Nonreversible MCMC for latent phylogenetic trees

Jere Koskela

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EPSRC
Engineering and Physical Sciences Research Council

Warwick Statistics

Outline

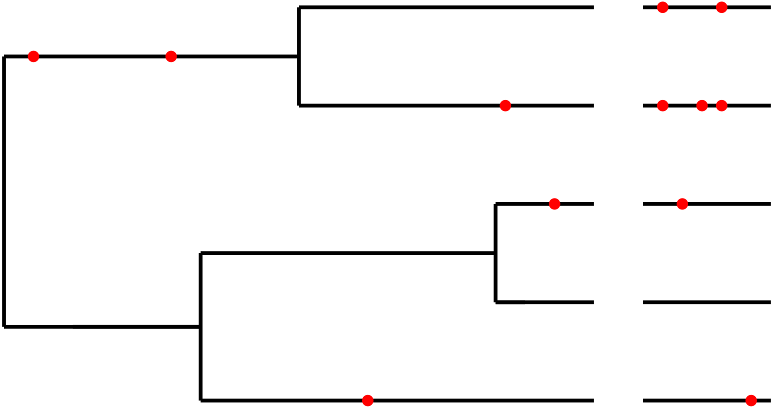
The coalescent

Metropolis-Hastings

The zig-zag process

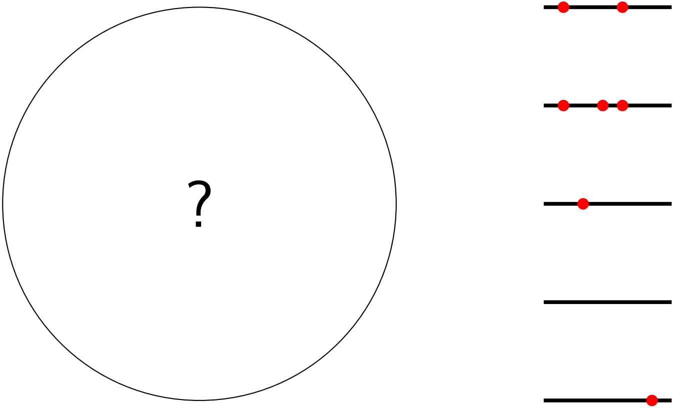
Zig-zag for the coalescent

The coalescent[1]



[1] J F C Kingman. The coalescent, Stoch Proc Appl 13(3):235–248, 1982.

The coalescent as missing data



$$P(D|\theta) = \int_A P(D|A,\theta)P(A|\theta)dA$$

Metropolis–Hastings[2]

```
1. Set $X_1 \leftarrow x$.
2. For $i \in \{2, \dots, m\}$ do
    2.1 Sample $Y \sim q(X_{i-1}, \cdot)$.
    2.2 Sample $U \sim U(0, 1)$.
    2.3 If $U \leq \min\left\{1, \frac{\pi(Y) q(Y, X_{i-1})}{\pi(X_{i-1}) q(X_{i-1}, Y)}\right\}$, set $X_i \leftarrow Y$.
    2.4 Else set $X_i \leftarrow X_{i-1}$.
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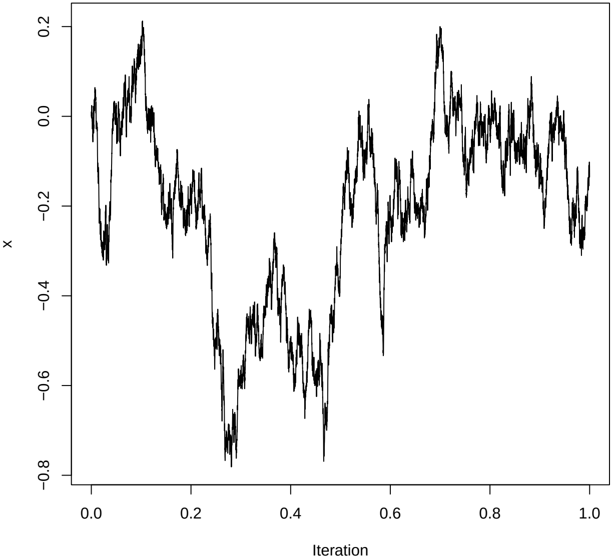
[2] W K Hastings. Monte Carlo sampling methods using Markov chains and their applications, Biometrika 57(1):97–109, 1970.

Reversibility ⇒ diffusive behaviour



The zig-zag process[3]

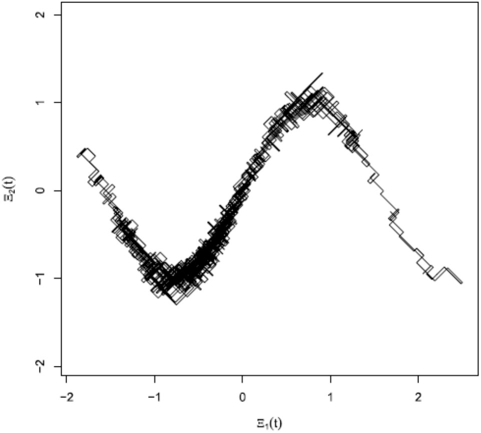
```
1. Set $(x, v) \in \mathbb{R}^n \times \{-1, 1\}^n$.
2. Set $t \leftarrow 0$.
3. While $t < T$ do
    3.1 Sample $Y \sim \mathrm{Exp}(1)$.
    3.2 Set $\rho$ such that $\sum_{i=1}^{n} \int_t^{t+\rho} \lambda_i(x + sv, v)\mathrm{d}s = Y$.
    3.3 Set $x \leftarrow x + \rho v$.
    3.4 Set $t \leftarrow t + \rho$.
    3.5 Sample $I \sim \mathrm{Categorical}(\lambda_1(x, v), \ldots, \lambda_n(x, v))$.
    3.6 Set $v_I \leftarrow -v_I$.
```

- Between switches, x moves with constant velocity v.
- Target density π is invariant if

$$\lambda_i(x, v) = v_i \partial_i \log \pi(x) \vee 0.$$

[3] J Bierkens, P Fearnhead and G Roberts. The zig-zag process and super-efficient sampling for Bayesian analysis of big data, Ann Stat 47(3):1288–1320, 2019.

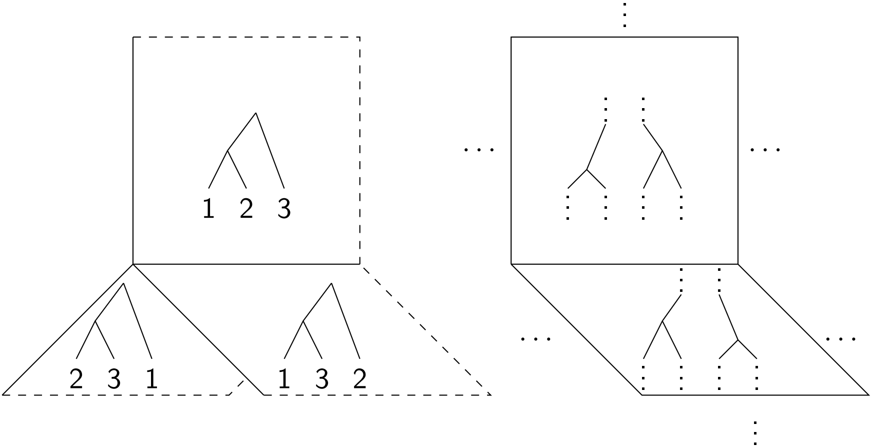
The zig-zag process



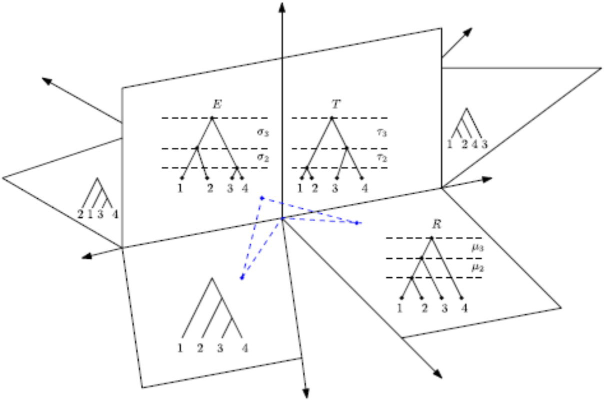
(d) 2D S-shaped density

[3] J Bierkens, P Fearnhead and G Roberts. The zig-zag process and super-efficient sampling for Bayesian analysis of big data, Ann Stat 47(3):1288–1320, 2019.

The three leaf τ-space



One third of the four leaf τ-space[4]



[4] A Gavryushkin and A J Drummond. The space of ultrametric phylogenetic trees, J Theor Biol 403:197–208, 2016.

Simulation study[5,6,7]

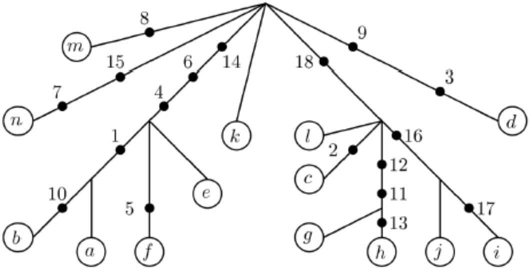


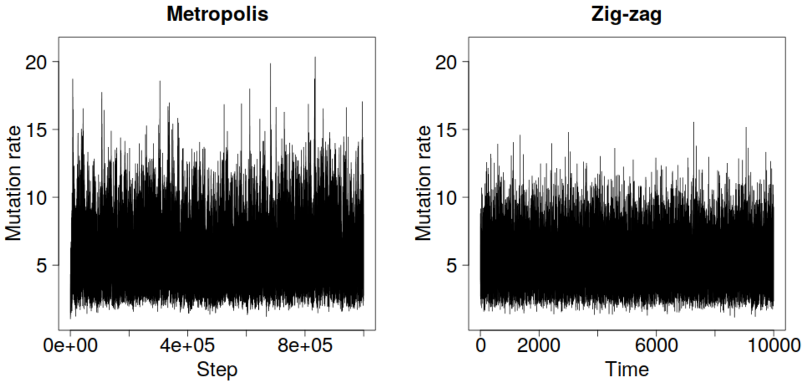
Figure 3.
Perfect phylogeny of the Griffiths and Tavaré (1994) data set.

[5] A Hobolth, M K Uyenoyama and C Wiuf. Importance sampling for the infinite sites model, Stat Appl Genet Mol Biol 7(1) Article 32, 2008.

[6] R C Griffiths and S Tavaré. Ancestral inference in population genetics, Stat Sci 9:307–319, 1994.

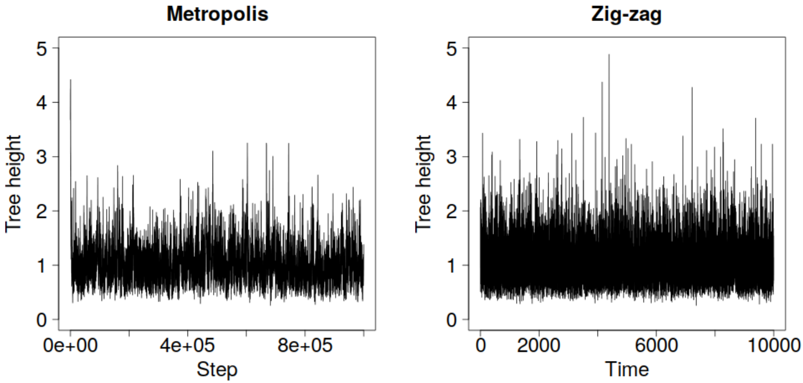
[7] R H Ward, B L Frazier, K Dew and S Pääbo. Extensive mitochondrial diversity within a single Amerindian tribe, Proc Natl Acad Sci USA 88:8720–8724, 1991.

Mutation rate (55 samples, 18 segregating sites)



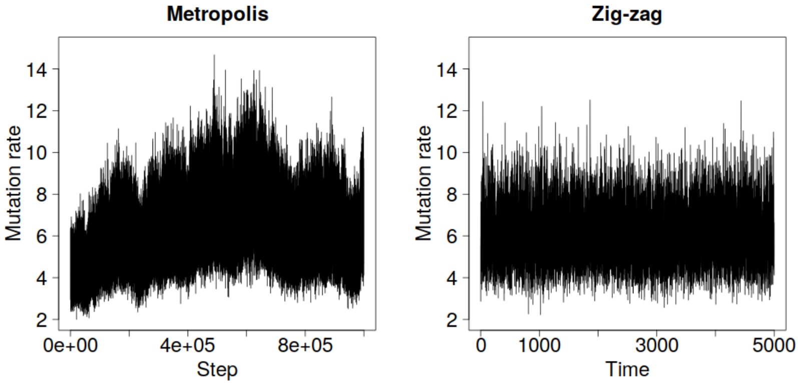
Run times: 3.5 min vs. 0.5 min.

Tree height (55 samples, 18 segregating sites)



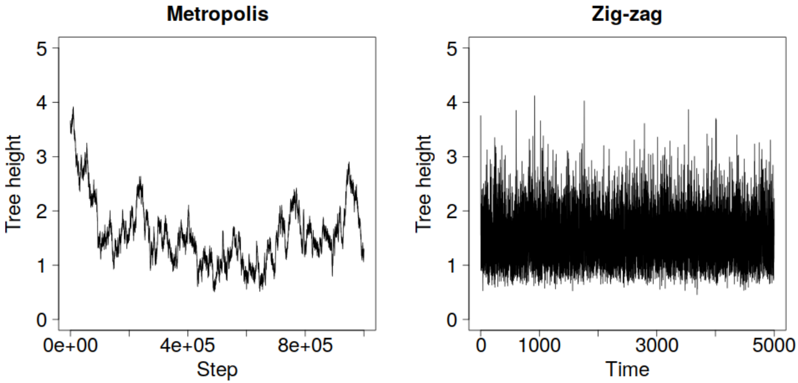
Run times: 3.5 min vs. 0.5 min.

Mutation rate (550 samples, 38 segregating sites)



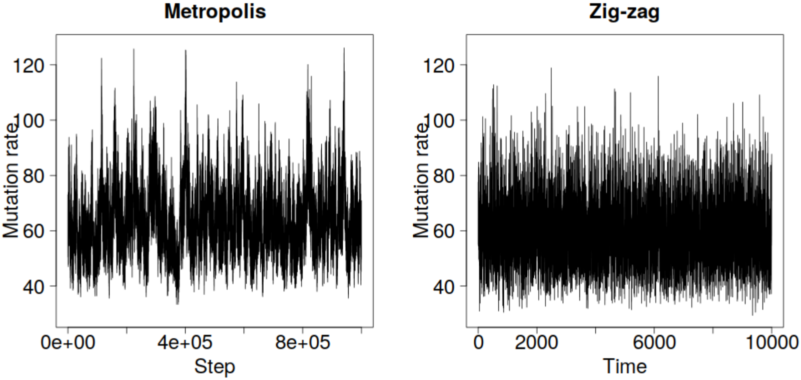
Run times: 70 min vs. 45 min.

Tree height (550 samples, 38 segregating sites)



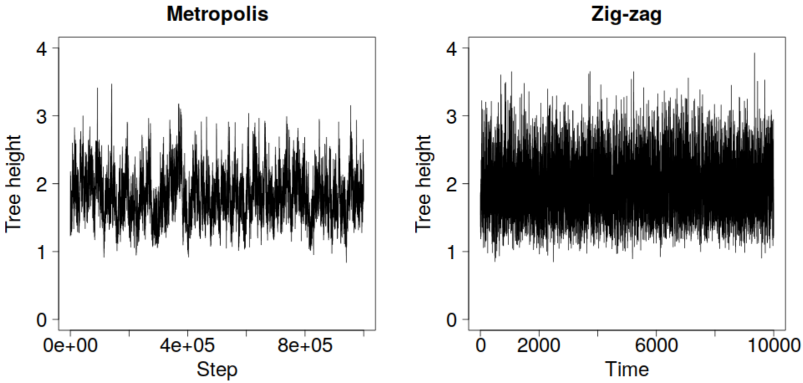
Run times: 70 min vs. 45 min.

Mutation rate (55 samples, 252 segregating sites)



Run times: 50 min vs. 1 min.

Tree height (55 samples, 252 segregating sites)



Run times: 50 min vs. 1 min.