SimTreeSDD: **Sim**ulating Phylogenetic **Tree**s Under **S**tate-**D**ependent **D**iversification

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Contents

Background

Preliminaries

Branching processes are often used as macroevolutionary null models or for fitting empirical data. In the process considered here, each lineage (species or other taxonomic level) at each time has a specified probability of giving rise to a new lineage (speciation/origination/birth), going extinct (extinction/death), or changing its state from one value of a character to another. This is "state-dependent diversification" when the value of the character affects the probabilities of speciation and extinction.

The purpose of this simulator is to produce trees under state-dependent diversification processes. Probabilities of birth, death, and character transition are assumed to be constant over time and across taxa in this implementation. The two processes available now are BiSSE (binary state speciation and extinction; Maddison, Midford & Otto (2007) SystBiol) and GeoSSE (geographic state speciation and extinction; Goldberg, Lancaster & Ree (in review) SystBiol).

As may be clear already, some terms are used interchangeably here:

lineage = species = taxon
birth = speciation = origination
death = extinction
trait value = (character) state

Methods

Two types of characters are possible here. First, for BiSSE, you can have a single binary character. For example, eyes may be present or absent, or breeding system may be self-compatible or self-incompatible. In this first case, there are (obviously) two possible states. Second, for GeoSSE, the character in question can be geographic location. In the two-region model implemented here, there are three possible states: a species may be present in both regions, it may be present only in the first region, or it may be present only in the second region. Transitions between these states occur through dispersal (a species present only in one region that disperses becomes present in both regions) or local extinction (a species present in both regions that went extinct in the first region becomes present only in the second region). Character state changes can also happen during speciation events if the parent lineage is in both regions.

Each tree is simulated beginning with a single lineage (GeoSSE) or a branching point (BiSSE) at an initial time and ending at a specified final time (or before then, if the tree goes extinct). Six rates must be specified for the branching process. For a binary character, these rates are

speciation in state 0
speciation in state 1
extinction in state 0
extinction in state 1
transition from state 0 to state 1
transition from state 1 to state 0

and for a geographic character, these rates are

speciation in region A
speciation in region B
extinction in region A
extinction in region B

dispersal from region A to region B
dispersal from region B to region A

A lineage present in both regions (AB) is subject to speciation in A (daughters are AB and A) or B (daughters are AB and B), or additionally, a between-region speciation rate may be given (daughters are A and B).

The simulations are carried out in continuous time, and the results can be written to a variety of output file types. The program is called from the command line, so it is easy to automate it to produce many trees organized however you like. It is quite fast: performance obviously depends on hardware and parameter values, but I have never waited more than a couple seconds for a batch of thousands of reasonably large trees.

How to use the program

`SimTreeSDD` is written in C, and the program is command line-based, so the instructions below assume you are working from a terminal (e.g. `xterm` in Linux or `Terminal` in Mac OS X). There is no reason why it shouldn't work under Windows, but I haven't tried—if you have, please send me a howto and I will incorporate it here.

Commands you should issue in the terminal are displayed like this:

```
type this command
then type this command
```

and the contents of input or output files are displayed like this:

File contents: `example.txt`

```
this is the first line of the file
this is the next line
```

Installation

`SimTreeSDD` is available as C source code, so first download `SimTreeSDD_xxx.tar.gz` from my website (currently `http://www.uic.edu/~eeg`; `xxx` is the date). Put this archive wherever you like and navigate there in the terminal. Then, unpack the files and compile the code:

```
tar zxvf SimTreeSDD_xxx.tar.gz
cd SimTreeSDD_xxx/src/
make
```

This will create an executable called `SimTreeSDD`. You may want to copy this to somewhere in your path, e.g.

```
cp SimTreeSDD /usr/local/bin/
```

If you don't do this, then in the examples below, replace `SimTreeSDD` with the relative or full path, which might be something like ~`yourname/SimTreeSDD_xxx/src/SimTreeSDD`.

Input options

SimTreeSDD can be told what to do (i.e. what parameter values to use in the simulation and what output to write) in two ways. First, you can use an input file, and second, you can pass options on the command line.

Input file

An input file to SimTreeSDD consists of lines of the form `option = value`. The comment character is #, so all text that follows a # on a line is ignored. A minimum input file might look like this:

File contents: `simple_sim_input.dat`

```
trait_type = character # for a binary character
birth0 = 0.5
birth1 = 0.3
death0 = 0.2
death1 = 0.2
alpha  = 0.4
beta   = 0.1
end_t  = 5
```

To simulate a tree with these values, type

```
SimTreeSDD simple_sim_input.dat
```

(giving the path to SimTreeSDD if necessary).

A sample input file with more options and comments is included as `SimTreeSDD_xxx/work/sim-params.dat`. Here is a complete list of options and their possible values:

`trait_type` the type of character to model
  = `character` a single binary character
  = `region` geographic location in a two-region system
`birth0` the speciation rate for trait 0 or region A
  = any real non-negative number
`birth1` the speciation rate for trait 1 or region B
  = any real non-negative number
`death0` the extinction rate for trait 0 or region A
  = any real non-negative number
`death1` the extinction rate for trait 1 or region B
  = any real non-negative number
`alpha` the transition rate from trait 0 to 1, or the dispersal rate from region A to B
  = any real non-negative number
`beta` the transition rate from trait 1 to 0, or the dispersal rate from region B to A
  = any real non-negative number
`root_state` the state of the initial node or lineage
  = `-1` for `trait_type=character`, draw the root state from the stationary distribution [default]
  = `0` for `trait_type=character`, root state is 0;
    for `trait_type=region`, root state is present in both regions [default]
  = `1` for `trait_type=character`, root state is 1;
    for `trait_type=region`, root state is present only in region A
  = `2` for `trait_type=region`, root state is present only in region B

`min_tips` the minimum number of tips a tree must have to be kept as a successful run; you can set this to whatever seems convenient, but keep in mind that this may introduce bias in some analyses
  `=` any non-negative integer [default is `0`]

`num_trees` the number of (successful) trees to simulate
  `=` any non-negative integer [default is `1`]

`file_prefix` a prefix to give output files
  `=` any text string [default is `run`]; this can include a path, e.g. `sim-runs/run1`

`num_start` the number with which to start labeling output files (if `num_trees` is greater than 1); for example, you could produce trees named run-1.tre, run-2.tre, run-3.tre
  `=` any non-negative integer [default is `1`]

`verbosity` how much information to print to the terminal as the program is running
  `= 0` print nothing
  `= 1` print some stuff
  `= 2` print lots [default]

`write_newick` create an output file containing the simulated tree in Newick format
  `= 0` don't create a `.tre` file for each tree
  `= 1` do create a `.tre` file for each tree [default]

`write_nexus` create an output file containing the simulated tree and character states in NEXUS format
  `= 0` don't create a `.nexus` file for each tree
  `= 1` do create a `.nexus` file for each tree [default]

`write_bmstrait` create an output file containing the tip character states in a format useable with BayesMultiState
  `= 0` don't create a `.bmstrait` file for each tree [default]
  `= 1` do create a `.bmstrait` file for each tree

`write_ttn` create an output file containing the simulated tree and character states in TTN format (see below)
  `= 0` don't create a `.ttn` file for each tree
  `= 1` do create a `.ttn` file for each tree [default]

Command-line options

Any option that can be given in the input file can also be given on the command line. This is sometimes handy when calling many runs of the program from a script. If an option is specified in both places, the value on the command line takes precedence. Options are separated by spaces. Spaces can *not* be used around the = sign on the command line. An input file *must* be given as the *first* argument. Here is an example in which the values in `simple_sim_input.dat` (above) are used but `end_t` is set to 2.5 instead and 10 trees are created:

```
SimTreeSDD simple_sim_input.dat end_t=2.5 num_trees=10
```

Output options

Depending on what you want to do with your simulated trees, you may want the output written in various forms. For viewing trees with, for example, R or TreeViewX, set `write_newick=1`. The tree string written contains tip and node labels showing the character states. Here is an example file for a small, 4-tip tree (but note that this is a single line in the real file):

File contents: `small_tree.tre`

```
(((0_tip0:0.051603,0_tip1:0.051603)0_n4:0.002604,0_tip2:0.054207)0_n5:
0.045793,1_tip3:0.100000)1_n6:0.000000;
```

For use with Mesquite, set `write_nexus=1`. For use with HyPhy, set `write_newick=1` and `write_nexus=1`. For use with BayesMultiState, set `write_nexus=1` and `write_bmstrait=1`.

For use with my other code (TreeLike and SDD-MCMC, which may or may not be packaged together with SimTreeSDD), you need a TTN file (`write_ttn=1`). This consists of the tree as a Newick string, a list of the tips and their trait values, and (optionally) a list of the nodes and their trait values. So TTN stands for Tree, Tips, Nodes. Here is an example file for the small tree used above:

File contents: `small_tree.ttn`

```
(((0:0.051603,1:0.051603):0.002604,2:0.054207):0.045793,3:0.100000):0.000000;
0 0
1 0
2 0
3 1
4 0
5 0
6 1
```

Large tree warning

It is rather easy to choose parameter values that lead to extremely large trees. This can cause trouble in (at least) three ways. First, output files may be unwieldy for other programs to handle. Second, `SimTreeSDD` itself may require a lot of memory, bogging down your computer. To avoid this, `SimTreeSDD` will abort itself if a tree reaches 50,000 nodes. This is an arbitrary cutoff, so if you need it to take a different value you can change the value of `TOO_BIG` in `build.h`. Third, the tree-building algorithm uses heavy recursion, so it is possible to get so deep in recursive layers as to exceed your stack size. `SimTreeSDD` can not check for this problem and so just dies with a segmentation fault. Sorry about that, but it should not be an issue for reasonable values of `birth0`, `birth1`, `death0`, `death1`, and `end_t`. If you have this problem and really need to use whatever extreme parameter values you have set, you can increase the stack size with `ulimit` or `limit`—consult the documentation for your shell.

Procedural stuff

Bugs and help

This code has been tested and used by me and others, and as far as I know it works as it should. But of course, any software may have bugs, so don't expect to hold me accountable if you do anything life-threatening with this program! If you encounter a bug, either an unexplainable crash or a result that seems incorrect, please let me know. You can either send me a good description of the problem or, better yet, fix it yourself and send me a patch.

I originally wrote this code because I needed it, but I wrote this documentation because I want it to be useful to other people. So if you have read the instructions here but are still having problems getting things working, just let me know and I will try to help. I would also be happy to hear if you have usability suggestions (e.g. making the documentation clearer or error-checking during use of the program), ideas for additional features that would be useful, or if you are making substantial changes to take the code in a new direction. And of course I would be especially glad to hear if the program just worked for your purposes!

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