Site rate logger with `babel.util.SiteRateLogger`

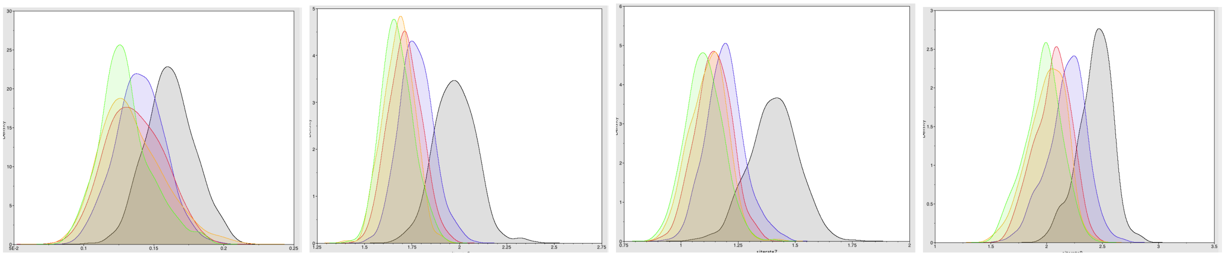
The `babel.util.SiteRateLogger` logs the rate for each site. It assume that more than 1 site category is used, typically through gamma rate heterogeneity with 4 or so categories. Let there be K categories, and let the rates be $r_1, \ldots, r_K$ with rate proportions $w_1, \ldots, w_K$ then for each site i and category j we can calculate the probability of the data at site i when the tree's branch lengths are weighted with rate r_i. Let p_{ij} be that probability, then the average rate for site i is

$$R_i = \int_{r=0}^{\infty} r_j p(r) p_i(r) dr \approx \frac{\sum_{j=1}^{K} r_j w_j p_{ij}}{\sum_{j=1}^{K} w_j p_{ij}}$$

(where $p_i(r)$ is the site probability at rate r, and $p(r)$ the probability of sampling rate r). The approximation is due to discretising the distribution $p(r)$ into K categories. The intuition is that for each rate there is a certain probability, and more likely categories (i.e. those with higher p_{ij}) indicate that rate is more likely. Rate proportions are usually equal ($w_i = 1/K$) and drop out of the equation above. This assumes the mean rate is one $\sum_{j=1}^{K} r_j w_j = 1$, however, in case this is not true, we can compensate for that by dividing by the mean rate:

$$R_i \approx \frac{\sum_{j=1}^{K} r_j w_j p_{ij}}{\sum_{j=1}^{K} w_j p_{ij} \sum_{j=1}^{K} r_j w_j}$$

Higher numbers of categories mean the rate distribution is approximated better and perhaps lead to more accurate estimates (with 1 category every R_i will be 1, 4 will be better, but not sure how high to go -- let me know if you have any experience).



Sample of rate estimates with 4 (black), 8 (blue), 16 (red), 32 (yellow) and 64 (green) rate categories when using gamma rate heterogeneity (shape=0.4).

Before you start

Make sure you have BEAST installed with the Babel package (see read me for details).

Usage

If there is only a single partition, there will be a single treelikelihood, and you can simply add a logger containing just one `SiteRateLogger` like so:

```
<logger id="siteratelog" fileName="siterate.log" logEvery="1000">

  <log spec="babel.util.SiteRateLogger" likelihood="@treeLikelihood.dna"/>
```

```
</logger>
```

This will create a log file `siterate.log` and with Tn$ sites, it will contain entries `siterate0,... ,siterate`$(n-1)$. If you have multiple partitions, say p1, p2, p3, p4, with treelikelihoods treelikelihoods.p1, treelikelihoods.p2, treelikelihoods.p3, treelikelihoods.p4 you can use four `SiteRateLoggers` each referring to a different treelikelihood. Make sure each `SiteRateLogger` gets its own unique ID, since that is used in the log to differentiate between the different loggers.

```
<logger id="siteratelog" fileName="siterate.log" logEvery="1000">

  <log id="siteratep1" spec="babel.util.SiteRateLogger"
likelihood="@treeLikelihood.p1"/>

  <log id="siteratep2" spec="babel.util.SiteRateLogger"
likelihood="@treeLikelihood.p2"/>

  <log id="siteratep3" spec="babel.util.SiteRateLogger"
likelihood="@treeLikelihood.p3"/>

  <log id="siteratep4" spec="babel.util.SiteRateLogger"
likelihood="@treeLikelihood.p4"/>

</logger>
```

To minimise the XML, you can use plates:

```
<logger id="siteratelog" fileName="dna-rate.log" logEvery="1000">

  <plate var="n" range="p1,p2,p3,p4">

    <log id="siterate$(n)" spec="babel.util.SiteRateLogger"
likelihood="@treeLikelihood.$(n)"/>

  </plate>

</logger>
```

Options

To only log a range of sites, use the "from" and "to" inputs. These are indices of sites, where the first site is numbered 1. For example, to only log sites 10 to 20 use:

```
  <log spec="babel.util.SiteRateLogger" from="10" to="20"
likelihood="@treeLikelihood.dna"/>
```

Instead of having to match site numbers in the log to actual meaningful site labels, you can specify the site labels as space delimited list of entries inside the element. For example, the following will log 5 sites and the trace log contains columns for cognate_ant_1, cognate_ant_3, cognate_ant4, cognate_water_1 and cognate_water_6:

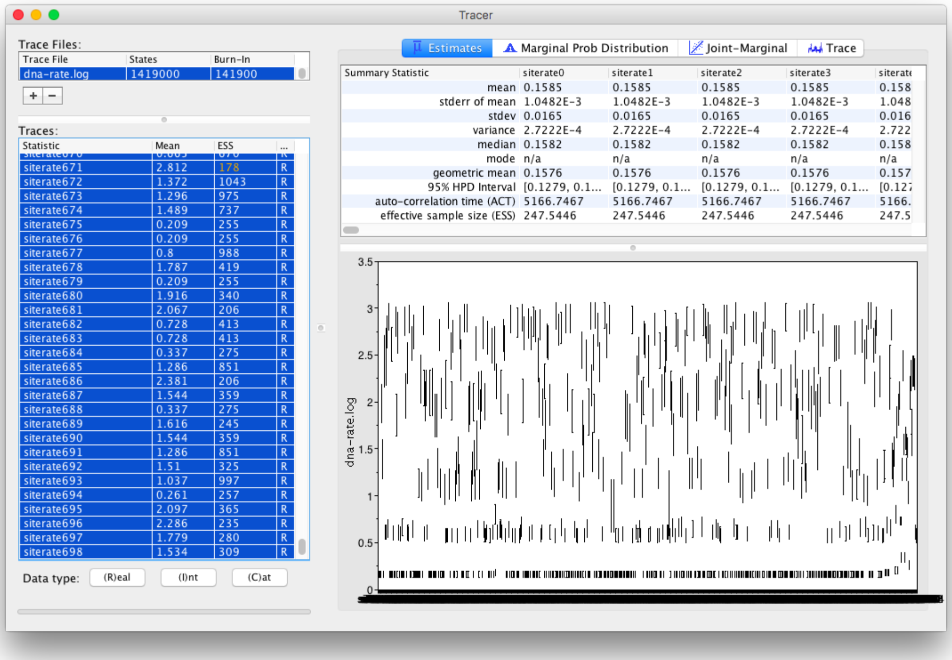
```
  <log spec="babel.util.SiteRateLogger" from="10" to="20"
likelihood="@treeLikelihood.dna">

    cognate_ant_1 cognate_ant_3 cognate_ant4 cognate_water_1 cognate_water_6

  </log>
```

Post processing

Just open the log file in tracer, and inspect the sites of interest.



Trace Files:

Trace File	States	Burn-In
dna-rate.log	1419000	141900

Traces:

Statistic	Mean	ESS	...
siterate671	2.812	178	R
siterate672	1.372	1043	R
siterate673	1.296	975	R
siterate674	1.489	737	R
siterate675	0.209	255	R
siterate676	0.209	255	R
siterate677	0.8	988	R
siterate678	1.787	419	R
siterate679	0.209	255	R
siterate680	1.916	340	R
siterate681	2.067	206	R
siterate682	0.728	413	R
siterate683	0.728	413	R
siterate684	0.337	275	R
siterate685	1.286	851	R
siterate686	2.381	206	R
siterate687	1.544	359	R
siterate688	0.337	275	R
siterate689	1.616	245	R
siterate690	1.544	359	R
siterate691	1.286	851	R
siterate692	1.51	325	R
siterate693	1.037	997	R
siterate694	0.261	257	R
siterate695	2.097	365	R
siterate696	2.286	235	R
siterate697	1.779	280	R
siterate698	1.534	309	R

Data type:

Summary Statistic	siterate0	siterate1	siterate2	siterate3	siterate
mean	0.1585	0.1585	0.1585	0.1585	0.158
stderr of mean	1.0482E-3	1.0482E-3	1.0482E-3	1.0482E-3	1.048
stdev	0.0165	0.0165	0.0165	0.0165	0.016
variance	2.7222E-4	2.7222E-4	2.7222E-4	2.7222E-4	2.722
median	0.1582	0.1582	0.1582	0.1582	0.158
mode	n/a	n/a	n/a	n/a	n/a
geometric mean	0.1576	0.1576	0.1576	0.1576	0.157
95% HPD Interval	[0.1279, 0.1...	[0.1279, 0.1...	[0.1279, 0.1...	[0.1279, 0.1...	[0.127
auto-correlation time (ACT)	5166.7467	5166.7467	5166.7467	5166.7467	5166.
effective sample size (ESS)	247.5446	247.5446	247.5446	247.5446	247.5