

# Ngesh: a Python library for synthetic phylogenetic data

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Software

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## Summary

This work presents [ngesh](#), a Python library for simulating phylogenetic trees and data, designed for usage in development, debugging, and benchmarking of analysis pipelines and methods for phylogenetic inference, particularly in historical linguistics and stemmatics. The package generates reproducible stochastic simulations of evolution according to various criteria, including character mutation rates and probability of horizontal transfer, and its results can include the simulation of inadequate data compilation and sampling. Different output formats are supported, both for visualization (such as plain text and with integrated graphical viewers) and for software interoperability (such as Newick and NEXUS).

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## Background

Computational phylogenetics is being increasingly accepted in fields beyond biology, such as historical linguistics (Bouckaert et al., 2012) and stemmatics (Robinson, 2016). Stochastic simulations, long advocated for natural sciences in general (Bailey, 1964) and genetics in specific (Foote, Hunter, Janis, & Sepkoski, 1999; Harmon, 2019), are not yet used often enough in these fields. However, they are highly desirable, allowing to evaluate evolutionary analogies and models, as well as methods' performance, through vast amounts of simulated histories, without limits imposed by data availability and collection time and with quantifiable precision of results. Simulations can also be used to perform basic fuzzy testing of software and to support studies on which evolutionary models, processes, and evolutionary parameters better match the observed phenomena.

The [ngesh](#) library is a tool that allows to perform such simulations, designed for easy integration into phylogenetic pipelines. It can generate reproducible trees and correlated data from random seeds, following both user-established parameters, such as ratios of birth and death, and constrains, such as branch lengths and minimum number of taxa. The library can label taxa progressive enumeration or with random names that are easy to pronounce (e.g. "Sume" and "Fekobir") or which imitate the binominal nomenclature (e.g. "Sburas wioris" and "Zurbata pusso"). Character evolution related to the tree topology can likewise be simulated, including *ex novo* mutations and horizontal gene transfers. Results can be manipulated in diverse manners, for example by pruning extinct leaves or simulating uneven sampling. The simulated trees are standard ETE3 objects (Huerta-Cepas, Serra, & Bork, 2016) and may be exported into different formats such as Newick trees, ASCII-art representation, and tabular lists.

As a building block for evaluating pipelines of analysis, the library is a curated alternative to the basic technique of randomizing taxa placement in existing cladograms, and to simpler tools such as the one by Noutahi (2017) or the `populate()` method of ETE3's `Tree` class (Huerta-Cepas et al., 2016). Within its intended scope, it compares to popular alternatives, including the R `TreeSim` (Stadler, 2011) and `geiger` packages (Pennell et al., 2014) and the `rtree()` function of `ape` (Paradis & Schliep, 2018), however with specific support for historical linguistics and stemmatics.

## Installation, Usage, & Examples

Users can install the library with the standard pip tool for managing Python packages. Trees can be generated from the command-line, defaulting to small phylogenies in Newick format:

```
$ ngesh
(Ukis:1.11985,(Koge:0.880823,(Rozkob:0.789548,(Meu:0.706601,
(((Felbuh:0.189693,Kefa:0.189693)1:0.117347,((Epib:0.153782,
Vugog:0.153782)1:0.0884745,Puluk:0.242256)1:0.0647836)1:0.0469885,
Efam:0.354028)1:0.352573)1:0.0829465)1:0.0912757)1:0.23903);
```

The tool supports both configuration files and command-line flags that take precedence over the former. Here we specify a model to generate Nexus data for a reproducible Yule tree, with a birth rate of 0.75, at least 5 leaves, "human" labels, and 20 presence/absence features:

```
$ cat my_tree.conf
[Config]
labels=human
birth=0.75
death=0.0
output=nexus
min_leaves=5
num_chars=20
$ ngesh -c my_tree.conf --seed 12345
begin data;
  dimensions ntax=6 nchar=33;
  format datatype=standard missing=? gap=-;
  matrix
Buza      111110110111011011010101000100110
Lenlar    11111101011011110110100010010011001
Mukom     111110111011011011011101001000100110
Pagil     111110110111011011011100100100100110
Suglu     111110110111011011011100011001001010
Wite      111110110111011011011100101000100110
;
end;
```

Despite the benefit of a stand-alone tool, the package is designed to be run as a library. The two primary functions are `gen_tree()`, which returns a random tree, and `add_characters()`, which adds character evolution data to a tree. Users can generate random trees without character information or simulate character evolution within existing trees, including non-simulated ones.

```
>>> import ngesh
>>> tree = ngesh.gen_tree(1.0, 0.5, max_time=0.3, labels="bio",
                        seed="135")
>>> print(tree)

    /-Lubedsas larpes
--|
  | /-Rasso wimapudda
  \-|
    \-Sbaes rapis
>>> print(tree.write())
(Lubedsas larpes:0.201311,(Rasso wimapudda:0.0894405,Sbaes rapis:0.0894405)
1:0.11187);
>>> tree = ngesh.add_characters(tree, 15, 2.0, 0.5)
```

Besides the `write()` method of the example above, which outputs Newick trees, results can be exported in NEXUS format with the `tree2nexus()` function and in a tabular output expected by tools such as BEASTling (Maurits, Forkel, Kaiping, & Atkinson, 2017), with the `tree2wordlist()` function.

## Code and Documentation Availability

The `ngesh` source code is available on GitHub at <https://github.com/tresoldi/ngesh>.

User documentation is available at <https://ngesh.readthedocs.io/>.

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