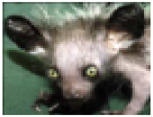
Beast 2 basics
Plugins
Inputs
MCMC library
Loop
Classes
Evolution library
Design patterns
Ways to mess up

Beast II 101: Part 1



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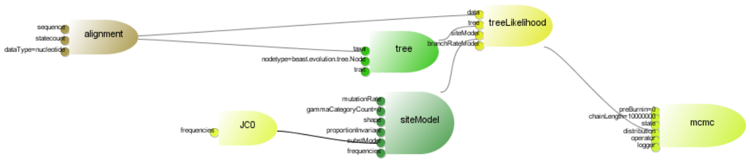
Jukes Cantor



All objects are Plugins - connected to each other through Inputs

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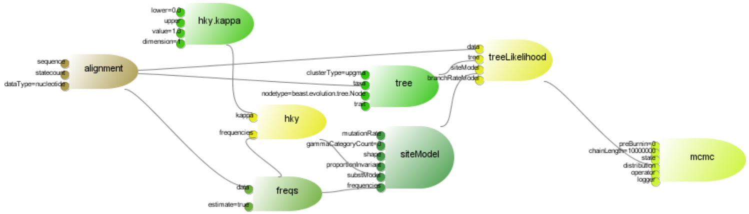
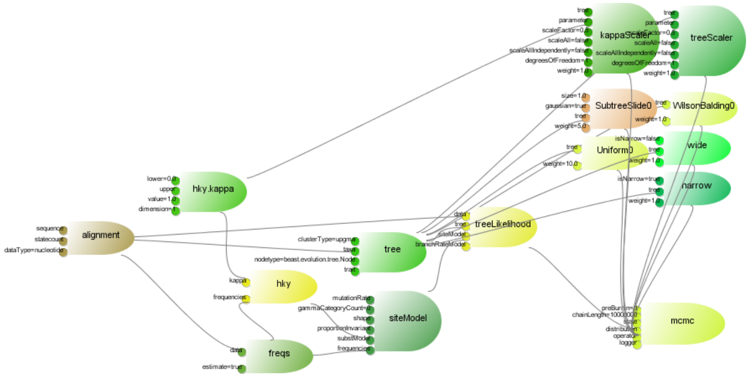
HKY



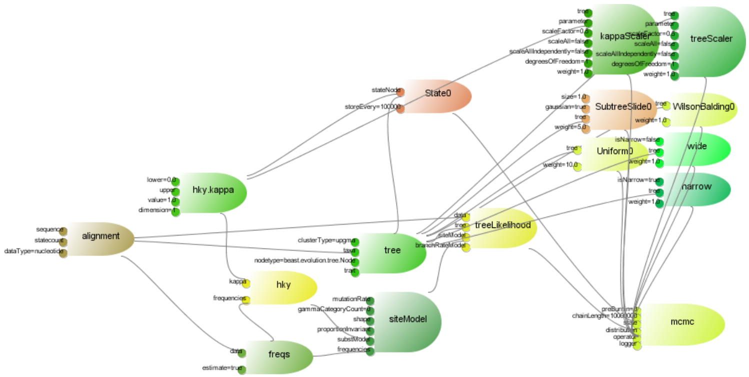
Adding kappa parameter and frequencies

Adding operators



Operate on kappa parameter and tree

Adding State



The state contains every Plugin that operators work on

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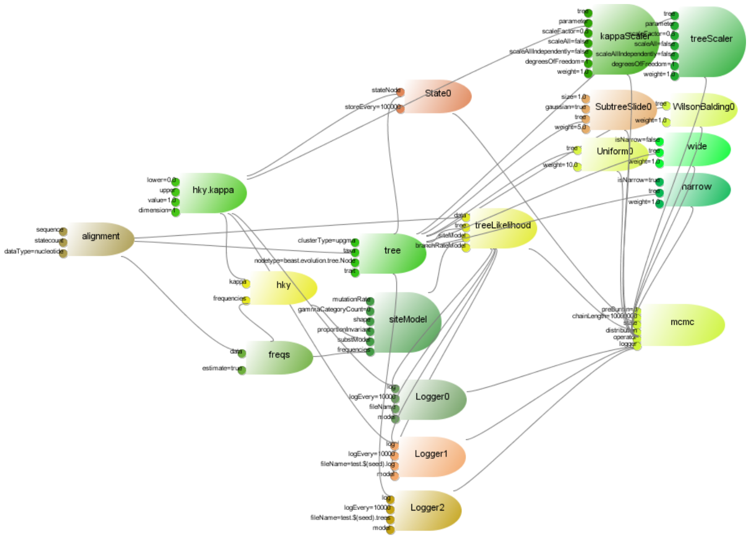
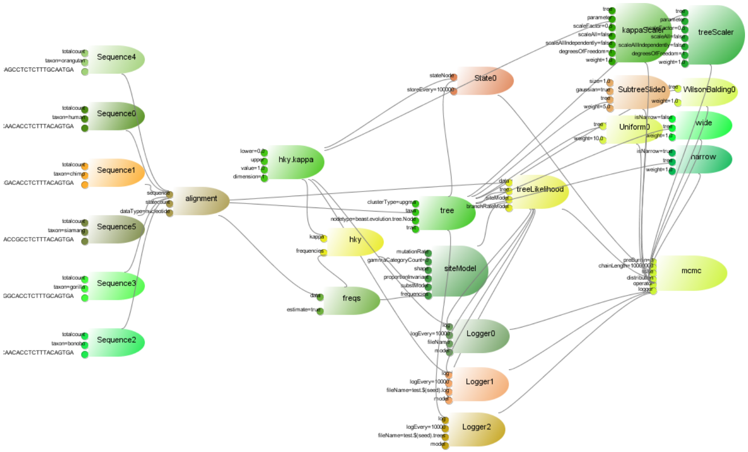
Adding Loggers



3 loggers: screen, trace and trees

Adding Sequences



Inputs to alignments, which takes care of the patterns, DataType and set of Taxon names

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What Beast 2 does

...supposed to do...

- The kind of Bayesian analysis as per citations on the Beast 1 wiki.
- Beauti 2: GUI to specify analysis.
- Provide a platform to develop add-ons - powerful interface, easy extensible XML, templates for Beauti.
- Sequence generator for simulation studies.
- Documentation for all the above – from user to developer, XML tweaker, etc.

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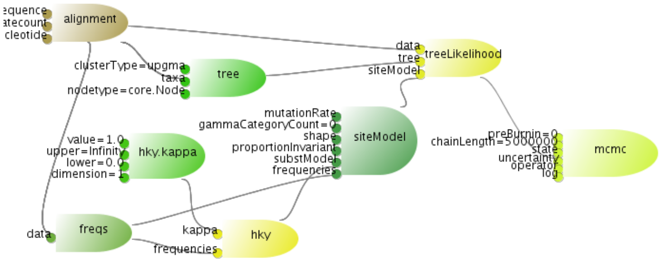
What Beast 2 doesn't

- Post-analysis processing like Tracer, tree annotator, tree log analyser, DensiTree, KML producer
- Most non-Bayesian analysis
- Laundry

Phylosophy

Everything is a plug-in



Plug-ins provide...

- connection with with other plug-ins/values through ’inputs’
- validation
- documentation
- ’XML parsing’

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Plugin class

```
@Description("Description␣goes␣here")
public class Plugin {
    public void initAndValidate()

    public String getDescription()
    public String getCitations()

    public String getID()
    public void setID(String sID)

} // class Plugin
```

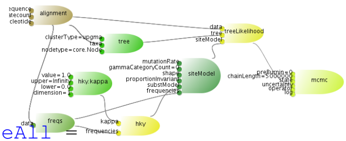
A minimal plugin

```
@Description("Description␣of␣MyPlugin␣goes␣here")
public class MyPlugin extends Plugin {
    public Input<Integer> m_value = new Input<Integer>("value",
        "value␣used␣by␣my␣plugin");

    public void initAndValidate() throws Exception {
        // go check stuff and
        // do stuff that normally goes in a constructor
    }

} // class MyPlugin
```

HKY Plugin

```
@Description("HKY85␣(Hasegawa,␣Kishino␣&␣Yano,␣1985)␣substitution␣model␣o
@Citation("Hasegawa,␣M.,␣Kishino,␣H␣and␣Yano,␣T.␣1985.␣Dating␣the␣human-a
        "Journal␣of␣Molecular␣Evolution␣22:160-174.")
public class HKY extends 'Plugin' {
    public Input<Frequencies> m_freqs = new Input<Frequencies>("frequenci
    public Input<Parameter> m_kappa = new Input<Parameter>("kappa", "kapp

    @Override public void initAndValidate() throws Exception {
        initialiseEigen();
    }

     public void getTransitionProbabilities(Node node,
                double fStartTime,
                double fEndTime,
                double fRate,
                double[] matrix) {...}

    @Override
    protected boolean requiresRecalculation() {...}

    @Override public void store() {...}
    @Override public void restore() {... }
} // class HKY
```

Inputs



Simple primitives

```
public Input<Boolean> m_pScaleAll =
    new Input<Boolean>("scaleAll",
        "if␣true,␣all␣elements␣of␣a␣parameter␣are␣scaled,␣otherwise␣one␣i
```

Other plugins

```
public Input<Frequencies> m_freqs =
    new Input<Frequencies>("frequencies",
        "frequencies␣of␣nucleotide␣letters");
```

Multiple inputs

```
public Input<List<Parameter>> m_pParameters =
    new Input<List<Parameter>>("parameter",
        "parameter,␣part␣of␣the␣state",
        new ArrayList<Parameter>());
```

Inputs

Enumerations

```
final static String [] UNITS =  {"year", "month", "day"};

public Input<String> m_sUnits = new Input<String>("units",
        "name␣of␣the␣units␣in␣which␣values␣are␣posed,␣" +
                "used␣for␣conversion␣to␣a␣real␣value.␣This␣can␣be␣" +
        Arrays.toString(UNITS) + "␣(default␣'year')",
        "year",
        UNITS);
```

Input validation

Default: OPTIONAL (see previous slide)

If input is REQUIRED:

```
public Input<Parameter> m_kappa =
    new Input<Parameter>("kappa",
        "kappa␣parameter␣in␣HKY␣model",
        Validate.REQUIRED);

public Input<List<Operator>> m_operators =
    new Input<List<Operator>>("operator",
        "operator␣for␣generating␣proposals␣in␣MCMC␣state␣space",
        new ArrayList<Operator>(), Validate.REQUIRED);
```

If input is XOR:

```
public Input<Tree> m_pTree =
    new Input<Tree>("tree",
        "if␣specified,␣all␣tree␣branch␣length␣are␣scaled");
public Input<Parameter> m_pParameter =
    new Input<Parameter>("parameter",
        "if␣specified,␣this␣parameter␣is␣scaled"
        , Validate.XOR, m_pTree);
```

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State

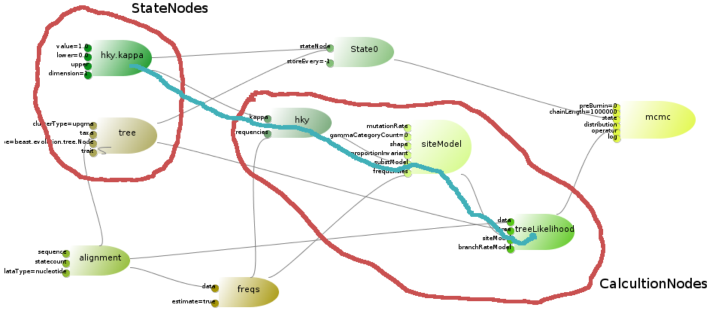
- State is explicit in XML & as object (unlike Beast 1)
- Contains StateNodes, e.g., parameters and trees
- Operators work on the StateNodes

```
public double proposal() throws Exception {...}
```

- State can be stored to disk/restored
- State can store/restore itself for MCMC proposals

MCMC Library

StateNode vs CalculationNode



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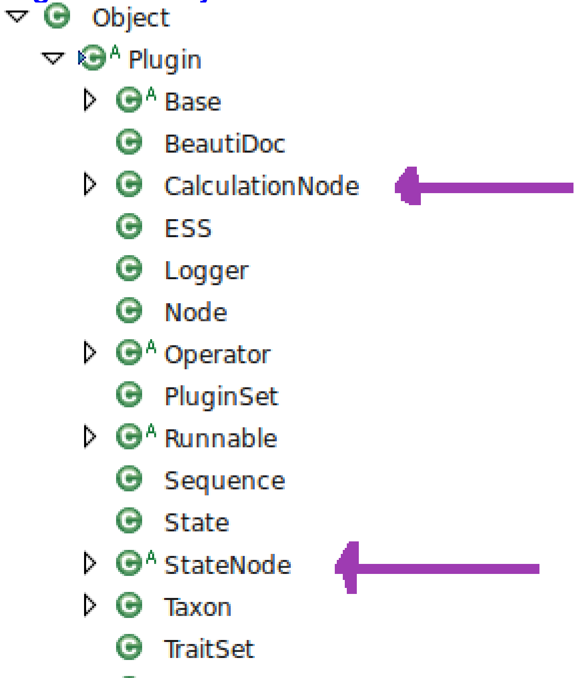
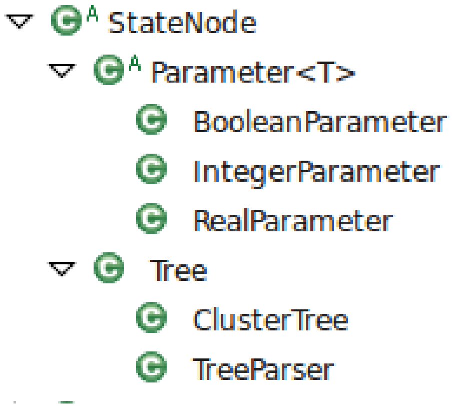
Plugin hierarchy



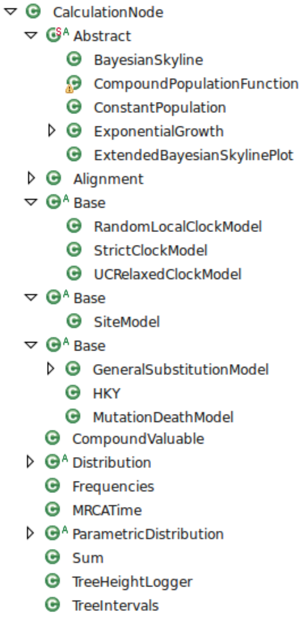
- Object
  - Plugin
    - Base
    - BeautiDoc
    - CalculationNode
    - ESS
    - Logger
    - Node
    - Operator
    - PluginSet
    - Runnable
    - Sequence
    - State
    - StateNode
    - Taxon
    - TraitSet

StateNode hierarchy



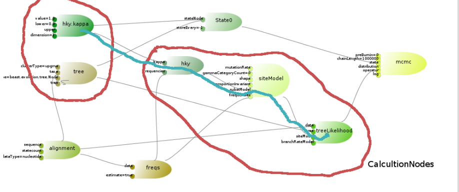
```
▽ StateNode
    ▽ Parameter<T>
        BooleanParameter
        IntegerParameter
        RealParameter
    ▽ Tree
        ClusterTree
        TreeParser
```

CalculationNode hierarchy



- CalculationNode
  - Abstract
    - BayesianSkyline
    - CompoundPopulationFunction
    - ConstantPopulation
    - ExponentialGrowth
    - ExtendedBayesianSkylinePlot
  - Alignment
  - Base
    - RandomLocalClockModel
    - StrictClockModel
    - UCRelaxedClockModel
  - Base
    - SiteModel
  - Base
    - GeneralSubstitutionModel
    - HKY
    - MutationDeathModel
  - CompoundValuable
  - Distribution
  - Frequencies
  - MRCATime
  - ParametricDistribution
  - Sum
  - TreeHeightLogger
  - TreeIntervals

MCMC loop

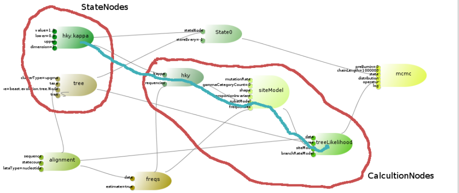


```
Propose new state


logP = calculateLogP();
if (new state is acceptable)
        // do something


else
        // do something else
```

MCMC loop effect on state nodes



```
Store state
Propose new state


logP = calculateLogP();
if (new state is acceptable)
    accept state

else
    restore state

mark state clean
```

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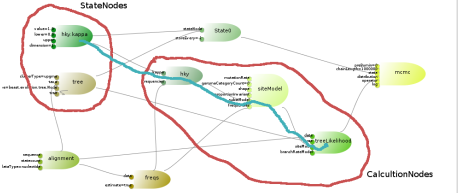
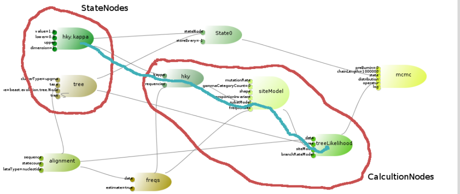
MCMC loop effect on calculation nodes



```
Store state
Propose new state
store calculation nodes
check dirtyness calculation nodes
logP = calculateLogP();
if (new state is acceptable)
    accept state
    mark calculation nodes clean
else
    restore state
    restore calculation nodes
mark state clean
```

MCMC loop
CalculationNode method calls



```
Store state
Propose new state
store calculation nodes store()
check dirtyness  requiresRecalculation()
logP = calculateLogP();
if (new state is acceptable)
        accept state
        mark calculation nodes clean accept()
else
        restore state
        restore calculation nodes restore()
mark state clean
```

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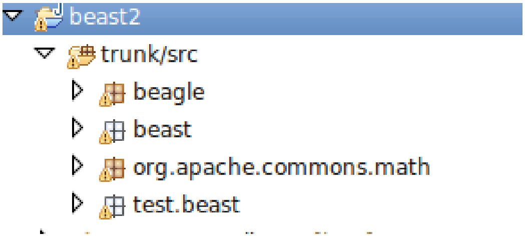
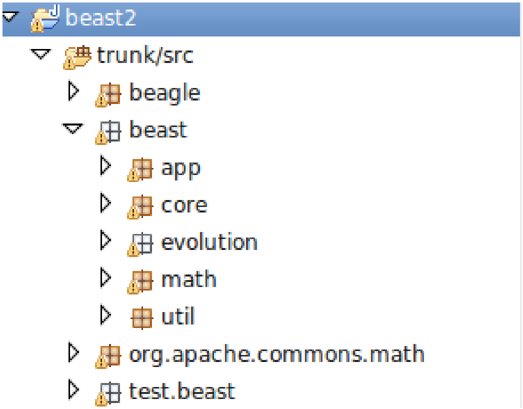
Beast class structure


beast2
trunk/src
beagle
beast
org.apache.commons.math
test.beast

beast - main beast classes
beagle and apache libraries
test - for junit tests

Beast core class structure



```
beast2
  trunk/src
    beagle
    beast
      app
      core
      evolution
      math
      util
    org.apache.commons.math
    test.beast
```

app - applications like BeastMCMC, Beauti, SequenceGenerator
core, evolution - MCMC and evolution libraries
math - mathematical classes
util - utilities like parsers, XML producers, random nr generator, class discovery.

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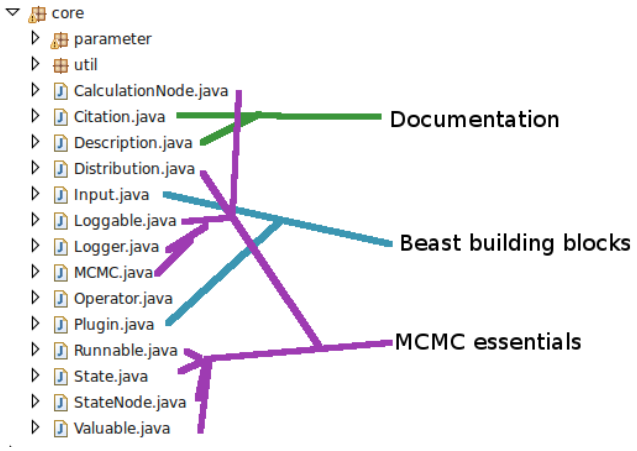
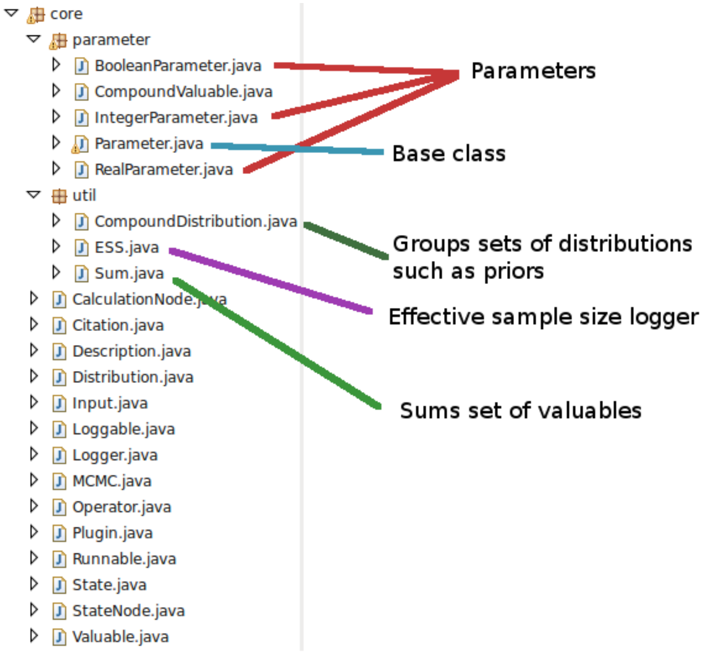
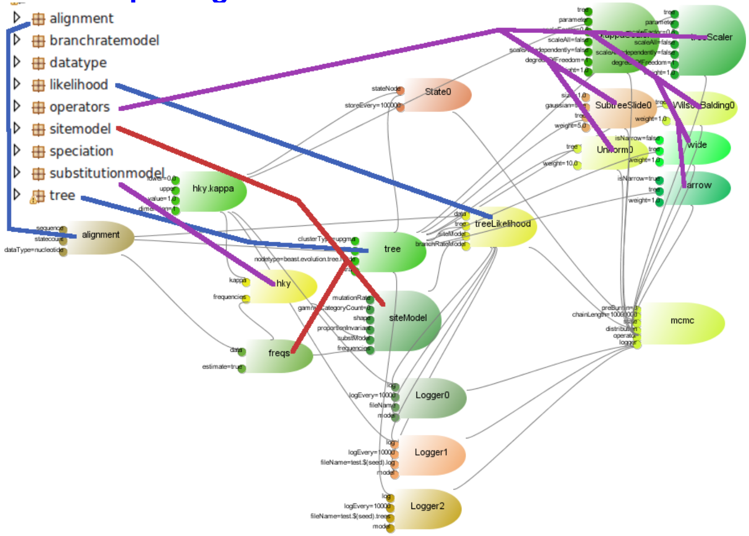
Beast core class structure



Beast core class structure



Evolution packages



Important classes you might want to derive from: SubstitutionModel, Operator, BranchRateModel, Coalescent, SpeciationLikelihood, (DataType, Alignment, SiteModel).

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Evolution - alignment classes

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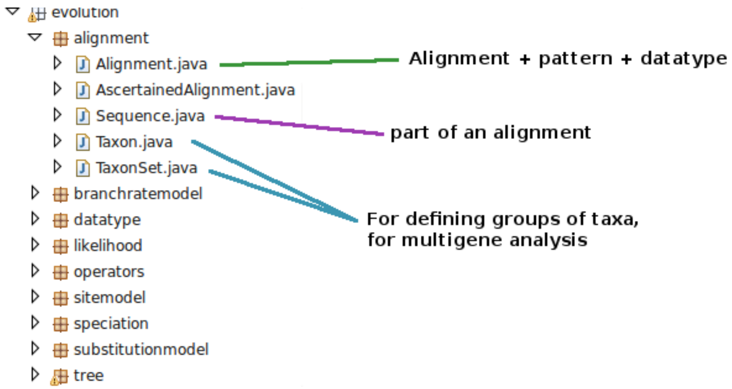
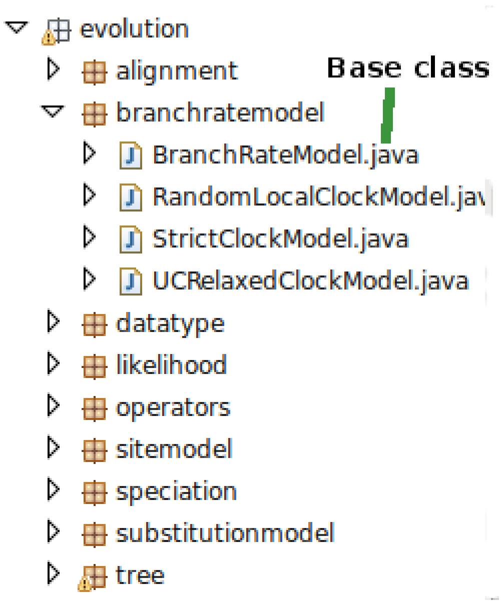


Evolution - branch rate model classes



```
▽ evolution
    ▷ alignment
    ▽ branchratemodel
        ▷ BranchRateModel.java
        ▷ RandomLocalClockModel.jav
        ▷ StrictClockModel.java
        ▷ UCRelaxedClockModel.java
    ▷ datatype
    ▷ likelihood
    ▷ operators
    ▷ sitemodel
    ▷ speciation
    ▷ substitutionmodel
    ▷ tree
```

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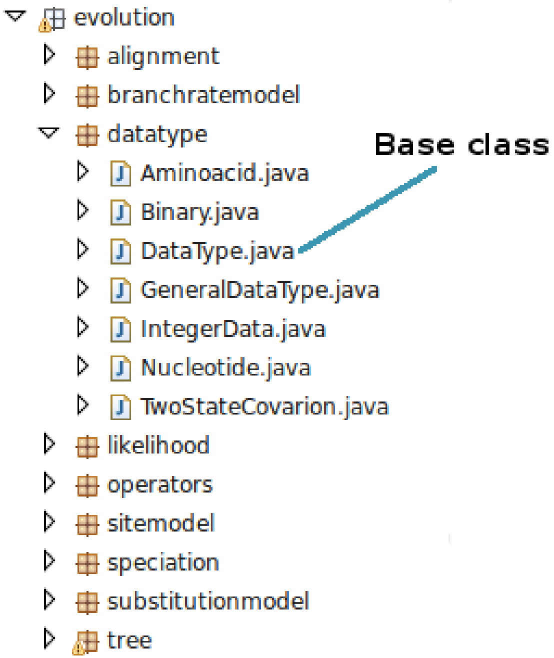
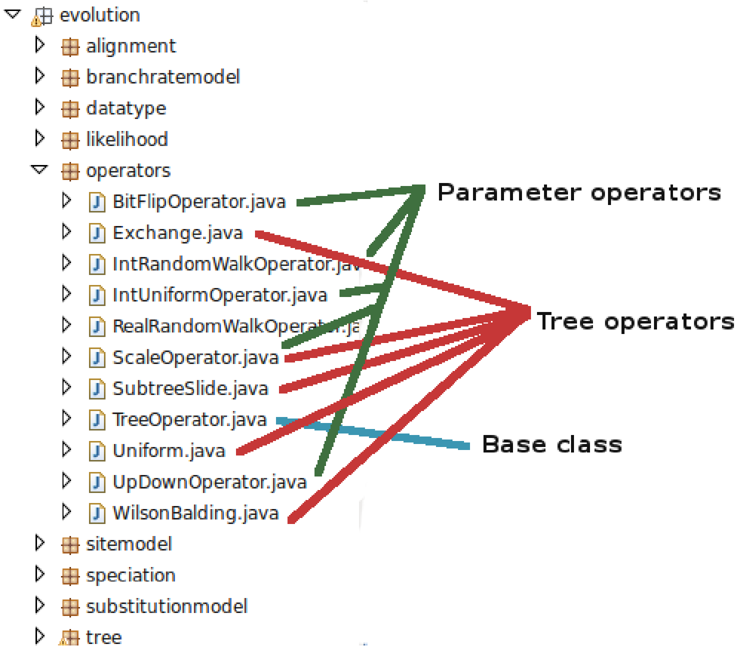
Evolution - data type classes



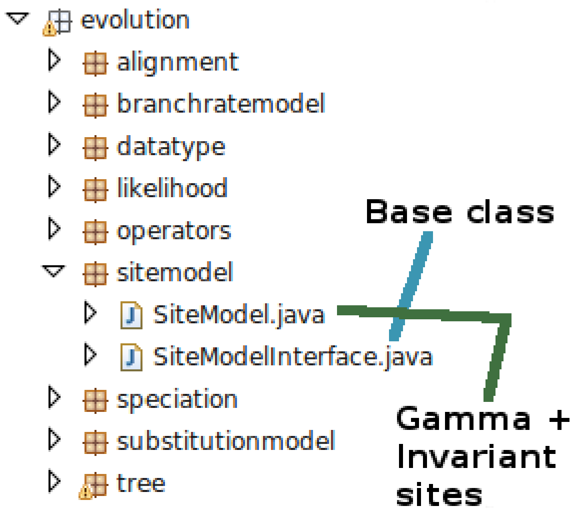
- evolution
  - alignment
  - branchratemodel
  - datatype
    - Aminoacid.java
    - Binary.java
    - DataType.java
    - GeneralDataType.java
    - IntegerData.java
    - Nucleotide.java
    - TwoStateCovarion.java
  - likelihood
  - operators
  - sitemodel
  - speciation
  - substitutionmodel
  - tree

Evolution - operator classes

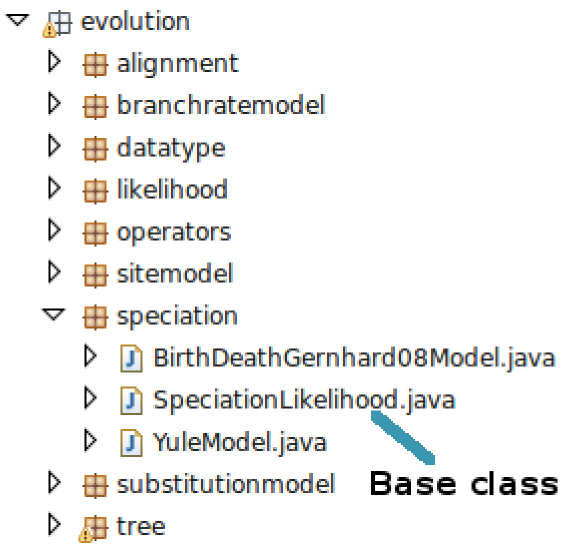


- evolution
  - alignment
  - branchratemodel
  - datatype
  - likelihood
  - operators
    - BitFlipOperator.java
    - Exchange.java
    - IntRandomWalkOperator.jav
    - IntUniformOperator.java
    - RealRandomWalkOperator.ja
    - ScaleOperator.java
    - SubtreeSlide.java
    - TreeOperator.java
    - Uniform.java
    - UpDownOperator.java
    - WilsonBalding.java
  - sitemodel
  - speciation
  - substitutionmodel
  - tree

Evolution - site model classes

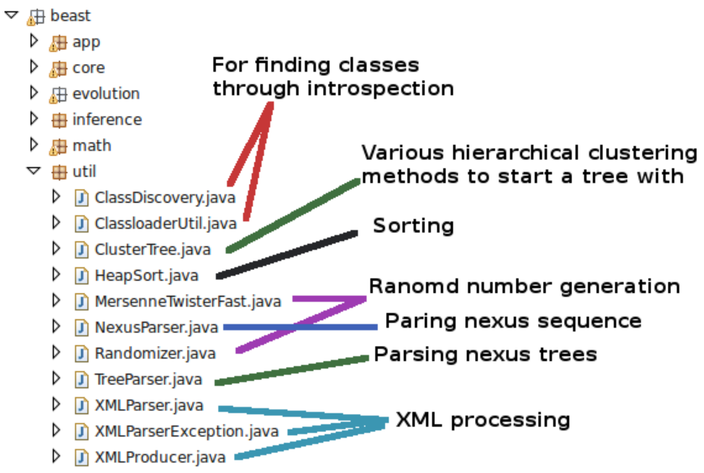


Evolution - speciation classes



evolution
- alignment
- branchratemodel
- datatype
- likelihood
- operators
- sitemodel
- speciation
  - BirthDeathGernhard08Model.java
  - SpeciationLikelihood.java
  - YuleModel.java
- substitutionmodel
- tree

Utility classes



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Variable naming

In case you wondered where those funny names came from...

Variable name format: `<scope><type><name>`

scope

- `m_` prefix for member variables
- `g_` globals = static member variables
- none otherwise

type

- `s` string
- `f` floating point number (double or float)
- `n` number
- `i` indicator
- `b` boolean
- `p` pointer to object

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Basic plugin layout

```
@Description("Some␣sensible␣description␣of␣the␣Plugin")
public class MyPlugin extends Plugin {
    <!-- inputs first -->
    public Input<RealParamater> m_p = new Input<>...;

    <!-- members next -->
    private Object m_o;

    <!-- initAndValidate -->
    @Override
    public void initAndValidate() {...}

    <!-- class specific methods -->

    <!-- Overriding methods -->
}
```

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Accessing inputs *for reading, not writing!*

Let there be an input:

```
public Input<RealParamater> m_p = new Input<>...;
```

To get the parameter of input `m_p`, use `m_p.get()`.

To get the value of the parameter, use `m_p.get().getValue()`.

Alternatively

```
    RealParamater p = m_p.get();
    double fValue = p.getValue();
```

requiresRecalculation()

```
public boolean requiresRecalculation() {
        // for StateNode inputs only
        if (m_stateNodeInput.get().somethingIsDirty()) {
                return true;
        }

        // for CalculationNode inputs only
        if (m_calculationNodeInput.get().isDirtyCalculation()) {
                return true;
        }
        return false;
}
```

Lean CalculationNode

```
boolean m_bNeedsUpdate; // flag to indicate internal state is up to date
public void initAndValidate() {m_bNeedsUpdate = true;}
// CalculationNode specific interface that returns results
public Object calculateSomeThing() {
        if (m_bNeedsUpdate) {
                update();
        }
        return someThing;
}
void update() {
        someThing = ...;
        m_bNeedsUpdate = false;
}
public boolean requiresRecalculation() {
        if (someInputIsDirty()) {
                m_bNeedsUpdate = true;
                return true;
        }
        return false;
}
public void store() {super.store();}
public void restore() {
        m_bNeedsUpdate = true;
        super.restore();
}
```

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Fat CalculationNode

As lean CalculationNode, but actually storing something

```
Object m_intermediateResult;
Object m_storedIntermediateResult;

public void initAndValidate() {
        // reserve space for result objects
        m_intermediateResult = new ...;
        m_storedIntermediateResult = new ...;
}

public void store() {
        // copy m_intermediateResult to m_storedIntermediateResult
        ...
        super.store();
}
public void restore() {
        // m_bNeedsUpdate = true; <- don't need this now
        Object tmp = m_intermediateResult;
        m_intermediateResult = m_storedIntermediateResult;
        m_storedIntermediateResult = tmp;
        super.restore();
}
```

Adding a Substitution model

Extend SubstitutionModel.Base class

- A substitution model should implement `getTransitionProbabilities(Node node, double fStartTime, double fEndTime, double fRate, double[] matrix)`
- Typically, `fRate * (fEndTime - fStartTime)` is the distance t in e^{Qt} and `Node` can be ignored.
- Results should go in the `matrix`: note this is represented as array.
- `SubstitutionModel` is a `CalculationNode`, so it may be worth implementing `store/restore/requireRecalculation`

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Adding an Operator: Extend Operator class

- An operator should have at least one input with a `StateNode` to operate on.
- An operator should implement `proposal()` which changes the State.
- `proposal()` should return the Hastings ratio.
- Return `Double.NEGATIVE_INFINITY` if the proposal is invalid/doomed (don't throw Exceptions).
- Implement `optimize()` if auto-optimization applies.
- Note: use **m_parameter.get(this)** in `proposal()` not `m_parameter.get()` **iff you want to change the value of the** `StateNode`

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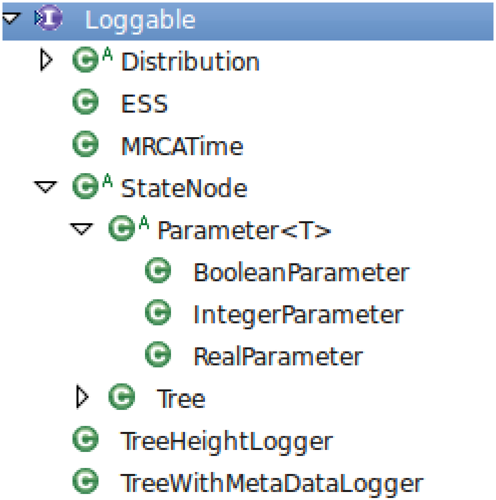
Adding a logger: Implement Loggable interface

```
void init(PrintStream out) throws Exception;

void log(int nSample, PrintStream out);

void close(PrintStream out);
```



```
Loggable
    Distribution
    ESS
    MRCATime
    StateNode
        Parameter<T>
            BooleanParameter
            IntegerParameter
            RealParameter
        Tree
    TreeHeightLogger
    TreeWithMetaDataLogger
```

Shadowing inputs

Never shadow a StateNode

```
public Input<RealParamater> m_p = new Input<>...;
private RealParameter m_pShadow;
```

Shadow CalculationNodes, primitives (Integer, Double, String, Boolen) inputs, and others is fine.

```
public Input<Integer> m_p = new Input<>...;
private Integer m_pShadow;
```

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Input rule of base class is not what you want.

If an Input is REQUIRED for a base class you want to override, but for the derived class this Input should be OPTIONAL, set the Input to OPTIONAL in the constructor. E.g. for a SNPSequence that derives from Sequence, but for which m_sData is optional, add a constructor

```
public SNPSequence() {
        m_sData.setRule(Validate.OPTIONAL);
}
```

Note that the constructor needs to be public, to prevent IllegalAccessExceptions on construction by e.g. the XMLParser.

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Input parameter dimension is unknown...

...but a CalculationNode can easily find out.

Then, in the `initAndValidate()` method of the `CalculationNode`, create a new Parameter `X`, and use `m_input.get().assignFrom(X)`

```
@Override
public void initAndValidate() throws Exception {
    // determine dimension, number of Nodes in a tree here
        int nNodes = m_tree.get().getNodeCount();

    // create new Parameter
        IntegerParameter positions = new IntegerParameter("0", 0, Integer
        for (int i = 0; i < nNodes; ++) {
                int iPosX = ...;
                positions.setValue(i, iPosX);
        }

    // make sure we maintain the correct ID
        positions.setID(m_positionsX.get().getID());

    // copy values to the input
        m_positions.get().assignFrom(positions);

}
```

Trees with traits

For a tree with n leaf nodes, so $2n - 1$ nodes in total

- Easiest: associate a parameter with dimension $2n - 1$ to the tree
  - Leaf nodes are numbered $0, \ldots, n - 1$
  - Internal nodes are numbered $n, \ldots, 2n - 1$
  - Root node is not treated as special internal node (no number guaranteed)
- Harder: Derive from class `Node` and process as meta-data

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Common errors

1. `Input` **is not declared public.**

If `Input`s are not public, they cannot get values assigned by for instance the `XMLParser`.

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Common errors

1. **`Input` is not declared public.**
If `Input`s are not public, they cannot get values assigned by for instance the `XMLParser`.

2. **`Operator` calls `input.get()` instead of `input.get(this)`.**
When an `Operator` does a proposal, it should change a `StateNode`. This `StateNode` needs to be one of its inputs. So, to get the `StateNode` normally a call to `input.get()` would give the value. However, for the `State` to know that a `StateNode` changes, the method `input.get(this);` should be called.
Note that this only applies to the `proposal()` method, not to `initAndValidate()` (though it does not hurt in the latter) since only in `proposal()` a `StateNode` should be changed.

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Common errors

3. **Shadow a `StateNode` in a `CalculationNode`.**
It is tempting to use a pattern like this:

```
public Input<RealParamater> m_p = new Input<>...;
    private RealParameter m_pShadow;

    public void initAndValidate() {
        m_pShadow = m_p.get();
    }

    double calculateSomethingOld() {
        // uses non-current value
        return m_pShadow.getValue() * 2.0;
    }

    double calculateSomethingNew() {
        // uses current value
        return m_p.get().getValue() * 2.0;
    }
```

in a Plugin. However, `StateNode`s like `RealParameter` can change their value and the `m_p.get()` may return a different object next time it is called. So, the method `calculateSomethingOld()` above may return the same initial value every time, while

Common errors

4. **Type of input is a template class (other than `List`).** Thanks to limitations of Java introspection and the way Beast II is set up, Inputs should be of a type that is concrete, and apart from `List<T>` no template class should be used.

Common errors

4. **Type of input is a template class (other than `List`).** Thanks to limitations of Java introspection and the way Beast II is set up, Inputs should be of a type that is concrete, and apart from `List<T>` no template class should be used.

5. **Store/restore do not call `super.store()/super.restore()`.** Obviously, not calling store/restore on super classes may result in unexpected behavior.

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