A short course on Approximate Bayesian Computation

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February 2017

What is ABC about?

- Stochastic models of biological phenomena are often complicated
- Statistical inference for such models is a challenge
- Likelihood-based methods are commonly used . . .
- . . . but likelihoods are often intractable
- What do we do?

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Overview of Course

- Bayesian preliminaries. Rejection methods. Population genetics example. Likelihood-free inference.
- ABC. Connection with sufficiency. Examples. Regression-based methods.
- Bayesian model choice. MCMC methods. Sequential MC methods.
- Hierarchical models, substantive examples.

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Bayesian Preliminaries 4

Notation (1)

$\mathcal{D}$ — data (usually discrete)

θ — parameters (often high-dimensional)

$\pi(\theta)$ — *prior* for θ

Aim is to study the *posterior* $f(\theta|\mathcal{D})$ given by

$$f(\theta|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|\theta)\,\pi(\theta)}{\mathbb{P}(\mathcal{D})}$$

where

$$\mathbb{P}(\mathcal{D}) = \int \mathbb{P}(\mathcal{D}|\theta)\,\pi(\theta)\,d\theta$$

is the *normalising constant*

Posterior is proportional to likelihood times prior

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Notation (2)

The *marginal likelihood* is

$$f(\mathcal{D}) = \int f(\mathcal{D}|\theta)\,\pi(\theta)\,d\theta$$

The *prior predictive distribution* of a random variable $Y = h(\mathcal{D})$ is

$$f_{\text{prior}}(y) = \int f_Y(y|\theta)\,\pi(\theta)\,d\theta$$

The *posterior predictive distribution* of Y is

$$f_{\text{post}}(y) = \int f_Y(y|\theta)\,f(\theta|\mathcal{D}_0)\,d\theta$$

where $\mathcal{D}_0$ denotes the observed data, and f_Y the distribution of Y.

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Example (1)

Suppose X is a Poisson random variable with mean θ, so that

$$\mathbb{P}(X = j) := f(j|\theta) = \frac{e^{-\theta}\theta^j}{j!}, j = 0, 1, \ldots$$

We write $X \sim \mathrm{Po}(\theta)$.
Recall that $\mathbb{E}X = \theta = \mathrm{Var}(X)$

Assume π is the gamma density with parameters r and λ

$$\pi(\theta) = \frac{\lambda^r\, \theta^{r-1} e^{-\lambda\theta}}{\Gamma(r)}, \quad \theta > 0$$

We write $\theta \sim \mathrm{Gamma}(r, \lambda)$.
Recall that $\mathbb{E}\theta = r/\lambda$ and $\mathrm{Var}(\theta) = r/\lambda^2$.

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Example (2)

It is easy to show that

$$\mathcal{L}(\theta|j) \sim \mathrm{Gamma}(j + r, \lambda + 1)$$

and that the normalising constant is

$$\mathbb{P}(j) = \frac{\Gamma(r + j)}{\Gamma(r)\, j!} \left(\frac{1}{\lambda + 1}\right)^j \left(\frac{\lambda}{\lambda + 1}\right)^r \tag{1}$$

We say X has a Negative Binomial distribution with parameters r and p if

$$\mathbb{P}(X = j) = \binom{j + r - 1}{j} (1 - p)^r\, p^j, \quad j = 0, 1, 2, \ldots$$

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Example (3)

We write $X \sim \mathrm{NegBin}(r, p)$.
Recall that $\mathbb{E}X = rp/(1-p)$ and $\mathrm{Var}(X) = rp/(1-p)^2$.

(1) shows that the prior predictive distribution is Negative Binomial with parameters r and $p = 1/(1+\lambda)$.

You should check that the posterior predictive distribution is Negative Binomial with parameters $r + j_0$ and $p = 1/(\lambda + 2)$, where j_0 is the observed value.

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The Rejection Algorithm 10

Rejection method

We now turn to methods for simulating observations from the posterior $f(\theta|\mathcal{D})$ The simplest is the *Rejection Method*:

1. Generate $\theta \sim \pi(\cdot)$
2. Accept θ with probability $h = \mathbb{P}(\mathcal{D}|\theta)$; return to [1.]

Observations accepted by this algorithm have density

$$\propto \pi(\theta)\, \mathbb{P}(\mathcal{D}|\theta) = f(\theta|\mathcal{D})$$

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Hitting the target

How long does it take to get an accepted observation?

$$\begin{aligned}\mathbb{P}(\text{ accept first observation}) &= \int_\theta \pi(\theta)\,\mathbb{P}(\mathcal{D}|\theta)d\theta \\ &= \mathbb{P}(\mathcal{D}) := p\end{aligned}$$

Because the simulations are independent, it follows that

$$\mathbb{P}(\text{first observation accepted on the } r\text{th trial}) = (1-p)^{r-1}p, r = 1, 2, \ldots$$

The expected number of trials to get n accepted observations is n/p

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Hitting the target quicker

If you can find a constant c such that

$$\mathbb{P}(\mathcal{D}|\theta) \leq c, \quad \forall\theta \tag{2}$$

then can replace step [2.] with

2. Accept θ with probability h/c

The mean number of trials to get n accepted observations is then nc/p

Note: the acceptance rate can be used to estimate the normalizing constant $\mathbb{P}(\mathcal{D})$.

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Example from Population Genetics 14

The coalescent (1)

The setting: a random sample of n sequences is taken at random from a population and the locations of the segregating sites (or SNPs) are recorded.

Think of the sequences as copies of the unit interval. SNPs in them arise as a consequence of mutation. We will ignore all sorts of things, such as recombination, variable population size, and selection.

For a sample from a stationary population of constant size, the genealogy of the sample is provided by Kingman's *coalescent*.

We model the ancestry of the n sequences as a random tree. It starts from n tips, waits a time T_n and then chooses two sequences at random to join. There are now $n-1$ ancestors of the sample.

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The coalescent (2)

We then wait time T_{n-1} and choose two of the ancestral sequences to merge. Continuing in this way, the sample spends a time T_2 with two ancestors, finally tracing back to the most recent common ancestor (MRCA).

In this simple model, the random variables $T_n, T_{n-1}, \ldots, T_2$ are independent and exponentially distributed, with

$$\mathbb{E}T_j = \frac{2}{j(j-1)}$$

The time scale is measured in units of $2N$ generations, N being the population size.

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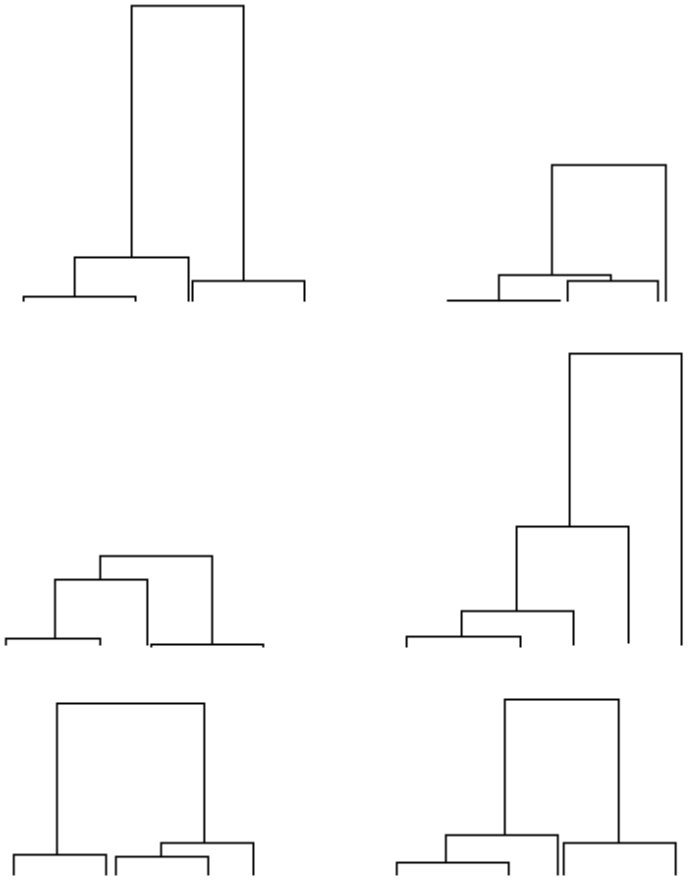
Coalescent trees (1)



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Coalescent trees (2)

Fig. 4.2. Coalescent trees for samples of size 6 and 32 from a population of constant size

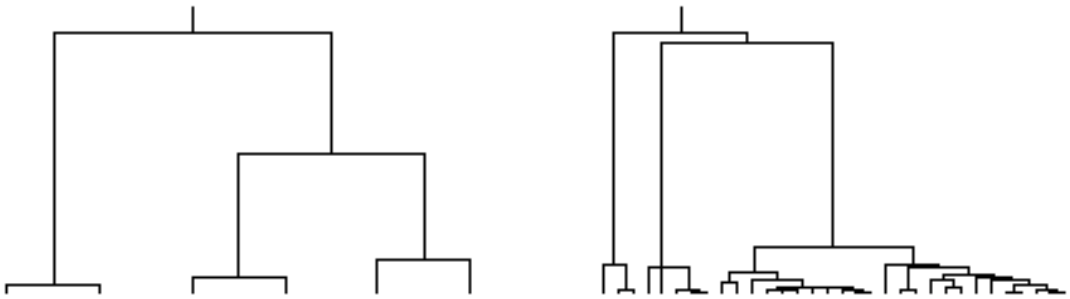
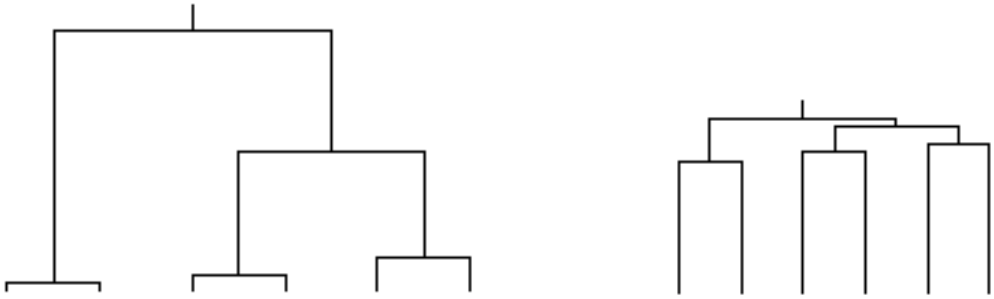


Fig. 4.3. The coalescent tree of a sample of size 6 (constant population size in left panel, exponentially growing population in right panel)



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Mutations in the coalescent (1)

Mutations are superimposed on the coalescent tree according to points of independent Poisson processes of rate $\theta/2$. In the *infinitely-many sites model*, each mutation introduces a segregating site into the sample. In this setting, θ is the compound parameter $\theta = 4Nu$, where u is the per generation mutation rate.

Note that, given the times $T_n, T_{n-1}, \ldots, T_2$, the number of segregating sites introduced while the sample has $n, n-1, \ldots, 2$ distinct ancestors have independent Poisson distributions with means

$$n\,\frac{\theta}{2}\,T_n, (n-1)\,\frac{\theta}{2}\,T_{n-1}, \ldots, 2\,\frac{\theta}{2}\,T_2.$$

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Mutations in the coalescent (2)

It follows that, given $T_n, \ldots, T_2$, the total number of SNPs, S_n, in the sample satisfies

$$\mathcal{L}(S_n|T_n, \ldots, T_2) \sim \mathrm{Po}\left(\frac{\theta}{2}\sum_{j=2}^{n} jT_j\right)$$

This gives what we need to find the posterior distribution of $\theta, T_n, \ldots, T_2$ given $S_n = s$, the observed number of segregating sites.

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The posterior distribution of T_{MRCA} (1)

Our rejection algorithm is

1. Generate $\theta \sim \pi(\cdot)$
2. Generate $T_n, \ldots, T_2$ from model. Calculate $L_n = \sum_{j=2}^{n} jT_j$
3. Accept $\theta, T_n, \ldots, T_2$ with probability

$$h = \mathrm{Po}\left(\frac{\theta}{2} L_n\right)\{s\}$$

   Return to [1.]

We get the posterior of $T_{\mathrm{MRCA}} = T_2 + \cdots + T_n$ from the accepted values in this algorithm

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Homework

See problem set on course moodle.

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Likelihood-free Inference 23

What, no likelihood?

In our earlier examples, we were able to calculate the *likelihood* $\mathbb{P}(\mathcal{D}|\theta)$

What if we can't?

This leads us to the field of likelihood-free inference, and this relies on our ability to simulate observations from the underlying model.

We begin with a result from Don Rubin (1984)

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Rejection method, revisited (1)

The analogue of the rejection method is:

1. Generate $\theta \sim \pi(\cdot)$
2. Generate $\mathcal{D}'$ from the model with parameter θ
3. Accept θ if $\mathcal{D}' = \mathcal{D}$; return to [1.]

Observations accepted by this algorithm have density

$$\begin{aligned} &\propto \pi(\theta)\,\mathbb{P}(\mathcal{D}' = \mathcal{D}|\theta) \\ &= \pi(\theta)\mathbb{P}(\mathcal{D}|\theta) \\ &= f(\theta|\mathcal{D}) \end{aligned}$$

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Rejection method, revisited (2)

- No likelihoods ...
- No analogue of c (?)
- Rubin DB (1984) Bayesianly justifiable and relevant frequency calculations for the applied statistician. *Ann Statist* 12: 1151-1172

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The posterior distribution of T_{MRCA} (2)

To implement this in our genetics example we replace the h step with a simulation step:

1. Generate $\theta \sim \pi(\cdot)$
2. Generate $T_n, \ldots, T_2$ from model. Calculate $L_n = \sum_{j=2}^{n} jT_j$
3. Simulate S' from $\mathrm{Po}(\theta L_n/2)$
4. Accept $\theta, T_n, \ldots, T_2$ if $S' = s$

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