Efficient brute-force marginalisation of discrete variables in Stan: an epidemic model of sub-critical transmission as a case study

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Motivation

As is widely known, the HMC algorithm underlying Stan cannot handle discrete latent variables (parameters). Thus, when for one to be able to fit a model containing latent variables in Stan, these need to be marginalised over, either analytically or by brute-force. Let X be the discrete latent variables of interest, $\boldsymbol{Y}$ be the data and other variables in the model and $\boldsymbol{\theta}$ be the model parameters. We can write

$$\Pr(\boldsymbol{\theta} \mid \boldsymbol{Y}) \propto \sum_{i \in \boldsymbol{\Omega}} \Pr(\boldsymbol{\theta} \mid \boldsymbol{Y}, X = i) = \sum_{i \in \boldsymbol{\Omega}} \Pr(\boldsymbol{Y}, X = i \mid \boldsymbol{\theta})\, \pi(\boldsymbol{\theta}),$$

which usually takes the more familiar form

$$\Pr(\boldsymbol{\theta} \mid \boldsymbol{Y}) \propto \sum_{i=0}^{\infty} \Pr(\boldsymbol{Y}, X = i \mid \boldsymbol{\theta})\, \pi(\boldsymbol{\theta}). \tag{1}$$

Here we will discuss a few ways to do the marginalisation in (1) and discuss what is, to the best of our knowledge, **a new technique for truncating infinite sums** while controlling approximation error.

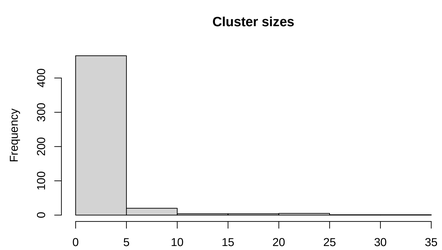
A motivating example: sub-critical transmission chains

Here are interested in the model Blumberg & Lloyd-Smith, (2013a), in which subcritical transmission leads to "stuttering" chains of transmission.

- **Birth-death.** The model assumes a birth-death process in which an initial single infection results in a distribution of offspring infections.
- **Secondary infection** distribution for each infection follows a negative binomial distribution with mean R_0 and over-dispersion parameter ω. When $\omega \to \infty$, the secondary infection distribution is Poisson distributed and when $\omega = 1$ the secondary infection distribution is an exponential distribution.
- **Total number of cases** within a transmission chain, c, that are caused by a single introduction (including the index case) has limiting distribution:

$$\Pr(C = c \mid R_0, \omega) = \frac{\Gamma(\omega c + c - 1)}{\Gamma(\omega c)\Gamma(c+1)} \frac{(R_0/\omega)^{c-1}}{(1 + R_0/\omega)^{\omega c + c - 1}}. \tag{2}$$

- **An outbreak** may be comprised of multiple concurrent transmission chains resulting from multiple introduction events. Each chain i comprises a count of cases c_i and the vector of case counts within distinct transmission chains is $\mathbf{C} = (c_1, \ldots, c_K)$.
- **Total number** of cases in the outbreak by $N = \sum_{i=1}^{K} c_i$.
- **MLE.** When $\mathbf{C}$ are observed directly, the maximum likelihood estimator of R_0 is $\widehat{R_0}^{\text{MLE}} = 1 - \frac{K}{N}$.



Modelling observation error

The main issue with estimating $\{R_0, \omega\}$ from data is that the clusters (and cluster sizes) are observed imperfectly. Here we explore the so-called size-independent model of observation error, which motivates the employment of truncation techniques.

Binomial (size-independent) observation error

Each case in chain/cluster c_i is observed independently with probability ψ such that we now observe a set $\mathbf{S} = (s_1, \ldots, s_J)$ of cases. Thus we have

$$P(S = s_i \mid C = c_i, \psi) = \binom{c_i}{s_i} \psi^{s_i} (1 - \psi)^{c_i - s_i}. \tag{3}$$

When $s_i = 0$, the cluster is not observed. The conditional probability that a cluster is not observed is $\Pr(S = 0 \mid C = c_i, \psi) = (1 - \psi)^{c_i}$, while the marginal probability is

$$\Pr(S = 0 \mid \psi, R_0, \omega) = \sum_{j=1}^{\infty} \Pr(S = 0 \mid C = j, \psi) \Pr(C = j \mid R_0, \omega). \tag{4}$$

After some manipulation we get

$$\sum_{k=1}^{\infty} \kappa(k, \omega) b^k = \frac{a}{1 + a}, \tag{5}$$

with $a := R_0/\omega$, $b = a/(1+a)^{(1+\omega)}$ and $\kappa(c, \omega) := \frac{\Gamma(\omega c + c - 1)}{\Gamma(\omega c)\Gamma(c+1)}$. Whilst the mapping $a \mapsto b$ is not invertible analytically, it can be easily inverted numerically *via* Newton solver. Hence for the case $s_i = 0$, we can write

$$\begin{aligned} P(S = 0 \mid R_0, \omega, \psi) &= \sum_{k=1}^{\infty} \frac{1 + a}{a} \kappa(k, \omega) b^k (1 - \psi)^k, \\ &= \frac{\omega + R_0}{R_0} \frac{u}{(1 + u)}, \end{aligned} \tag{6}$$

where $b \cdot (1 - \psi) = u/(1 + u)^{(1+\omega)}$ and u can be obtained by numerical inversion. The marginal probability when $S > 0$ is not available in closed-form, and we discuss a strategy to marginalisation in **Adaptive truncation**.

Adaptive truncation

Let $p(j) := \Pr(\boldsymbol{\theta} \mid \boldsymbol{Y}, X = j)$ let $Q = \sum_{j=s}^{\infty} p(j)$ be the sum of interest, with ϵ the desired approximation error. Define $L := \lim_{n \to \infty} \frac{p(n+1)}{p(n)}$. The algorithm can be summarised as follows:

1. Find $\dot{N}$ such that $p(j+1)/p(j) < 1$ for all $j > \dot{N}$;
2. Compute $\dot{Q} = \sum_{j=s}^{\dot{N}} p(j)$;
3. Let $z_j = \frac{p(j+1)p(j)}{p(j) - p(j+1)}$;
4. Find $\ddot{N} \geq \dot{N}$ such that $p(j) \left(\frac{L}{1-L}\right) + z_j =: \Delta_j < 2\epsilon$ for all $j > \ddot{N}$;
5. Compute $\ddot{Q} = \sum_{j'=\dot{N}}^{\ddot{N}} p(j')$;
6. Compute the estimate $\hat{Q} = \dot{Q} + \ddot{Q} + \frac{1}{2}\Delta_{\ddot{N}}$.

For the model discussed here, $L = [(1+\omega)/(R_0 + \omega)]^{1+\omega} R_0 (1 - \psi)$, but usually we have $L = 0$.

Priors

- **Independent priors.** $\pi(R_0, \omega, \psi) = \pi_R(R_0)\pi_H(\omega)\pi_S(\psi)$;
- **Reproduction number**: $\pi_R(R_0)$, $\text{Beta}(1,1)$ or a boundary-avoiding $\text{Beta}(2,2)$ – reference prior is available when ω is fixed;
- **Dispersion**: $\pi_H(\omega)$, $\text{Gamma}(1,1)$;
- **Observation probability**: $\pi_S(\psi)$, $\text{Beta}(1,1)$;

Including information about the number of unobserved clusters

- **How many unobserved clusters?** We do not observe the number of size zero clusters, $n_0 = K - J$, directly. Since we know the number of observed clusters J, we can also choose to model the true number of clusters K instead of n_0, and this is the route we take here.
- **Marginalising over K**
  - Let $p_0 := \Pr(S = 0 \mid R_0, \omega, \psi)$;
  - Then for $k > J$ we have $\Pr(K = k \mid \boldsymbol{\theta}) = \Pr(K = k \mid p_0) = p_0^{k-J}$;
  - Fix a total (case) count sum: $N = \sum_{i=1}^{K} c_i$;
  - Then $K \in [J, U]$, where $U = J + N - T$ and $T = \sum_{i=1}^{J} s_i$.

  Using a doubly-truncated Poisson prior on K, the marginalisation is now

$$\begin{aligned} m''(J, U, p_0, \lambda_K) &:= \sum_{k=J}^{U} \Pr(K = k \mid p_0) \pi_2(K = k \mid \lambda_K) \\ &= \frac{\exp(\lambda_K(p_0 - 1))}{p_0^J}. \end{aligned}$$

Prelimnary results

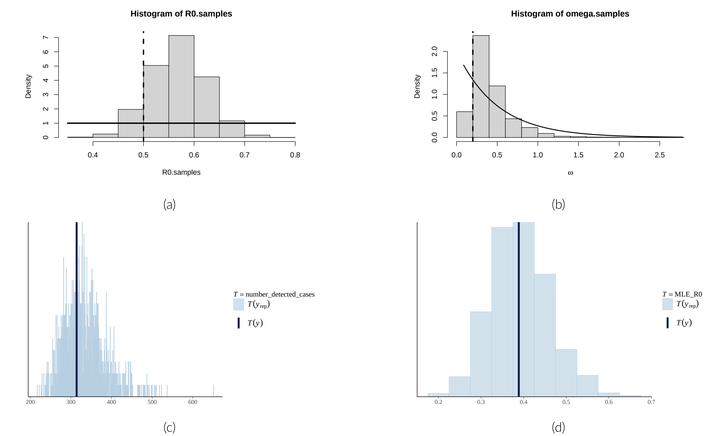


Figure 1. Posterior distributions and posterior predictives for quantities of interest in the model.

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