Deterministic Bayesian inference methods for the Naomi model

HIV Inference Lab Group Meeting

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Bayesian modelling and inference

- As a statistical modeller, the bulk of our job is in constructing a generative model for data y using parameters ϑ
- This is the joint distribution $p(y, \vartheta) = p(y \mid \vartheta)p(\vartheta)$
- Then, we want to compute (ideally without having to think much about it) the posterior $p(\vartheta \mid y)$ which is just[1]

$$p(\vartheta \mid y) = \frac{p(y, \vartheta)}{p(y)} = \frac{p(y \mid \vartheta)p(\vartheta)}{p(y)}$$

- The central problem of Bayesian inference is doing the following integral

$$p(y) = \int p(y, \vartheta) \mathrm{d}\vartheta$$

[1] I've highlighted this with sarcasm in mind: it's a difficult problem

Numerical integration

- If you want to integrate something deterministically, you could use numerical integration, otherwise called quadrature
- Select nodes $\vartheta \in \mathcal{Q} \subset \Theta$ and weights $\omega : \Theta \to \mathbb{R}$ then compute the sum

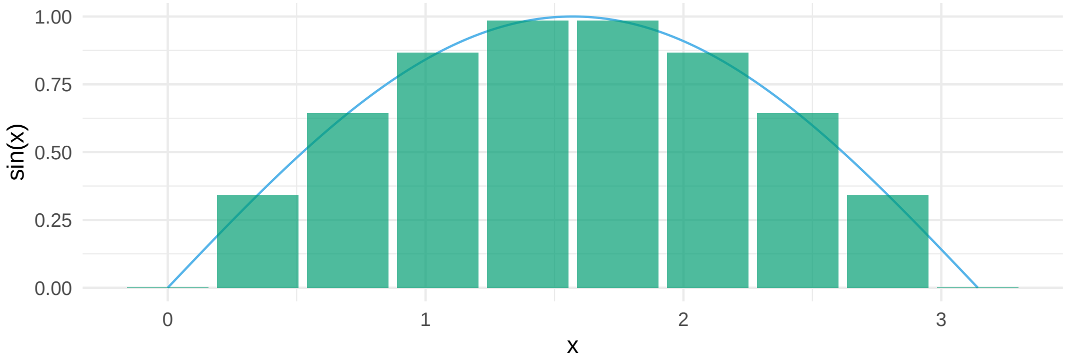
$$\tilde{p}(y) = \sum_{\vartheta \in \mathcal{Q}} p(y, \vartheta)\omega(\vartheta)$$

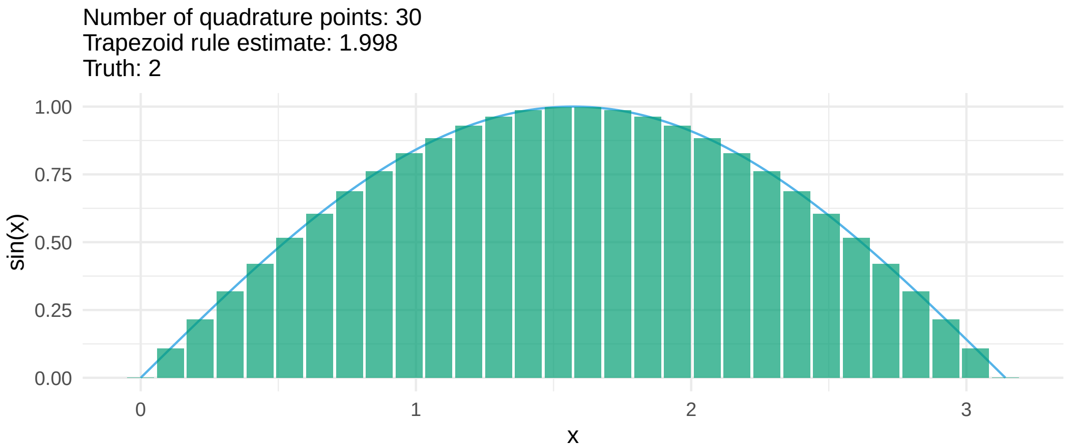
Naive quadrature example

- Remember how integration is taught? (Rienmann sums)
- Try computing $\int_0^\pi \sin(x)\mathrm{d}x = 2$ using trapezoid rule

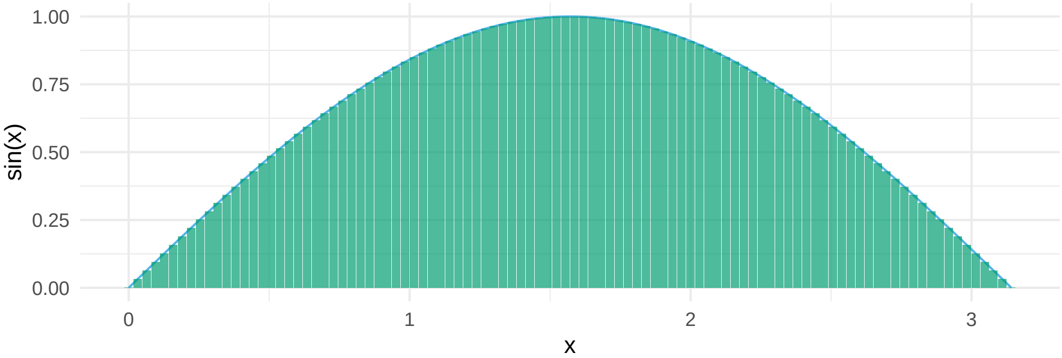
```
trapezoid_rule <- function(x, spacing) {
  w <- rep(spacing, length(x))
  w[1] <- w[1] / 2
  w[length(x)] <- w[length(x)] / 2
  sum(w * x)
}
```

Number of quadrature points: 10
Trapezoid rule estimate: 1.98
Truth: 2




Number of quadrature points: 30
Trapezoid rule estimate: 1.998
Truth: 2
1.00
0.75
0.50
0.25
0.00
sin(x)
0
1
2
3
x

Number of quadrature points: 100
Trapezoid rule estimate: 2
Truth: 2



Monte Carlo as an example of numerical integration

- Suppose we can sample $\vartheta_i \sim p(y, \vartheta)$ for $i = 1, \dots, N$
- If we set $\omega(\vartheta_i) = 1/N$ for all i then we get a **Monte Carlo** (MC) estimate

$$\tilde{p}(y) = \frac{1}{N} \sum_i p(y, \vartheta_i)$$

- For complicated models[2] it's not possible to sample directly from $p(y, \vartheta)$, but we can usually sample from a Markov chain which if you squint a bit is good enough (MCMC)

[2] Or not even that complicated

Monte Carlo is fundamentally unsound

- "Monte Carlo ignores information" according to O'Hagan (1987)
- Suppose $N = 3$ and we sample $\vartheta_1, \vartheta_2, \vartheta_3$ with $\vartheta_2 = \vartheta_3$ then our MC estimate is
$$\tilde{p}(y) = \frac{1}{3}\left(p(y, \vartheta_1) + p(y, \vartheta_2) + p(y, \vartheta_3)\right)$$
- This is despite the fact that nothing new about the function has been learned by adding $\{\vartheta_3, p(y, \vartheta_3)\}$

Application to HIV survey sampling

- This is a digression but...
- Say we're running a household survey, and sample the same individual twice
- We didn't learn anything new about HIV by surveying them again!
- This doesn't just bite for nodes or individuals which are exactly the same: an analogous argument can be made if they are close together and we expect their function evaluations to be similar

$\implies$ Bayesian quadrature, Bayesian survey design
For some half-baked thoughts, see athowes.github.io/fourth-gen/paper.pdf

Latent variables and hyperparameters

- Quadrature doesn't work very well when $\dim(\vartheta)$ gets even moderately sized
  - If you're using k points per dimension it's $k^{\dim(\vartheta)}$
- Previously all of the parameters were under the symbol ϑ – what if we split them up as being $\vartheta = (x, \theta)$
- The key part about this is that $\dim(x) = N$ is big and $\dim(\theta) = m$ is small

Names for x	Names for θ
Latent variables, random effects, latent field	Hyperparameters, fixed effects

Spatio-temporal statistics

- There is nothing inherently special about spatio-temporal statistics, but we do often end up in similar situations because of the structures of the problems we tackle
- We have observations indexed by space $s \in \mathcal{S}$ and time $t \in \mathcal{T}$
- Usually we associate parameters to spatio-temporal locations as well as observations
- This ends up with us having something like $\{x_{s,t}\}$

What's important about this?

1. There might be a lot of spatio-temporal locations, so $\dim(x)$ might be pretty big! If you have 100 districts and 10 years, that's already $100 \times 10 = 1000$ parameters
2. Perhaps we're willing to make quite strong assumptions about how things vary over space-time[3]

- Not IID anymore!

[3] Are there any slides about spatial statistics that don't describe Tobler's first law of geography?

Latent Gaussian models

- A latent Gaussian model (LGM) (Rue, Martino, and Chopin 2009) looks along these lines:

$$\begin{aligned}
&\text{(Observations)} && y \sim p(y \mid x, \theta), \\
&\text{(Latent field)} && x \sim \mathcal{N}(x \mid \mu(\theta), Q(\theta)^{-1}), \\
&\text{(Hyperparameters)} && \theta \sim p(\theta).
\end{aligned}$$

- Many models are LGMs, especially in spatio-temporal statistics
- $\dim(x) = n$, $\dim(x) = N$, $\dim(\theta) = m$

Laplace approximation

- Remember that we wanted to compute

$$p(y) = \int p(y, \vartheta) \mathrm{d}\vartheta$$

- One trick for doing this is to pretend $p(\vartheta \mid y)$ is Gaussian

  - Mode $\hat{\vartheta} = \arg\max_{\vartheta} \log p(y, \vartheta)$
  - Hessian $H(\hat{\vartheta}) = -\partial^2_{\vartheta} \log p(y, \vartheta)|_{\vartheta = \hat{\vartheta}}$
  - Gaussian approximation $\implies \tilde{p}_{\mathrm{G}}(\vartheta \mid y) = \mathcal{N}(\vartheta \mid \hat{\vartheta}, H(\hat{\vartheta})^{-1})$

Example of computing the Laplace approximation

- Consider the following model for $i = 1, \ldots, n$ with fixed a and b

$$y_i \sim \text{Poisson}(\lambda), \quad \lambda \sim \text{Gamma}(a, b).$$

- It's conjugate so we directly know that

$$\lambda \mid y \sim \text{Gamma}(a + \sum_i y_i, b + n)$$

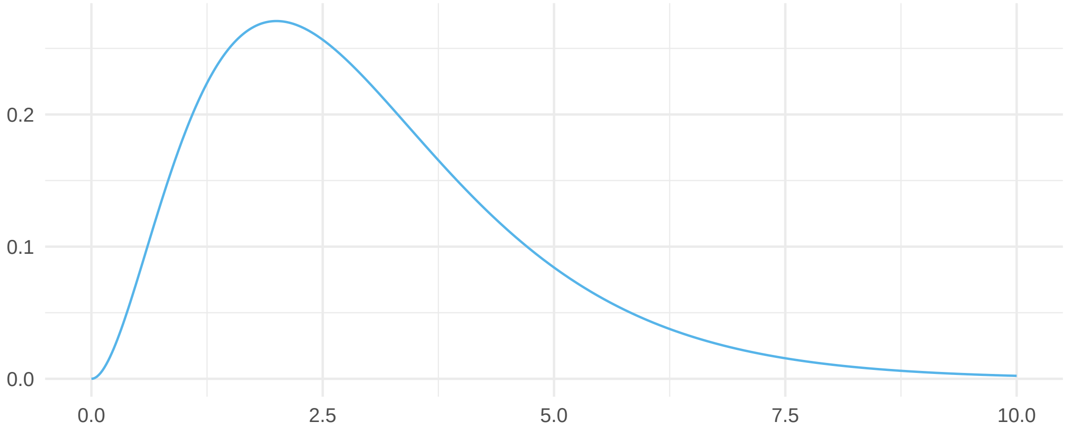


Figure 1: A Gamma prior with $a = 3$ and $b = 1$.

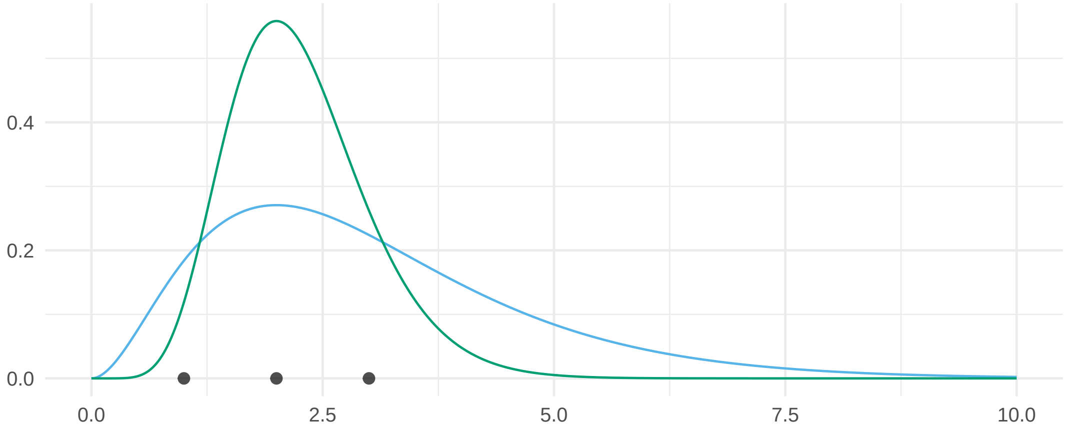


Figure 2: Draw 3 points from Poisson(3), then compute the posterior.

```r
fn <- function(x) dgamma(x, a + sum(y), b + length(y), log = TRUE)

# Here we are using numerical derivatives rather than automatic
ff <- list(
  fn = fn,
  gr = function(x) numDeriv::grad(fn, x),
  he = function(x) numDeriv::hessian(fn, x)
)

opt_bfgs <- aghq::optimize_theta(
  ff, 1, control = aghq::default_control(method = "BFGS")
)
```

Laplace approximation

```
laplace <- posterior +
  stat_function(
    data = data.frame(x = c(0, 10)),
    aes(x),
    fun = dnorm,
    n = 500,
    args = list(mean = opt_bfgs$mode, sd = sqrt(1 / opt_bfgs$hessian)),
    col = cbpalette[3]
  )
```

Laplace approximation

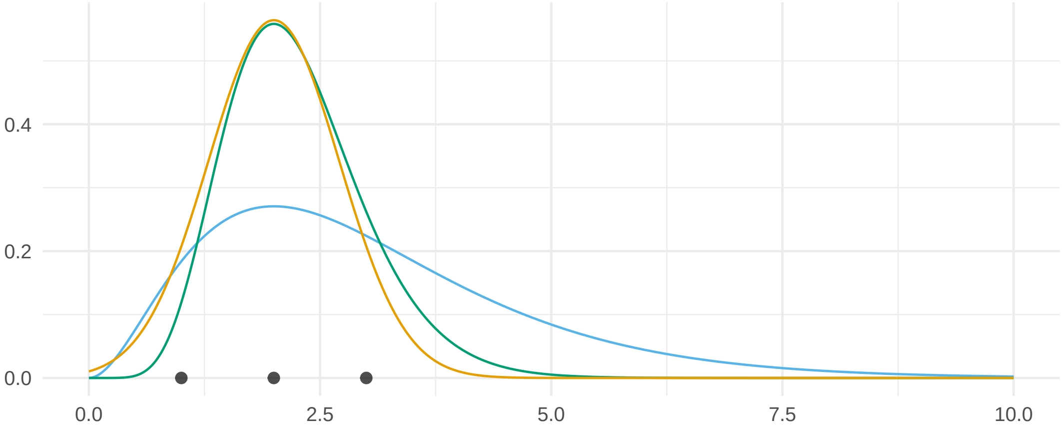


Figure 3: The Laplace approximation matches the true posterior near the mode but it's not great in the tails.

Laplace approximation

- Now
$$p(y) = \frac{p(\vartheta, y)}{p(\vartheta \mid y)} \approx \frac{p(\vartheta, y)}{p_{\mathrm{G}}(\vartheta \mid y)}$$
and we can evaluate RHS where we would like, so let's pick the point at which the Gaussian is most accurate, which is $\hat{\vartheta}$
$$p_{\mathrm{LA}}(y) = \frac{p(\vartheta, y)}{p_{\mathrm{G}}(\vartheta \mid y)}\Big|_{\vartheta=\hat{\vartheta}} = (2\pi)^{\mathrm{dim}(\vartheta)/2} \det(H(\hat{\vartheta}))^{-1/2} p(\hat{\vartheta}, y)$$

Marginal Laplace approximation

- Hey wait a second, is it reasonable to just assume $p(\vartheta \mid y)$ is Gaussian?
- No, not in general. But...

1. We just described a class of models (LGMs) where some subset of the parameters (x) have a Gaussian prior $\implies$ it's a lot more reasonable to think that they would have a marginal posterior which is close to Gaussian
2. We just talked about how big x is in comparison to θ! $\implies$ most of the work in our integral can be done using a **marginal Laplace** approximation to get rid of x

Generalist versus specialist methods

Dichotomy in statistical inference methods:

1. Generalist: works in all situations
2. Specialist: "exploits" properties of the problem at hand

We are taking approach 2!

Marginal Laplace approximation

- What does this look like? Instead of assuming $p(\vartheta \mid y) = p(x, \theta \mid y)$ is Gaussian we assume $p(x \mid \theta, y)$ is

$$\tilde{p}_{\mathrm{G}}(x \mid \theta, y) = \mathcal{N}(x \mid \hat{x}, H(\hat{x}))^{-1}$$

  where $\hat{x} = \hat{x}(\theta)$
- Now the marginal Laplace approximation is

$$p_{\mathrm{LA}}(\theta, y) = \frac{p(x, \theta, y)}{\tilde{p}_{\mathrm{G}}(x \mid \theta, y)}\Big|_{x=\hat{x}} = (2\pi)^{N/2} \det(H(\hat{x}))^{-1/2} p(\hat{x}, \theta, y)$$

Integrated nested Laplace approximation

- Now we can compute $p_{\mathrm{LA}}(\theta, y)$ but what we really want is still $p(y)$
- But hopefully[4] the dimension of θ is small enough that we can now tackle this with quadrature
- So pick some nodes $\mathcal{Q}$ and a weighting function ω and away we go

$$p(y) \approx \sum_{\theta \in \mathcal{Q}} p_{\mathrm{LA}}(\theta, y)\omega(\theta)$$

- This is the famous integrated nested Laplace approximation (INLA)

[4] Really: hopefully

Taking stock

1. Bayesian inference is integration
2. Spatial statistics has parameters (x, θ)
3. Integrate x cheaply using a Gaussian assumption
4. Try a bit harder with θ performing quadrature

Now let's apply this to a difficult problem in HIV inference!

The Naomi model

- Naomi is a spatial evidence synthesis model
- Used by countries to produce HIV estimates in a yearly process supported by UNAIDS
- Inference for Naomi is currently conducted using `TMB` by optimising $p_{\texttt{LA}}(\theta, y)$, and has to be pretty quick to allow for interactive review and development of estimates

Figure 4: A supermodel

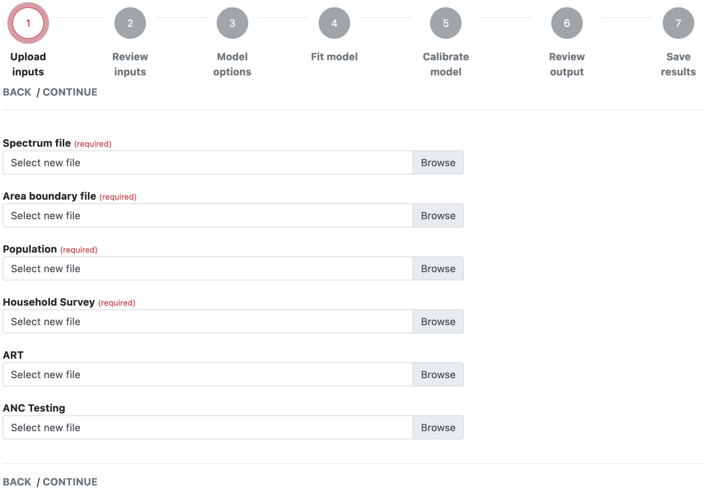


Figure 5: Example of the user interface from https://naomi.unaids.org/

Template Model Builder refresher

- TMB (Kristensen et al. 2015) is an R package which implements the Laplace approximation for latent variable models
- To use TMB, you write your objective function $-\log p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}) p(\mathbf{x} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})$ in TMB's C++ syntax
- For example, for the model $\mathbf{y} \sim \mathcal{N}(\mu, 1)$ with $p(\mu) \propto 1$ then the TMB user template looks as follows

```
#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);
}
```

Why do we use TMB

- It runs quickly, and is flexible enough to write the model
- Another answer: we don't have any better options
  - Markov chain Monte Carlo (MCMC) is accurate (eventually) but takes too long
  - Though Naomi is a spatial model with a large Gaussian latent field, it isn't technically a latent Gaussian model, and isn't compatible with the R-INLA implementation of INLA

Idea

- Implement an algorithm similar to INLA which

1. is compatible with Naomi
2. uses `TMB` to perform Laplace approximation

- Does this improves the quality of the inferences we get?

Not a new idea!

> *My main comment is that several aspects of the computational machineery that is presented by Rue and his colleagues* ***could benefit from the use of a numerical technique known as automatic differentiation (AD)*** *... By the use of AD one could obtain a system that is automatic from a user's perspective... the benefit would be a fast, flexible and easy-to-use system for doing Bayesian analysis in models with Gaussian latent variables*

– Hans J. Skaug (coauthor of `TMB`), RSS discussion of Rue, Martino, and Chopin (2009)

Meanwhile in Canada...

- Alex Stringer in Toronto $\to$ Waterloo had been thinking along similar lines, and made a lot of progress

1. Implementing an algorithm similar to INLA, using a specific quadrature rule $\mathcal{Q}$ called adaptive Gauss-Hermite quadrature (AGHQ) which he and others argue should be the default for this problem
2. Defining a class of models called extended latent Gaussian models (ELGMs) which Naomi fits into

- I will explain what both of these acronyms (AGHQ[5] and ELGM) mean!

[5] Amusingly similar to AGYW: adolescent girls and young women

Gauss-Hermite quadrature

- Recall

$$\int f(z)\mathrm{d}z \approx \sum_{z \in \mathcal{Q}} f(z)\omega(z)$$

- Replace $f(z)$ by $\phi(z)f(z)$ and say that f is a polynomial and ϕ is unknown
- Suppose that $\phi(z) = \exp(-z^2)$

Adaptation

- The nodes and weights we use should probably depend on the integrand
  - Especially when the integrand is also a function of y as in $p(y, \vartheta)$
- Let $z \in \mathcal{Q}(m, k)$ then $\theta(z) = \hat{\theta} + Lz$ where L is the lower Cholesky of $H(\hat{\theta})$

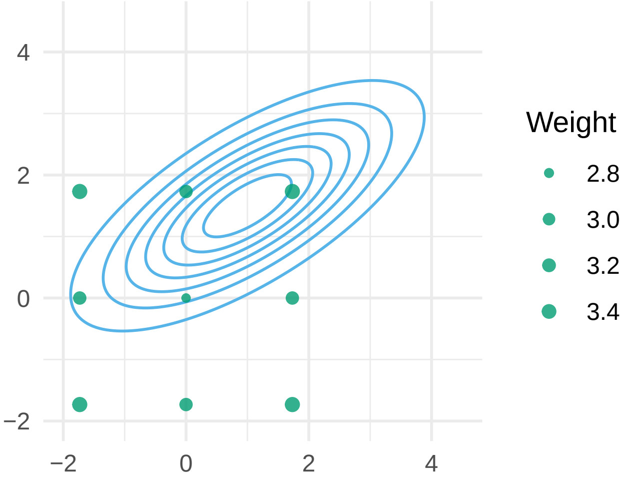


Figure 6: Unadapted points in two dimensions with $k = 3$.

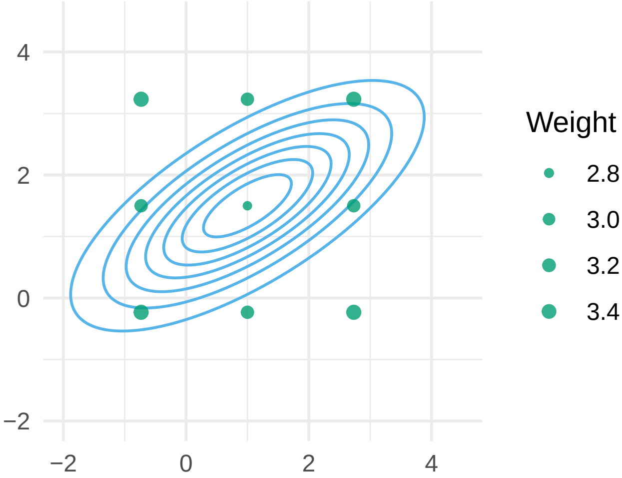


Figure 7: Add the mean.

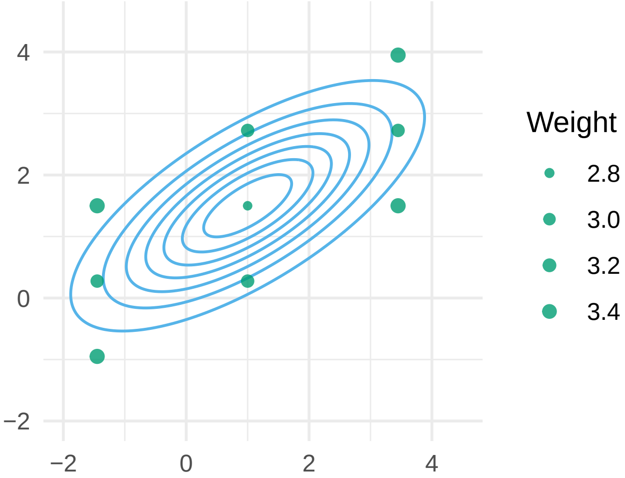


Figure 8: Rotate by the lower Cholesky.

Extended latent Gaussian models

- To explain what an extended latent Gaussian model (ELGM) is, we need a little more detail on LGMs
- In an LGM the conditional mean depends on exactly one structured additive predictor, specifically

$$
\begin{aligned}
y_i &\sim p(y_i \mid \eta_i, \theta_1), \quad i \in [n] \\
\mu_i &= \mathbb{E}(y_i \mid \eta_i) = g(\eta_i), \\
\eta_i &= \beta_0 + \sum_{l=1}^{p} \beta_j z_{ji} + \sum_{k=1}^{r} f_k(u_{ki}),
\end{aligned}
$$

Extended latent Gaussian models

- ELGM remove this requirement such that

$$\mu_i = g(\eta_{\mathcal{J}_i})$$

  where $g_i : \mathbb{R}^{|\mathcal{J}_i|} \to \mathbb{R}$ and $\mathcal{J}_\rangle$ is some set of indices
- This allow for a higher degree of non-linearity in the model

Why is Naomi an ELGM?

	Things I thought made Naomi an ELGM	Does it actually?
1	ANC offset from household survey	?
2	Incidence depends on adult prevalence and coverage	?
3	ART attendance is a product	?
4	ART attendance uses a multinomial	?
5	Aggregation of finer processes	?

- I will explain each of these, and whether or not they make Naomi an ELGM, in more detail in slides to follow
  - The notation may not have been introduced properly, but hopefully the gist will still make sense

ANC offset from household survey

$$\text{logit}(\rho^{\text{ANC}}_{x,a}) = \text{logit}(\rho_{x,F,a}) + \beta^{\rho^{\text{ANC}}} + u^{\rho^{\text{ANC}}}_{x} + \eta^{\rho^{\text{ANC}}}_{R_x,a},$$
$$\text{logit}(\alpha^{\text{ANC}}_{x,a}) = \text{logit}(\alpha_{x,F,a}) + \beta^{\alpha^{\text{ANC}}} + u^{\alpha^{\text{ANC}}}_{x} + \eta^{\alpha^{\text{ANC}}}_{R_x,a}.$$

- Here $\text{logit}(\rho_{x,F,a})$ and $\text{logit}(\alpha_{x,F,a})$ are Gaussian
- They have their own structured additive predictors, but by use of the `copy` feature this should be possible in R-INLA
- Conclusion: does not make Naomi an ELGM

Incidence depends on adult prevalence and coverage

$$\log(\lambda_{x,s,a}) = \beta_0^{\lambda} + \beta_S^{\lambda, s=\text{M}} + \log(\rho_x^{\text{15-49}}) + \log(1 - \omega \cdot \alpha_x^{\text{15-49}}) + u_x^{\lambda} + \eta_{R_x,s,a}^{\lambda}.$$

- Here $\log(\rho_x^{\text{15-49}})$ and $\log(1 - \omega \cdot \alpha_x^{\text{15-49}})$ are not going to be Gaussian – no matter your copy tricks
- Conclusion: does make Naomi an ELGM

ART attendance is a product

ART attendance uses the multinomial

Aggregation of finer processes

The algorithm

$$
\begin{tikzcd}
p(\theta, x, y) \arrow[d, "\text{Laplace}"] & \tilde{p}_{\texttt{AQ}}(\theta \mid y) \arrow[r, "\text{Marginalise}"] & \tilde{p}_{\texttt{AQ}}(\theta_j \mid y) \arrow[d, "\text{Spline}"] \\
\tilde{p}_{\texttt{LA}}(\theta, y) \arrow[r, "\text{AGHQ}"] & \tilde{p}_{\texttt{AQ}}(y) \arrow[u, "\text{Normalise}"'] & \text{Output}
\end{tikzcd}
$$

Figure 9: Inference for the hyperparameters. Shaped like a snake for no real reason.

$$
\begin{tikzcd}
p(\theta, x_i, x_{-i}, y) \arrow[d, "\text{Laplace}"] & \tilde{p}_{\texttt{AQ}}(x_i \mid y) \arrow[r, "\text{Spline}"] & \text{Output} \\
\tilde{p}_{\texttt{LA}}(x_i, \theta, y) \arrow[r, "\text{AGHQ}"] & \tilde{p}_{\texttt{AQ}}(x_i, y) \arrow[u, "\text{Normalise}"'] &
\end{tikzcd}
$$

Figure 10: Inference for the latent field.

Thanks for listening!

- Working on a paper "Fast approximate Bayesian inference for small-area estimation of HIV indicators using the Naomi model" based on this work, joint with Alex Stringer (Waterloo) and my PhD supervisors Seth Flaxman (Oxford) and Jeff Eaton (Imperial)
- Let me know if you'd be up for being an early reader!
- Code for this project is at `athowes.github.io/elgm-inf`

References I

Kristensen, Kasper, Anders Nielsen, Casper W Berg, Hans Skaug, and Brad Bell. 2015. "TMB: automatic differentiation and Laplace approximation." *arXiv Preprint arXiv:1509.00660*.

O'Hagan, Anthony. 1987. "Monte Carlo Is Fundamentally Unsound." *The Statistician*, 247–49.

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.