



Troubleshooting BEAST2 analyses

Joëlle Barido-Sottani
Slides adapted from Jūlija Pečerska



Possible scenarios

Beast analysis

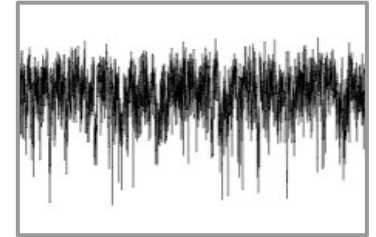
Initialisation failed

```
Start likelihood: -Infinity after
1000 initialisation attempts

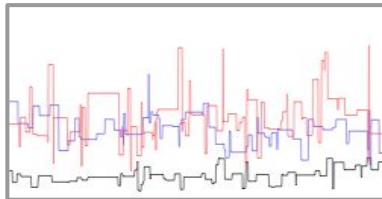
Fatal exception: Could not find a
proper state to initialise.
Perhaps try another seed.

P(posterior) = -Infinity (was
-Infinity)
```

Everything mixed



Nothing mixed



One parameter did not mix

kappa.noncoding	13.143	191
kappa.1stpos	6.28	376
kappa.2ndpos	8.643	372
kappa.3rdpos	27.988	92
mutationRate.noncodi...	0.347	273
mutationRate.1stpos	0.459	238
mutationRate.2ndpos	0.185	237

Failed initialisation

```
Start likelihood: -Infinity after 1000 initialisation attempts
Fatal exception: Could not find a proper state to initialise. Perhaps try another seed.
```

```
P(posterior) = -Infinity (was -Infinity)
  P(prior) = -Infinity (was -Infinity)
    P(BDMM) = -Infinity (was -Infinity)
      P(R0Prior) = -0.5586849541070393 (was -0.5586849541070393)
        P(rPrior) = -11.46042136866474 (was -11.46042136866474)
          P(rateMatrixPrior) = -0.14088025499381485 (was -0.14088025499381485)
            P(samplingProportionPrior) = -10.049507225748343 (was -10.049507225748343)
              P(becomeUninfectiousRatePrior) = -0.7811241751317991 (was -0.7811241751317991)
java.lang.RuntimeException: Could not find a proper state to initialise. Perhaps try another
seed.
at beast.core.MCMC.run(Unknown Source)
at beast.app.BeastMCMC.run(Unknown Source)
at beast.app.beastapp.BeastMain.<init>(Unknown Source)
at beast.app.beastapp.BeastMain.main(Unknown Source)
at beast.app.beastapp.BeastLauncher.main(Unknown Source)
```

```
Fatal exception: Could not find a proper state to initialise. Perhaps try another seed.
```

```
BEAST has terminated with an error. Please select QUIT from the menu.
```

Parameter prior is -Infinity

Example: $P(\text{rateMatrixPrior}) = -\text{Infinity}$ (was -Infinity)

Possible solutions:

- ✓ Increase initialization attempt number
- ✓ Check for incompatible priors
- ✓ Adjust initial conditions
- ✓ Talk to the BEAST2 support group!

Model prior is -Infinity

Example: $P(\text{BDMM}) = -\text{Infinity}$ (was -Infinity)

Possible solutions:

- ✓ Increase initialization attempt number
 - ✓ Check for incompatible priors
 - ✓ Adjust initial conditions
 - ✓ Talk to the BEAST2 support group
 - ✓ Talk to the model developers
- } Including the dependent parameters

Possible scenarios

Beast analysis

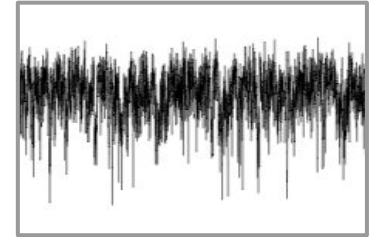
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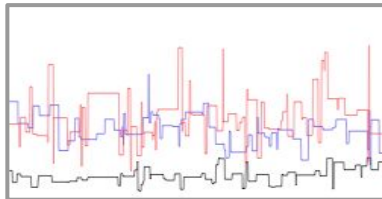
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-Infinity)
```

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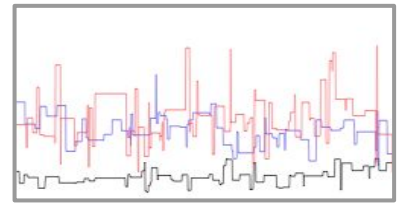
Nothing mixed



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mutationRate.noncodi...	0.347	273
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mutationRate.2ndpos	0.185	237

Nothing mixed



Possible solutions:

- ✓ Increase chain length
- ✓ Run multiple independent chains
- ✓ Increase sampling frequency (if ACT permits)
- ✓ Check for conflicts in the data / priors
- ✓ Check if the model is misspecified or too complex for the data

Possible scenarios

Beast analysis

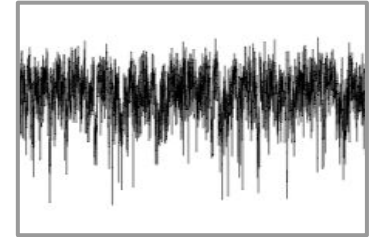
Initialisation failed

```
Start likelihood: -Infinity after
1000 initialisation attempts

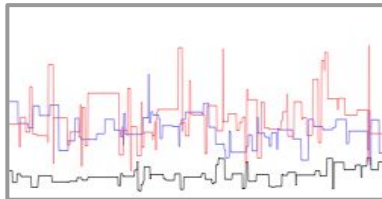
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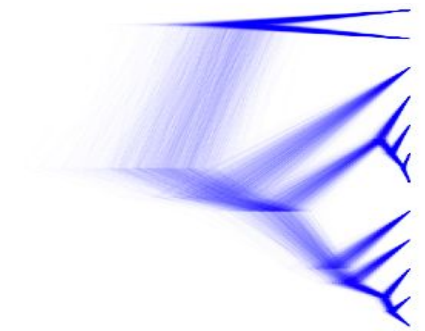
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mutationRate.1stpos	0.459	238
mutationRate.2ndpos	0.185	237

First: CHECK THE TREE

Possible solutions:

- ✓ Tweak the operator weights:
 - ✓ Increase the weight for low ESS parameters
 - ✓ Use an UpDown operator for correlated parameters
- ✓ Run longer (or combine several independent chains)
- ✓ Change the starting value
- ✓ Use a more informative prior

Tree space mixing



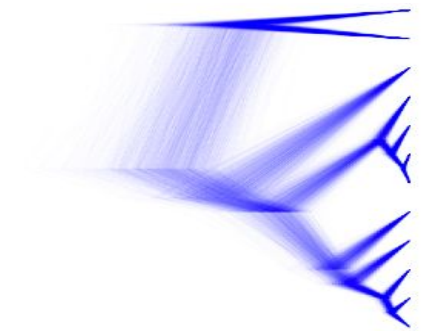
Bad news:

Tracer can not directly examine the ESS of the trees

Good news:

- Good mixing of the other parameters, posterior and likelihood is indicative
- Other tools are available:
 - RWTY (R package) to check the topology ESS
 - Convenience (R package) to check the ESS of clade splits

Tree not mixing



Possible solutions:

- ✓ Tweak the tree operator weights
- ✓ Run longer (or combine several independent chains)
- ✓ Use a good starting tree
- ✓ Add topological constraints and/or time calibration information
- ✓ Add data or simplify the analysis

Possible scenarios

Beast analysis

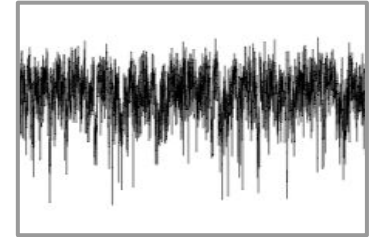
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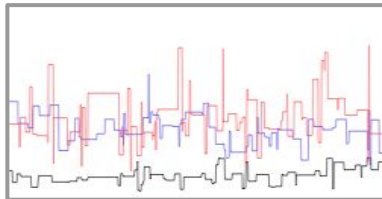
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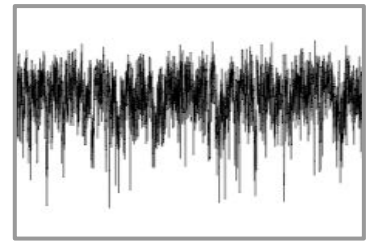
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Everything mixed



Final checks:

Comparison between chains

Multi-modal distributions

Are my results driven by the data?

Sampling from prior

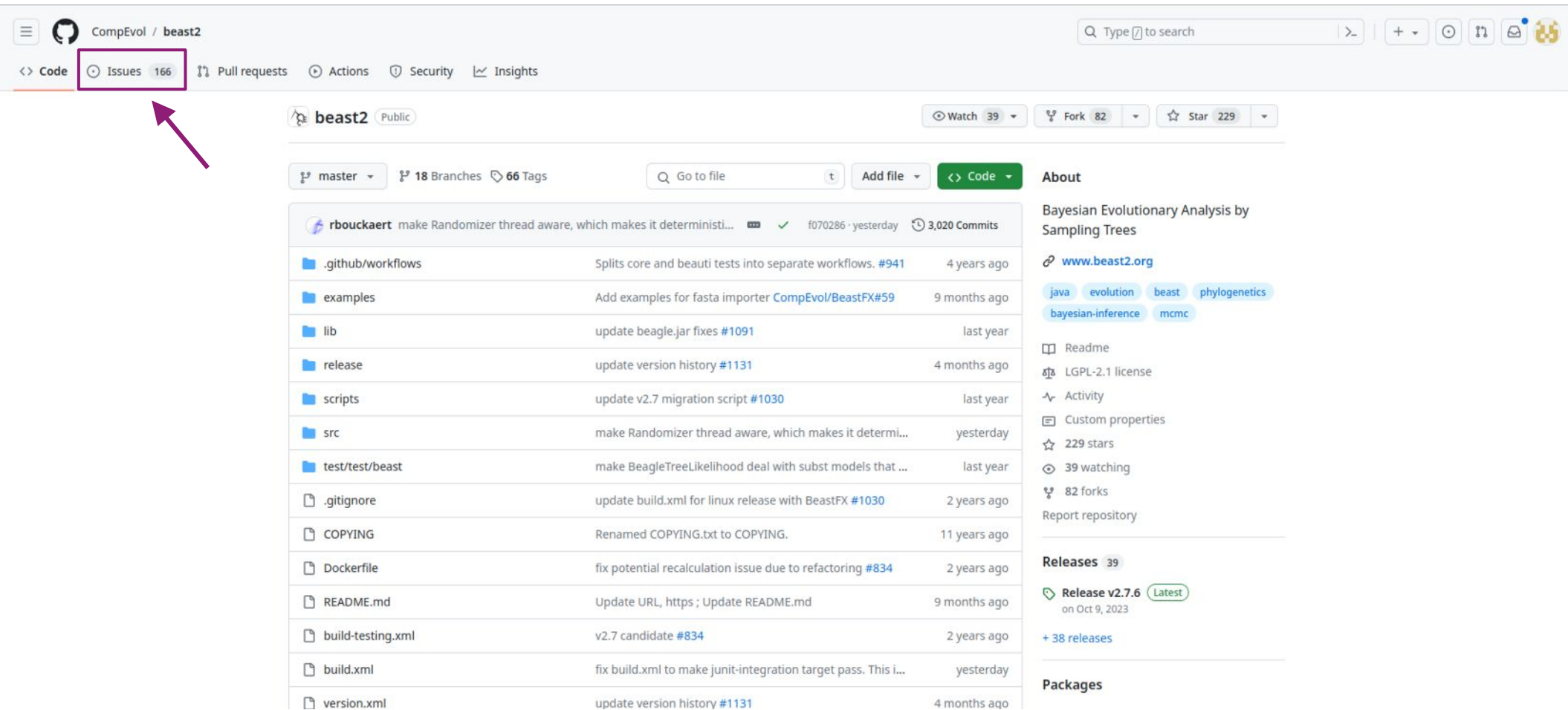
Keep in mind:

- The uncertainty is part of the result !
- The result is conditioned on the model !

Good places to look for help

- Taming the BEAST tutorials
- BEAST2 website (BEAST2 and some packages)
 - Additional tutorials <http://www.beast2.org/tutorials/>
 - Blog posts <http://www.beast2.org/blogindex.html>
- Users google group (BEAST2 and some packages)
<https://groups.google.com/g/beast-users>
- File an issue (BEAST2 and packages)
- Last resort – email developers directly

Reporting issues



CompEvol / **beast2**

Issues 166 Pull requests Actions Security Insights

beast2 Public Watch 39 Fork 82 Star 229

master 18 Branches 66 Tags

Go to file Add file Code

rbouckaert make Randomizer thread aware, which makes it deterministi... f070286 · yesterday 3,020 Commits

.github/workflows	Splits core and beauti tests into separate workflows. #941	4 years ago
examples	Add examples for fasta importer CompEvol/BeastFX#59	9 months ago
lib	update beagle.jar fixes #1091	last year
release	update version history #1131	4 months ago
scripts	update v2.7 migration script #1030	last year
src	make Randomizer thread aware, which makes it determi...	yesterday
test/test/beast	make BeagleTreeLikelihood deal with subst models that ...	last year
.gitignore	update build.xml for linux release with BeastFX #1030	2 years ago
COPYING	Renamed COPYING.txt to COPYING.	11 years ago
Dockerfile	fix potential recalculation issue due to refactoring #834	2 years ago
README.md	Update URL, https ; Update README.md	9 months ago
build-testing.xml	v2.7 candidate #834	2 years ago
build.xml	fix build.xml to make junit-integration target pass. This i...	yesterday
version.xml	update version history #1131	4 months ago

About

Bayesian Evolutionary Analysis by Sampling Trees

www.beast2.org

java evolution beast phylogenetics bayesian-inference mcmc

Readme LGPL-2.1 license Activity Custom properties 229 stars 39 watching 82 forks Report repository


Releases 39

Release v2.7.6 Latest on Oct 9, 2023

+ 38 releases

Packages

Reporting issues

 CompEvol / beast2

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<> Code Issues 166 Pull requests Actions Security Insights

Filters 🔽 🔍 is:issue is:open

🔖 Labels 20 📅 Milestones 6

New issue

🕒 166 Open ✓ 888 Closed

Author 🔽 Label 🔽 Projects 🔽 Milestones 🔽 Assignee 🔽 Sort 🔽

🕒 Randomizer per thread for deterministic behaviour when using threads

#1141 opened last week by rbouckaert

🕒 BEAST.base installation

#1140 opened 3 weeks ago by NRuizVargas

🕒 BEAST 2.7.6 not launching on Mac

#1139 opened last month by kbhoehn

🕒 Add CCD package to list of recommended packages

#1138 opened on Feb 1 by rbouckaert

💬 4

🕒 java.lang.Error: randomChoiceUnnormalized falls through -- negative components in input distribution?

#1135 opened on Dec 2, 2023 by Sikandar37

💬 2

🕒 How can I find out number of patterns and number of partitions from my input file without running Beast2?

#1134 opened on Nov 4, 2023 by mzhuangsdsc

💬 6

🕒 Robustify package manager

#1133 opened on Oct 26, 2023 by rbouckaert

🕒 BEAST2: fatal error has been detected by the Java Runtime Environment

#1132 opened on Oct 25, 2023 by Rutaiwan

💬 1

🕒 Prep for v2.7.6 release

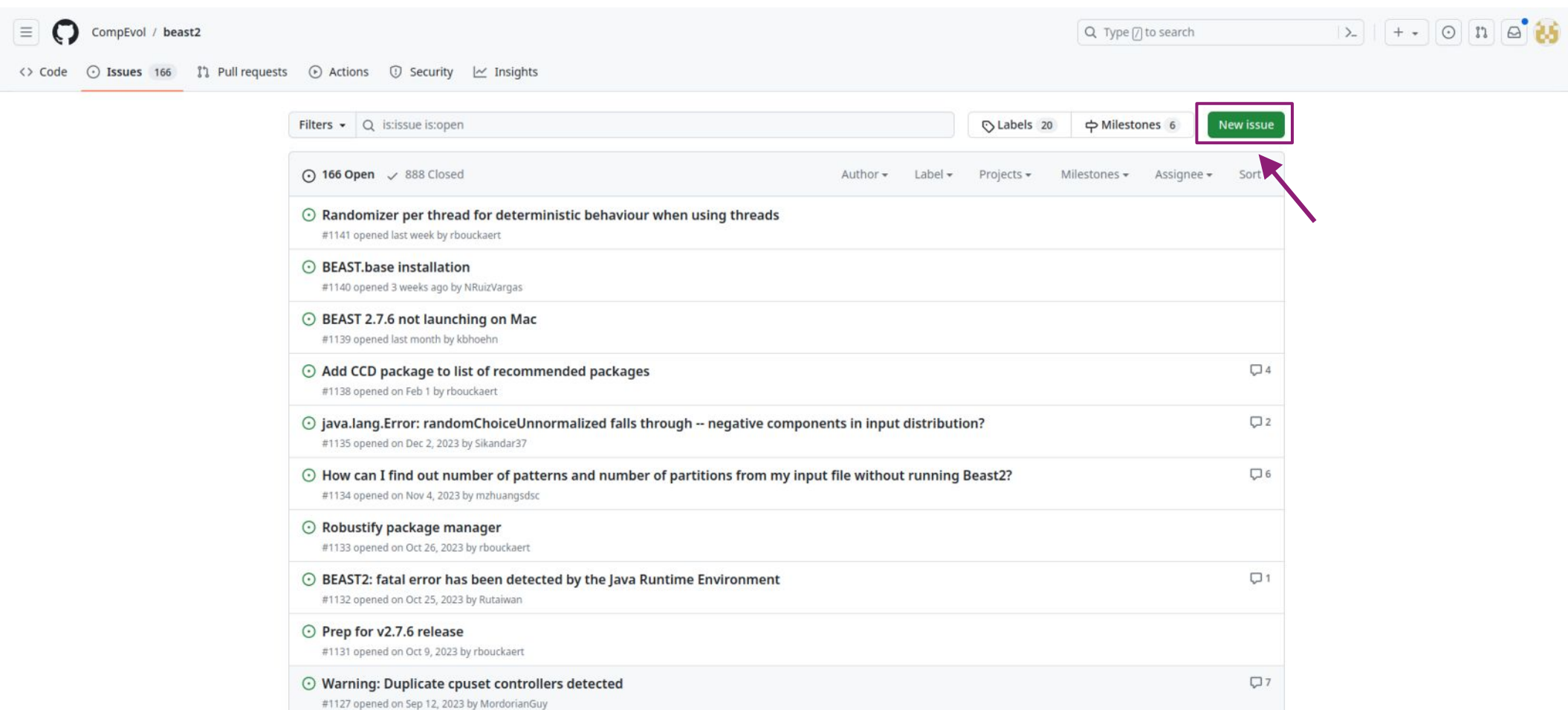
#1131 opened on Oct 9, 2023 by rbouckaert

🕒 Warning: Duplicate cpuset controllers detected

#1127 opened on Sep 12, 2023 by MordorianGuy

💬 7

Reporting issues



The screenshot displays the GitHub interface for the `CompEvol / beast2` repository. The top navigation bar includes links for `Code`, `Issues` (166), `Pull requests`, `Actions`, `Security`, and `Insights`. A search bar is located on the right. Below the navigation bar, the `Issues` section is active, showing a list of 166 open issues. The issues are sorted by 'Newest' (indicated by a green circle icon). A purple box highlights the `New issue` button, and a purple arrow points to it from the right.

Filters: `is:issue is:open`

Labels: 20 | Milestones: 6 | [New issue](#)

166 Open ✓ 888 Closed

Author ▾ | Label ▾ | Projects ▾ | Milestones ▾ | Assignee ▾ | Sort ▾

- Randomizer per thread for deterministic behaviour when using threads
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Reporting issues

CompEvol / beast2

Q Type to search

<> Code Issues 166 Pull requests Actions Security Insights

Add a title

title

Add a description

Write Preview

H B I

Add your description here...

Markdown is supported Paste, drop, or click to add files

Submit new issue

Assignees
No one assigned

Labels
None yet

Projects
None yet

Milestone
No milestone

Development
Shows branches and pull requests linked to this issue.

Helpful resources
[GitHub Community Guidelines](#)

Remember, contributions to this repository should follow our [GitHub Community Guidelines](#).

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Best practices when asking for help

- Use the latest version of everything
- Describe the problem (what you were trying to do, what should have happened, what happened)
- Give all information needed to debug....
 - **XML file for the analysis**
 - Output files if you have them
 - Screenshots for BEAUti issues
-but not more than that !!
 - Reduce the file size if possible
 - Narrow down the issue

Going further

Taming the BEAST tutorials (of course!)

METHOD ARTICLE 

Practical guidelines for Bayesian phylogenetic inference using Markov Chain Monte Carlo (MCMC)

[version 1; peer review: 2 approved, 1 approved with reservations]

Joëlle Barido-Sottani  , Orlando Schwery, Rachel C. M. Warnock, Chi Zhang, April Marie Wright

<https://open-research-europe.ec.europa.eu/articles/3-204>

```
<operator id="StrictClockRateScaler_morph" spec="ScaleOperator" parameter="@clockRate_morph" scaleFactor="0.75" weight="3.0"/>
<operator id="strictClockUpDownOperator" spec="UpDownOperator" scaleFactor="0.75" weight="3.0">
  <up idref="clockRate_morph"/>
  <up idref="clockRate"/>
  <down idref="Tree"/>
</operator>
```

BEAST2 XML files

Joëlle Barido-Sottani
Slides adapted from Tim Vaughan

```
  <log idref="likelihood"/>
  <log idref="prior"/>
</logger>
<logger id="treelog" spec="Logger" fileName="seed_1051_struct_upclock_all_samples_SA_10.trees" logEvery="10000" mode="tree">
  <log id="TreeWithMetaDataLogger" spec="beast.evolution.tree.TreeWithMetaDataLogger" tree="@Tree"/>
</logger>
```

What is a BEAST2 XML file ?

- Precise description of a BEAST2 analysis :
 - Data (alignment, sampling times, ...)
 - Model (substitution model, tree prior, ...)
 - Parameter priors
- Usually produced by BEAUti.
- Read by BEAST2 when the analysis is run.
- Makes BEAST2 results reproducible
 - => should be included in any research data archive

Why should I learn about BEAST2 XML ?

- Every BEAST2 analysis can be described using BEAST2 XML
=> **but...** many analyses cannot be set up using BEAUti!
- Some analyses best done by modifying the XML file :
 - Fixing parameters or the trees in the analysis.
 - Linking certain models (beyond the usual substitution, clock, or tree priors)
 - Adjusting initial values (e.g. for troubleshooting)
 - Modifying analyses that were not produced using BEAUti.

BEAST2 XML : A first look

```
<parameter id="clockRate_morph" spec="parameter.RealParameter" name="stateNode">1.0</parameter>
<parameter id="clockRate" spec="parameter.RealParameter" name="stateNode">0.01</parameter>
<parameter id="gammaShape" spec="parameter.RealParameter" name="stateNode">1.0</parameter>
<parameter id="kappa" spec="parameter.RealParameter" lower="0.0" name="stateNode">2.0</parameter>
<parameter id="birthRateFBD" spec="parameter.RealParameter" lower="0.0" name="stateNode">1.0</parameter>
<parameter id="deathRateFBD" spec="parameter.RealParameter" lower="0.0" name="stateNode">0.5</parameter>
<parameter id="samplingRateFBD" spec="parameter.RealParameter" lower="0.0" name="stateNode">0.5</parameter>
<parameter id="originFBD" spec="parameter.RealParameter" lower="0.0" name="stateNode">130.0</parameter>
<parameter id="freqParameter" spec="parameter.RealParameter" dimension="4" lower="0.0" name="stateNode" upper="1.0">0.25</parameter>
</state>
<init id="RandomTree" spec="beast.evolution.tree.RandomTree" estimate="false" initial="@Tree" taxa="@simdata">
  <populationModel id="ConstantPopulation0" spec="ConstantPopulation">
    <parameter id="randomPopSize" spec="parameter.RealParameter" name="popSize">1.0</parameter>
  </populationModel>
</init>
<distribution id="posterior" spec="util.CompoundDistribution">
  <distribution id="prior" spec="util.CompoundDistribution">
    <distribution id="FBD" spec="beast.evolution.speciation.SABirthDeathModel" conditionOnRhoSampling="true" birthRate="@birthRateFBD" origin="@originFBD" samplingRate="@samplingRateFBD" tree="@Tree" deathRate="@deathRateFBD">
      <parameter id="rFBD" spec="parameter.RealParameter" lower="0.0" name="removalProbability" upper="1.0">0.0</parameter>
      <parameter id="rhoFBD" spec="parameter.RealParameter" estimate="false" lower="0.0" name="rho" upper="1.0">1.0</parameter>
    </distribution>
    <prior id="birthRatePriorFBD" name="distribution" x="@birthRateFBD">
      <Exponential id="Exponential.1" name="distr">
        <parameter id="RealParameter.9" spec="parameter.RealParameter" estimate="false" name="mean">1.0</parameter>
      </Exponential>
    </prior>
    <prior id="ClockPrior" name="distribution" x="@clockRate">
      <Exponential id="Exponential.6" name="distr">
        <parameter id="RealParameter.7" spec="parameter.RealParameter" estimate="false" name="mean">0.1</parameter>
      </Exponential>
    </prior>
    <prior id="ClockPrior_morph" name="distribution" x="@clockRate_morph">
      <Exponential id="Exponential.7" name="distr">
        <parameter id="RealParameter.8" spec="parameter.RealParameter" estimate="false" name="mean">0.1</parameter>
      </Exponential>
    </prior>
    <prior id="KappaPrior" name="distribution" x="@kappa">
      <LogNormal id="LogNormalDistributionModel1.0" name="distr">
        <parameter id="RealParameter.4" spec="parameter.RealParameter" estimate="false" name="M">1.0</parameter>
        <parameter id="RealParameter.5" spec="parameter.RealParameter" estimate="false" name="S">1.25</parameter>
      </LogNormal>
    </prior>
    <prior id="originPriorFBD" name="distribution" x="@originFBD">
      <Uniform id="Uniform.5" name="distr" lower="80" upper="300"/>
    </prior>
    <prior id="samplingRatePriorFBD" name="distribution" x="@samplingRateFBD">
      <Exponential id="Exponential.3" name="distr">
        <parameter id="RealParameter.11" spec="parameter.RealParameter" estimate="false" name="mean">1.0</parameter>
      </Exponential>
    </prior>
    <prior id="deathRatePriorFBD" name="distribution" x="@deathRateFBD">
      <Exponential id="Exponential.2" name="distr">
        <parameter id="RealParameter.10" spec="parameter.RealParameter" estimate="false" name="mean">1.0</parameter>
      </Exponential>
    </prior>
  </distribution>
</distribution>
```


What is XML ?

- XML is a standard way of representing hierarchically structured data
- XML files are plain text files containing XML-formatted data
- XML file components :

```
<tag attributeOne="Attribute value" attributeTwo="Another attribute value">  
  <childTag childAttribute="10">  
  </childTag>  
  <childTag childAttribute="20"/>  
  <!-- This is a "comment" -->  
</tag>
```

A simple example model

BEAUti 2: Standard

Partitions Tip Dates Site Model Clock Model Priors MCMC

Link Site Models Unlink Site Models Link Clock Models Unlink Clock Models Link Trees Unlink Trees

Name	File	Taxa	Sites	Data Type	Site Model	Clock Model	Tree	...
h3n2	h3n2	150	1762	nucleotide	h3n2	h3n2	h3n2	

+ - r Split

BEAUti 2: Standard

Partitions Tip Dates Site Model Clock Model Priors MCMC

Gamma Site Model

Substitution Rate 1.0 ☐ estimate

Gamma Category Count 0

Proportion Invariant 0.0 ☐ estimate

Subst Model JC69

BEAUti 2: Standard

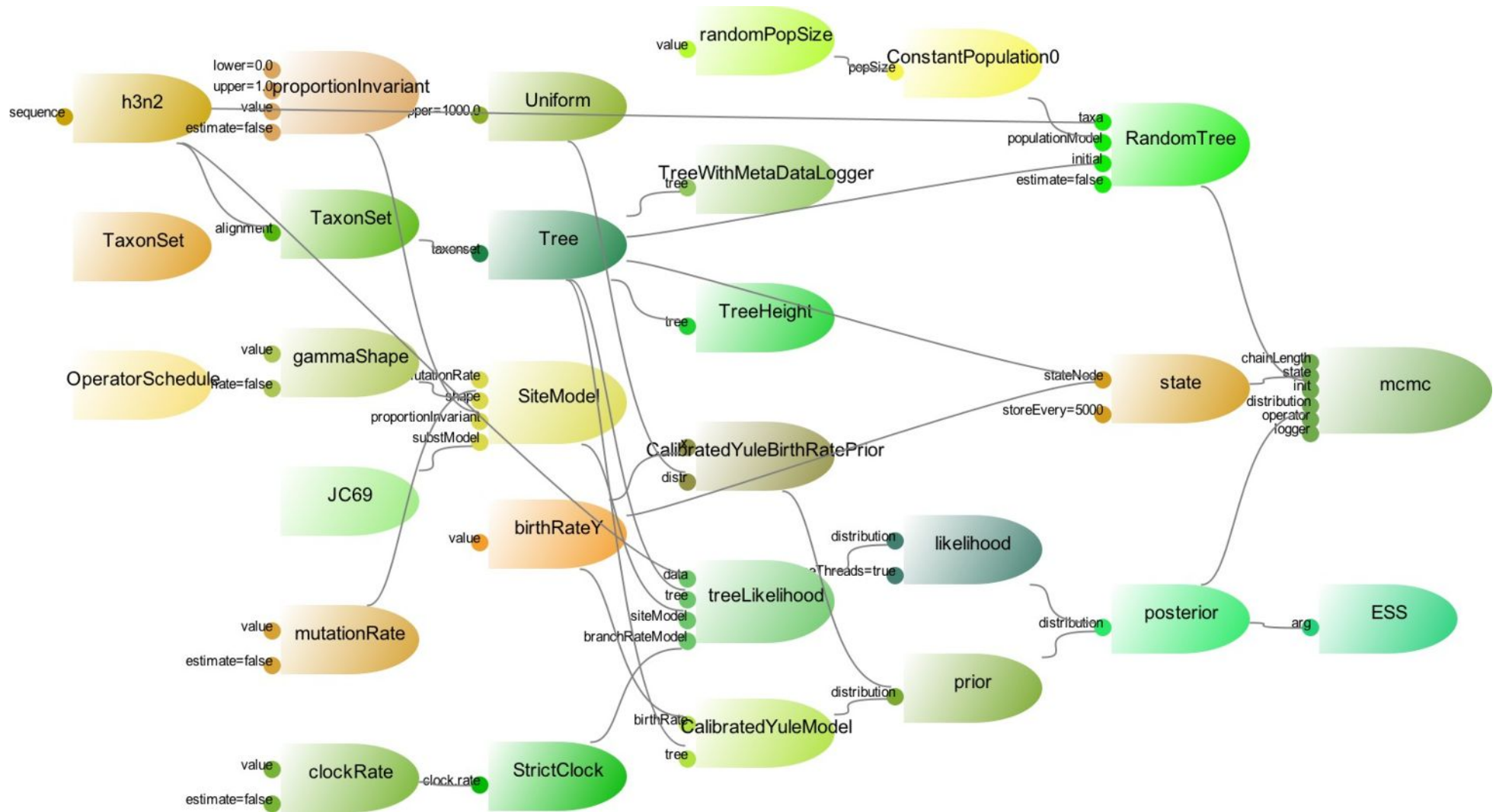
Partitions Tip Dates Site Model Clock Model Priors MCMC

Tree:t:h3n2 Calibrated Yule Model

birthRateY.t:h3n2 Uniform initial = [1.0] $[-\infty, \infty]$ Calibrated Yule speciation process birth rate for t:h3n2

+ Add Prior

The BEAST2 model graph



Relationships in the model graph



- Objects are connected through inputs
- There is a “**has a**” relationship between objects and their inputs
 - => E.g. the NormalDistribution object **has a** RealParameter input with the name “mean”

Relationships in the XML



```
<parentInput spec="BEASTObject">  
  <input1 .../>  
  <input2 .../>  
  ...  
</parentInput>
```

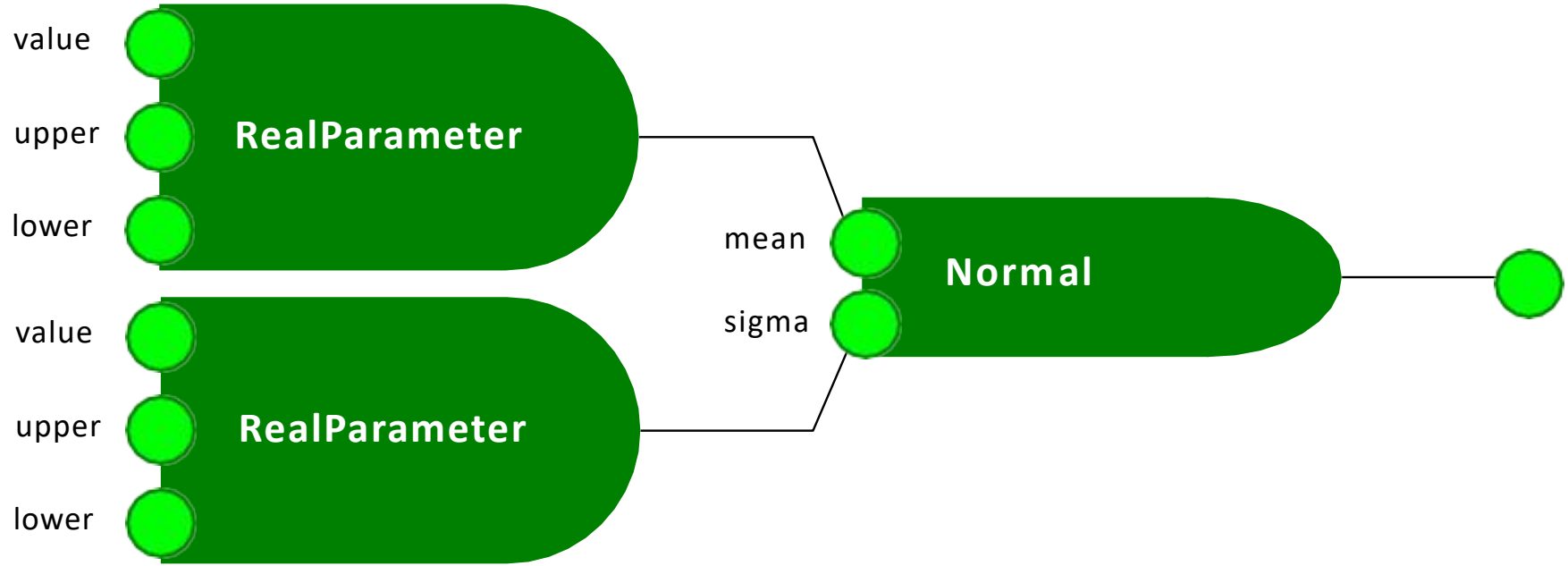
```
<distr spec="Normal" id="NormalDistribution">  
  <mean spec="RealParameter" estimate="false" value="1.0"/>  
</distr>
```

Simple inputs

- Some BEASTObjects take inputs with primitive types such as strings (i.e. text), boolean values (true/false) or numbers.
- These values are specified using attributes.

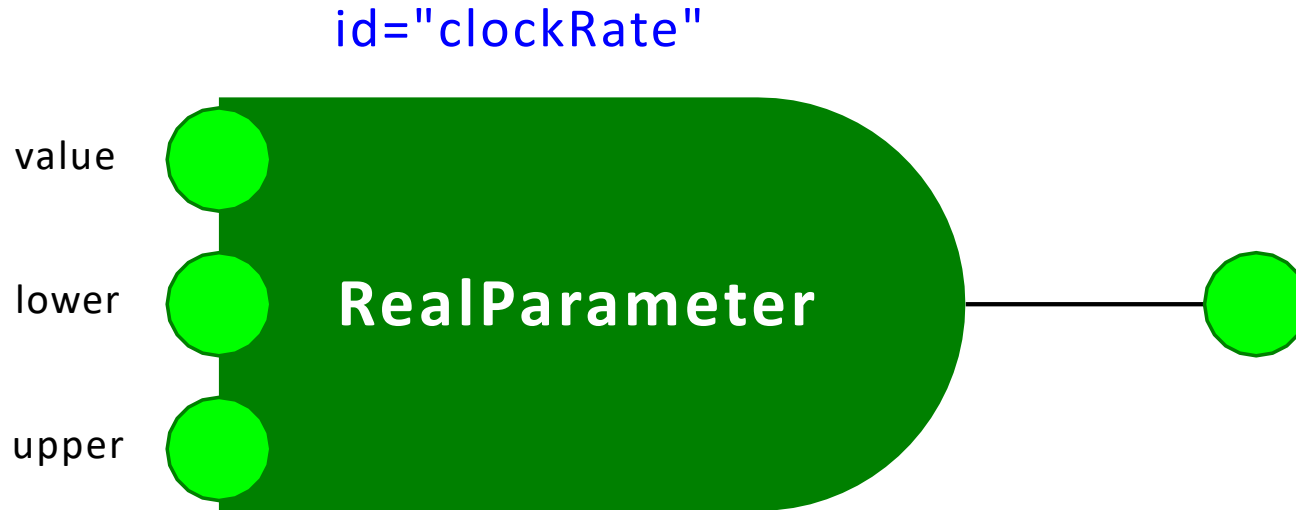
```
<mcmc spec="MCMC"  
      chainLength="100000000"  
      storeEvery="10000"  
      sampleFromPrior="true">  
  . . .  
</mcmc>
```

Connecting complex objects



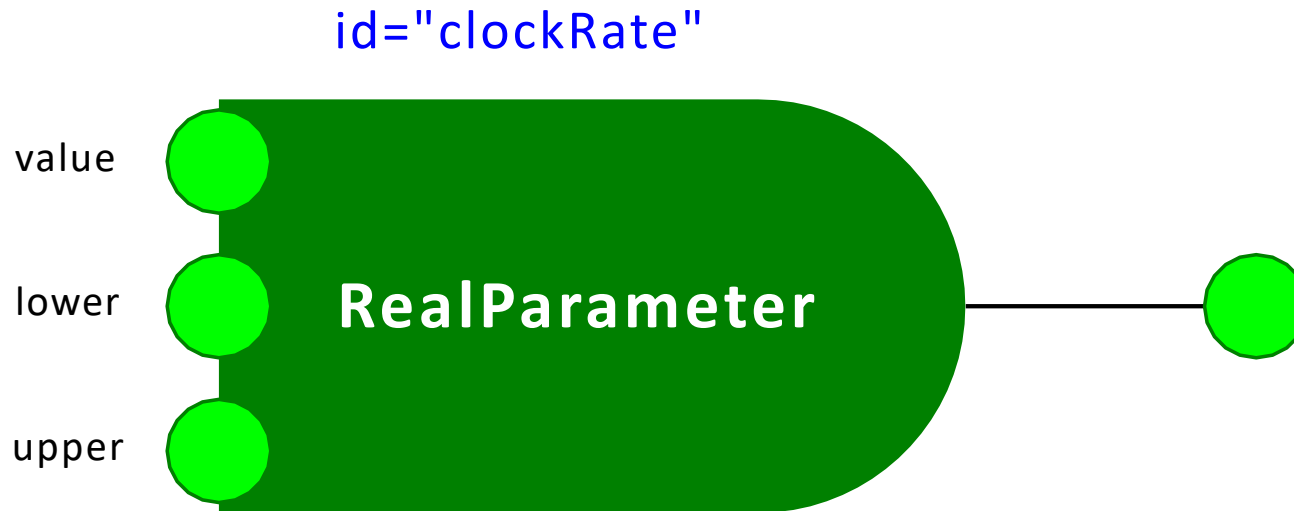
```
<parentInput spec="Normal">  
  <mean spec="RealParameter" value="1.0" lower="0.0" upper="5.0"/>  
  <sigma spec="RealParameter" value="0.5" lower="0.0" upper="5.0"/>  
</parentInput>
```

Referencing objects



```
<state>
  <stateNode spec="RealParameter" value="1.0" id="clockRate"/>
</state>
...
<logger logEvery="1000" fileName="logfile.log">
  <log idref="clockRate"/>
</logger>
```


Referencing objects – part 2



```
<state>
  <stateNode spec="RealParameter" value="1.0" id="clockRate"/>
</state>
...
<operator spec="ScaleOperator" parameter="@clockRate" weight="1">
</operator>
```

Final comments

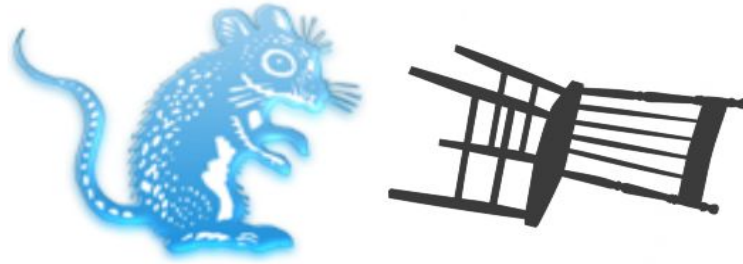
- These are equivalent forms of BEASTObject representation :

```
<parentInput spec="RealParameter" value="1.0"/>
```

```
<parameter name="parentInput" value="1.0"/>
```

- Object class names are in general prefixed by their location in the package, e.g. `beast.core.parameter.RealParameter` is equivalent to `RealParameter`

Troubleshooting time !



<https://taming-the-beast.org/tutorials/Troubleshooting-initialization-issues/>

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