(Particle) Markov chain Monte Carlo

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Inference and prediction

Once the model is fitted and the model fit assessed, we can use the model / parameter estimates in various ways:

- **Inference**: interpreting the parameter estimates.
- **Prediction**: to predict what might happen if the outbreak were to occur under the same conditions again.
- **Forecasting**: to predict what might happen in the future, based on data available now.

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- **Surveillance**: e.g. under-reporting, imperfect coverage, imperfect diagnosis, mis-diagnosis;
- **Rounding error**: e.g. data often collated daily / weekly;
- **Hidden states**: some epidemiological processes never observed (e.g. you might know *roughly* when you started feeling sick with flu, but not when you were infected or when you became infectious).

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Dealing with these challenges is **hard**! (But we will have a go!)

Intractable likelihoods

To deal with the **partially observed** data, we can introduce a set of **latent** variables, $\mathbf{x} = (\mathbf{t}, \delta)$, where $\mathbf{t}$ is a vector of **hidden** event *times*, and δ is a vector of **hidden** event *types*.

Then the **likelihood** can be expressed as:

$$f(\mathbf{y} \mid \theta) = \int_{\mathcal{X}} f(\mathbf{y} \mid \mathbf{x}, \theta) f(\mathbf{x} \mid \theta) d\mathbf{x},$$

where

- $f(\mathbf{y} \mid \mathbf{x}, \theta)$ is an **observation** process (or **measurement error** / **model discrepancy**);
- $f(\mathbf{x} \mid \theta)$ is the **likelihood function** based on the **latent** variables $\mathbf{x}$.

Intractable likelihoods

$$f(\mathbf{y} \mid \theta) = \int_{\mathcal{X}} f(\mathbf{y} \mid \mathbf{x}, \theta) f(\mathbf{x} \mid \theta) d\mathbf{x},$$

This **marginalises** (*averages*) across the hidden variables $\mathbf{x}$.

This is a complex integral, over all possible combinations of events, and all possible event times consistent with the data.

It may also be the case that the **number** of hidden events is **unknown**, in which can we have to repeat the integration for every possible number of hidden events.

Data augmentation

One approach is therefore to include the **hidden** variables $\mathbf{x}$ as **additional parameters** in the model.

We can then estimate the ***joint* posterior** distribution for $(\theta, \mathbf{x})$, and then derive the ***marginals*** for the parameters of interest (θ) *numerically*.

This is usually done using MCMC methods; an approach known as **data-augmented MCMC** (e.g. Gibson and Renshaw 1998; O'Neill and Roberts 1999; Jewell et al. 2009).

It is very powerful, but difficult to code, scale and optimise.

Simulation-based approaches

Alternatively, we can build inference algorithms around **simulating** directly from the model-of-interest, and then searching for parameter sets that are more consistent with the **observed data**.

These **simulation-based methods** are also powerful and flexible:

- Don't have to store all of the latent variables (so memory requirements are lower).
- Are often straightforward to parallelise.
- Simulation can often be easier than calculating the likelihood.
- Implementation often easier than DA (e.g. "plug-and-play")

However, there are also practical difficulties:

- The probability of matching the data exactly (i.e. getting a non-zero likelihood) is often very low.
- Often require some form of approximation to obtain a match.

Alternative fitting methods

Examples of latent variable methods:

- **Data-augmented MCMC** (e.g. Gibson and Renshaw 1998; O'Neill and Roberts 1999; S. Cauchemez and Ferguson 2008; Jewell et al. 2009)
- **Sequential Monte Carlo** (Simon Cauchemez et al. 2008)

Examples of simulation-based methods:

- **Maximum likelihood via iterated filtering** (Ionides, Bretó, and King 2006)
- **Approximate Bayesian Computation** (e.g. Toni et al. 2009; McKinley, Cook, and Deardon 2009; Conlan et al. 2012; Brooks Pollock, Roberts, and Keeling 2014)
- **Pseudo-marginal methods** (e.g. O'Neill et al. 2000; Beaumont 2003; Andrieu and Roberts 2009; McKinley et al. 2014)
- **Particle MCMC** (Andrieu, Doucet, and Holenstein 2010; Drovandi, Pettitt, and McCutchan 2016)
- **Synthetic likelihood** (Wood 2010)
- **History matching** (with **emulation**) (e.g. Andrianakis et al. 2015; McKinley et al. 2018)

Pseudo-marginal MCMC

Require: $\theta^{(0)}$.
  for $i = 1, \ldots, n$ **do**
    Propose **candidate** $\theta' \sim q\left(\cdot \mid \theta^{(i-1)}\right)$.
    Calculate the **acceptance probability**:

$$\alpha = \min\left(1, \frac{\hat{f}\left(\mathbf{y} \mid \theta'\right) f\left(\theta'\right)}{\hat{f}\left(\mathbf{y} \mid \theta^{(i-1)}\right) f\left(\theta^{(i-1)}\right)} \times \frac{q\left(\theta^{(i-1)} \mid \theta'\right)}{q\left(\theta' \mid \theta^{(i-1)}\right)}\right)$$

    Sample $u \sim U(0, 1)$
    if $u < \alpha$ **then**
      $\theta^{(i)} = \theta'$
    else
      $\theta^{(i)} = \theta^{(i-1)}$
    end if
  end for

One option is to simply plug this **estimate** into a standard Metropolis-Hastings algorithm in place of the true likelihood.

Remarkably, as long as this estimate is **unbiased**, this will still converge to the **true** posterior.

This approach is known as **pseudo-marginal MCMC**.

Beaumont (2003); Andrieu and Roberts (2009).

Simulation-based approximations

One option is to replace the likelihood, $f(\mathbf{y} \mid \theta)$, by a **Monte Carlo** estimate:

$$
\begin{aligned}
f(\mathbf{y} \mid \theta) &= \int_{\mathcal{X}} f(\mathbf{y} \mid \mathbf{x}, \theta) f(\mathbf{x} \mid \theta) d\mathbf{x} \\
&\approx \frac{1}{M} \sum_{i=1}^{M} f(\mathbf{y} \mid \mathbf{x}_i, \theta),
\end{aligned}
$$

where $\mathbf{x}_i \sim f(\mathbf{x} \mid \theta)$ are simulations from the underlying model.

This provides an **unbiased** estimate for $f(\mathbf{y} \mid \theta)$.

Efficiency of pseudo-marginal MCMC

The efficiency (i.e. **mixing**) of pseudo-marginal MCMC relies on the **variance** of the **estimator** $\widehat{f}(\mathbf{y} \mid \theta)$.

- If the variance is **small**, then mixing will be **improved**.
- If the variance is **large**, then mixing will be **poor**.

We can reduce the variance by:

- increasing the number of simulations $M \to$ higher computational burden;
- improving the estimator.

Particle MCMC

This leads on to the idea of **particle MCMC** (Andrieu, Doucet, and Holenstein 2010).

In essence this aims to use **Sequential Monte Carlo**[†] to produce an **unbiased** estimate of the likelihood that has **lower variance** than a vanilla Monte Carlo estimate.

One of the earliest and most widely used particle filters is known as the **bootstrap particle filter** (Gordon, Salmond, and Smith 1993).

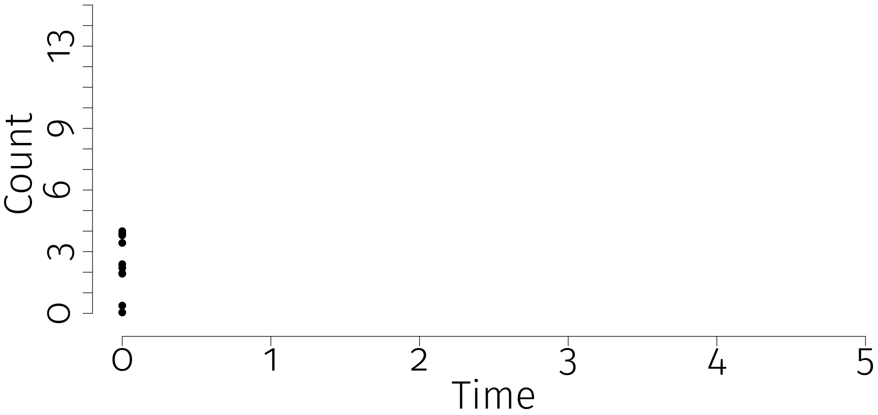
[†] i.e. **particle filtering**

Bootstrap particle filter

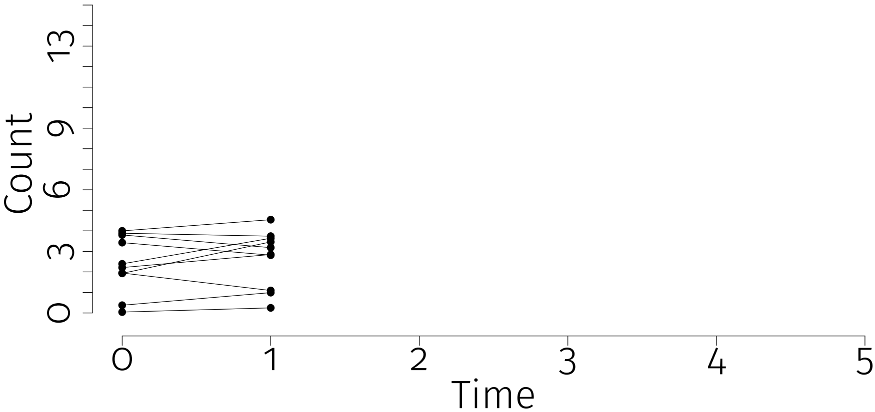
Each **particle** now corresponds to the **unobserved states** of the system at time 0, $\mathbf{x}_0 = (\mathbf{x}_0^1, \dots, \mathbf{x}_0^M)$. The parameters are **fixed**.

1. Each particle m is propagated forwards in time by **simulating** from the model $\mathbf{x}_1^m \sim f(\mathbf{x} \mid \mathbf{x}_0^m, \theta)$.
2. Each new particle is **weighted** according to the **observation process**, $f(\mathbf{y} \mid \mathbf{x}_1^m, \theta)$.
3. These weights are **normalised**, and a **re-sampling** step undertaken.
4. The new set of particles are propagated forwards to time $t + 1$ and so on...

Bootstrap particle filter



Bootstrap particle filter



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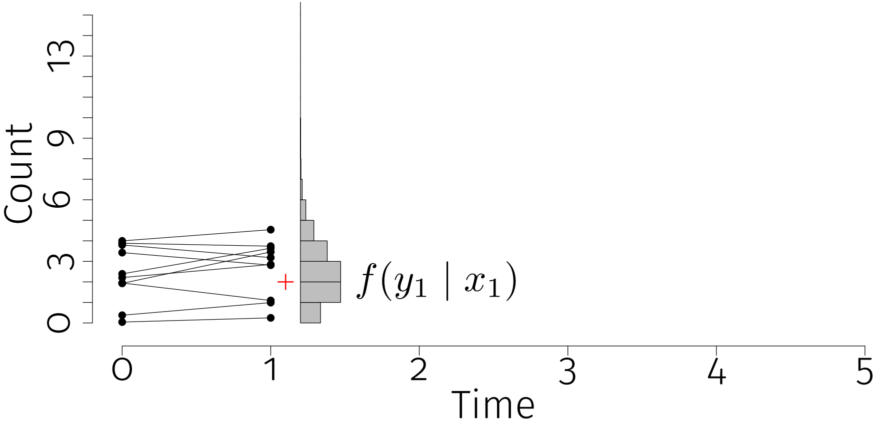

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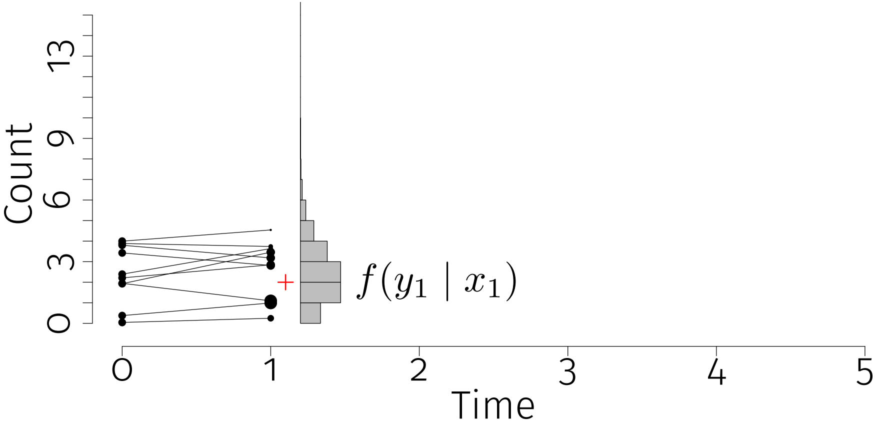

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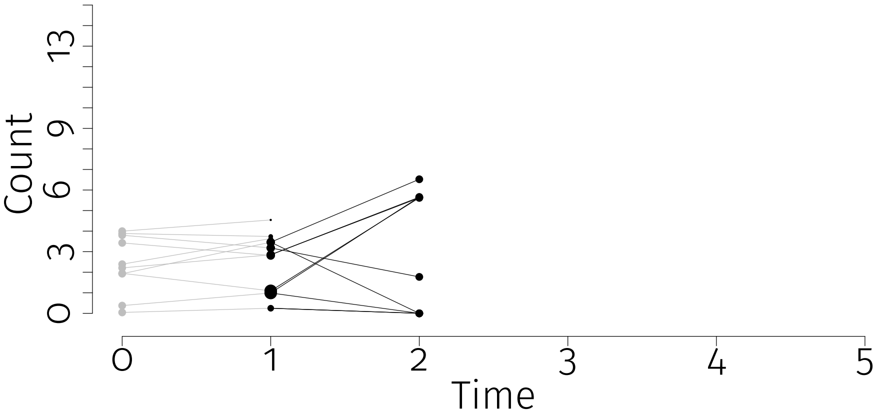

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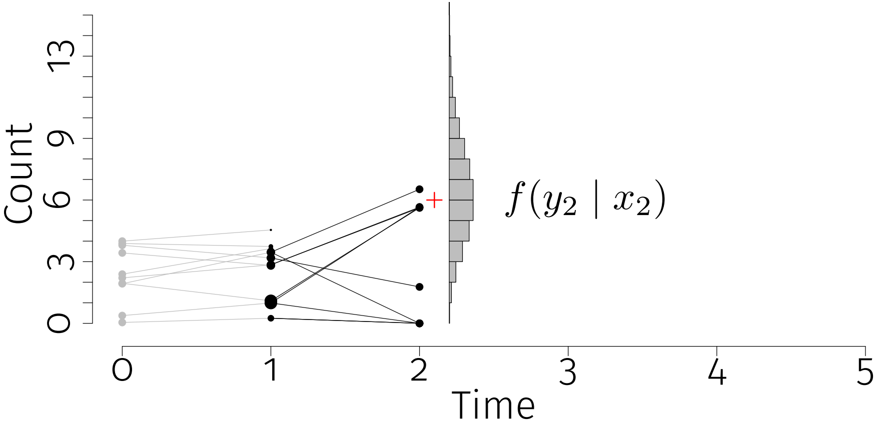

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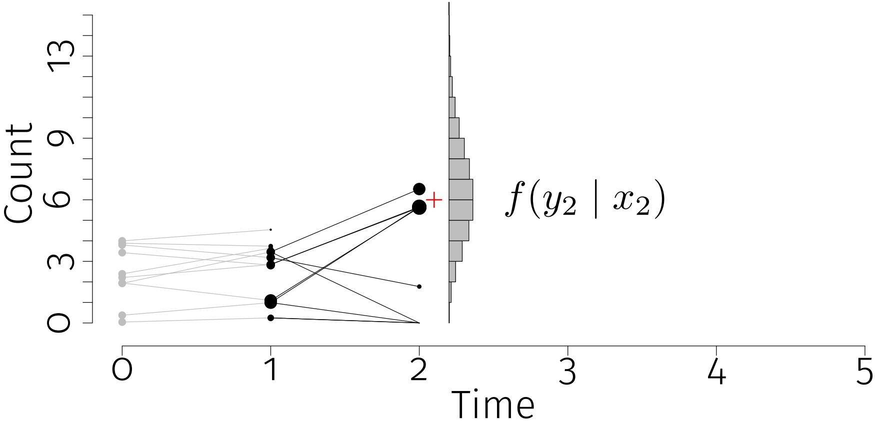

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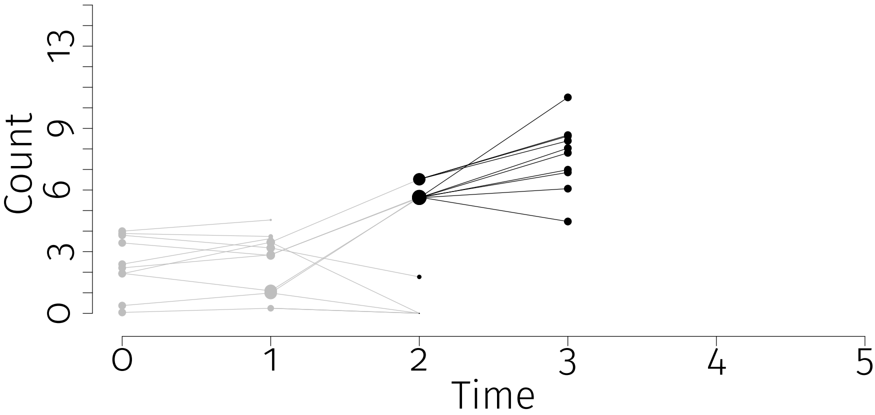

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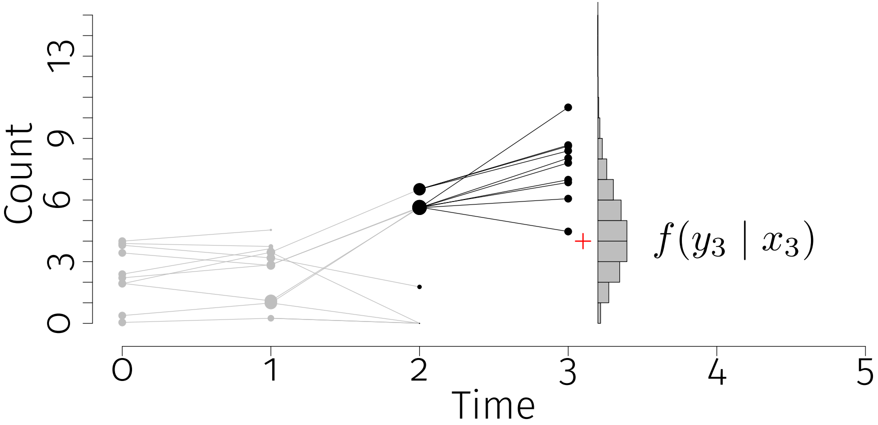

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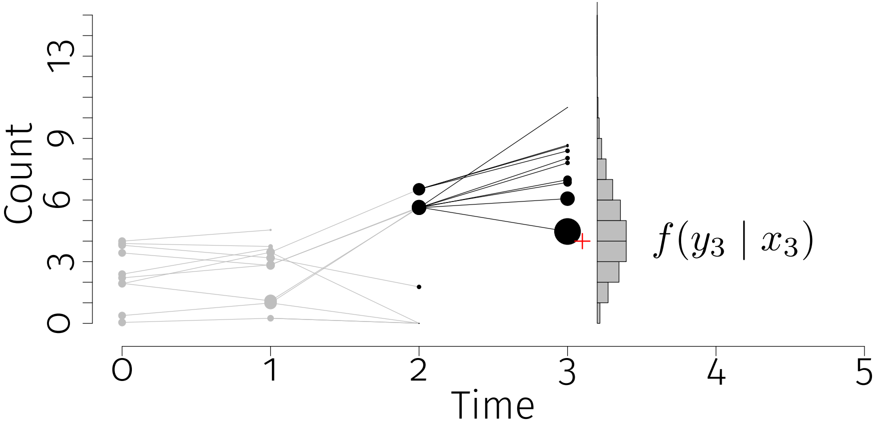

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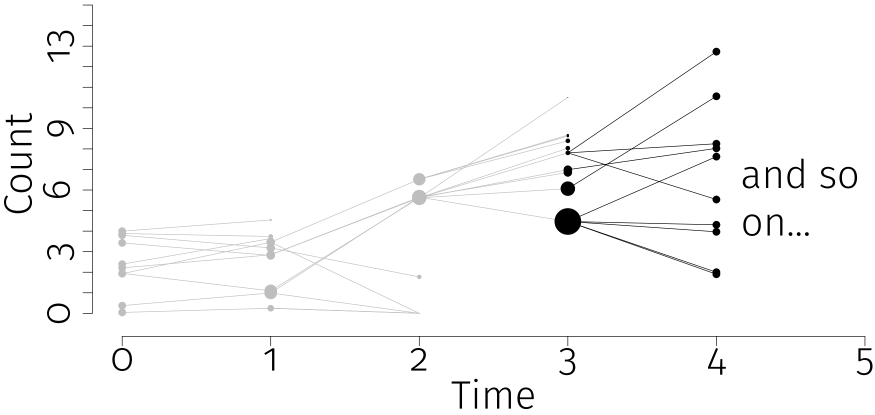


Bootstrap particle filter

We can generate an **unbiased estimate** of the conditional densities:

$$\hat{f}\left(y_t \mid y_{0:(t-1)}\right) = \frac{1}{M}\sum_{m=1}^{M} f\left(y_t \mid \mathbf{x}_t^m, \theta\right),$$

where $y_{0:(t-1)}$ corresponds to the observed time-series counts at time $t_0, t_1, \dots, t_{t-1}$.

It turns out that we can also derive an **unbiased** estimate of the overall **likelihood** as:

$$\hat{f}\left(\mathbf{y} \mid \theta\right) = f\left(y_0\right)\prod_{t=1}^{T}\hat{f}\left(y_t \mid y_{0:(t-1)}\right).$$

Particle MCMC

Hence we can generate an **unbiased** estimate of the likelihood which **numerically** integrates over the **hidden states**.

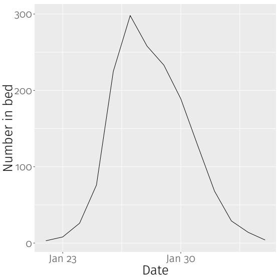
We can then plug this estimate into a standard Metropolis-Hastings algorithm to produce a **pseudo-marginal** MCMC routine that will converge to the *correct posterior distribution in probability*.

This approach only requires a **simulation** model, and an **observation process**.

The bootstrap particle filter we've used is defined for **time-series** counts, and can be extended in various ways.

Example: flu in boarding school

To illustrate some of these ideas we can use a case study of influenza in a boarding school. These data are from a paper in the BMJ in 1978 (Anonymous 1978) and provided in the `outbreaks` package. We use a simple $SIRR_1$ model:



The event probabilities are:

$$P\left[S_{t+\delta t} = S_t - 1, I_{t+\delta t} = I_t + 1\right] \approx \beta SI/N$$
$$P\left[I_{t+\delta t} = I_t - 1, R_{t+\delta t} = R_t + 1\right] \approx \gamma I$$
$$P\left[R_{t+\delta t} = R_t - 1, R_{1,t+\delta t} = R_{1,t} + 1\right] \approx \gamma_1 R$$

Example: flu in boarding school

Here we will place a Poisson error process around the R curve, such that:

$$R_t \sim \text{Po}(R'_t + 10^{-6}),$$

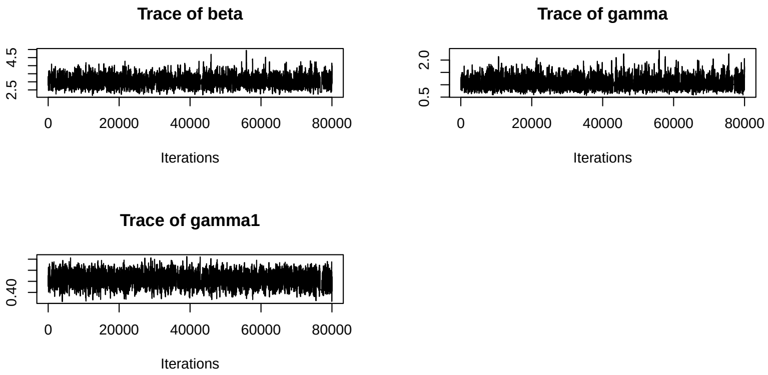
where R_t is the **observed** R count at time t, R'_t is the simulated count†.

The initial population size is 763 pupils, and we assume an initial introduction of infection of a single child at day 0.

†see e.g. Funk et al. (2016) or here for similar ideas in practice

Example: flu in boarding school

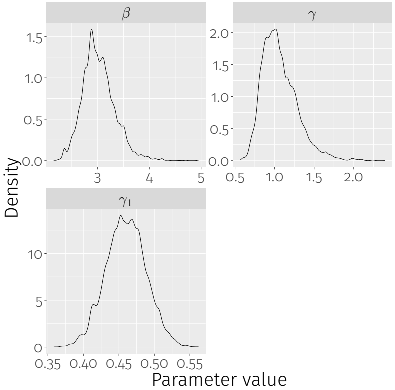
We ran a PMCMC algorithm for 100,000 iterations, discarding the first 20,000 as burn-in. We used 75 particles for the particle filter.



Example: flu in boarding school

Summaries of the marginal posterior distributions are:

Parameter	Mean	2.5%	97.5%
β	3	2.5	3.7
γ	1.1	0.73	1.6
γ_1	0.46	0.41	0.52



Summary

Particle MCMC is a powerful approach for inference in **partially observed** systems (see e.g Wilkinson 2012 or his associated blog for fantastic explanations of these methods).

It is often used when there is some form of **stochastic** discrepancy / observation process mapping the **hidden** states to the **observed** states.

Other particle filters exist, such as the **Alive Particle Filter** (Jasra et al. 2013), and the system can be extended to the **ABC** setting, where approximate matching around data points is used (Drovandi, Pettitt, and Lee 2014; McKinley et al. 2020).

Software

Partially Observed Markov Processes:

- `pomp`
- `SimBIID`[†]
- `SimInf`[‡]
- `nimble`[§]
- `hmer`[¶]

[†] designed mostly for teaching purposes, but should work for simple models
[‡] now implements ABC-SMC (e.g. Toni et al. 2009; McKinley, Cook, and Deardon 2009)
[§] now supports state-space models (although I've not used it for these)
[¶] hot-off-the-press! Implements emulation and history matching for epidemic models

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