theta}, \mathbf{y})$

- Simplest version (Rue and Martino 2007) is to marginalise the  $p_G(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y})$

$$\tilde{p}(x_i | \boldsymbol{\theta}, \mathbf{y}) = \mathcal{N}(x_i | \mu_i^*(\boldsymbol{\theta}), 1/q_i^*(\boldsymbol{\theta})) \quad (4)$$

- The above is referred to as method = "gaussian" in R-INLA
- There are two better, more complex approximations
  - Confusingly called "simplified laplace" and "laplace"

# Integrated Nested Laplace Approximation

4) Finally (!) use quadrature combining

- our approximation  $p(\boldsymbol{\theta} | \mathbf{y})$  from step 1),
- our integration points and weights  $\{\boldsymbol{\theta}^{(k)}, \Delta^{(k)}\}$  from step 2),
- and our approximation  $\tilde{p}(x_i | \boldsymbol{\theta}, \mathbf{y})$  from step 3) to give

$$\tilde{p}(x_i | \mathbf{y}) = \sum_{k=1}^K \tilde{p}(x_i | \boldsymbol{\theta}^{(k)}, \mathbf{y}) \times \tilde{p}(\boldsymbol{\theta}^{(k)} | \mathbf{y}) \times \Delta^{(k)} \quad (5)$$

# Experiments

- We would like to find an accurate way to do inference for the Naomi model
- It also needs to be fast enough to use in production!

# Experiments

- We wrote a simplified version of the Naomi model up in TMB
  - This allowed us to test three inference methods **all using precisely the same model and C++ code**
1. A direct Gaussian approximation via TMB
  2. Adaptive Gaussian Hermite quadrature via `aghq`
  3. No-U-Turn Sampling (NUTS – a type of Hamiltonian Monte Carlo) via `tmbstan`
- Note: using different software it is often very difficult to ensure the model is precisely the same, so we're very fortunate here

## Comparison approach

- You could look at the summaries like the mean and standard deviation of each of the posterior marginals
  - Any approximation method should be pretty good at getting the mean right
  - Gaussian approximations should be good at getting the second moment right
- It's probably better to compare the whole posterior distributions
- One way to do this is via Kolmogorov-Smirnov statistics, which give the maximum difference between two empirical CDFs

## References I

- Bilodeau, Blair, Alex Stringer, and Yanbo Tang. 2021. "Stochastic Convergence Rates and Applications of Adaptive Quadrature in Bayesian Inference." <https://arxiv.org/abs/2102.06801>.
- Blangiardo, Marta, and Michela Cameletti. 2015. *Spatial and spatio-temporal Bayesian models with R-INLA*. John Wiley & Sons.
- Griewank, Andreas, and Andrea Walther. 2008. *Evaluating derivatives: principles and techniques of algorithmic differentiation*. Vol. 105. Siam.
- Kristensen, Kasper, Anders Nielsen, Casper W Berg, Hans Skaug, and Brad Bell. 2015. "TMB: automatic differentiation and Laplace approximation." *arXiv Preprint arXiv:1509.00660*.
- Rue, Håvard, and Sara Martino. 2007. "Approximate Bayesian inference for hierarchical Gaussian Markov random field models." *Journal of Statistical Planning and Inference* 137 (10): 3177–92.

## References II

- Rue, Håvard, Sara Martino, and Nicolas Chopin. 2009. "Approximate Bayesian inference for latent Gaussian models by using integrated nested Laplace approximations." *Journal of the Royal Statistical Society: Series b (Statistical Methodology)* 71 (2): 319–92.
- Stringer, Alex. 2021. "Implementing Approximate Bayesian Inference Using Adaptive Quadrature: The Aghq Package."  
<https://arxiv.org/abs/2101.04468>.