Ngesh: a Python library for synthetic phylogenetic data

Tiago Tresoldi^{1, 2}

f 1 Department of Linguistics and Philology, Uppsala University f 2 Department of Linguistic and Cultural Evolution, Max Planck Institute for the Science of Human History

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).

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 an 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 of historical linguistics and stemmatics, it compares to popular alternatives, such as the R TreeSim (Stadler, 2011) and geiger packages (Pennell et al., 2014) and the rtree() function of ape (Paradis & Schliep, 2018), by using default parameters that produce trees closer to those found in these fields. The library also addresses the need of a tool that can be used to teach phylogenetics in these fields by focusing on the

DOI:

Software

- Review 🗗
- Repository 🗗
- Archive 🗗

Editor: 2

Submitted: Published:

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License (CC-BY).

generation of data, such as random cognate classes, which fit existing pipelines better than the results of tools developed with a focus on biology.

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
          1111110101101111101100010010011001
Lenlar
Mukom
          111110111011011011101001000100110
          111110110111011011100100100100110
Pagil
          111110110111011011100011001001010
Suglu
          111110110111011011100101000100110
Wite
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.

```
(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/.

Acknowledgements

The author has received funding from the Riksbankens Jubileumsfond (ID: MXM19-1087:1, "Cultural Evolution of Texts") and from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (No. ERC #715618, "Computer-Assisted Language Comparison").

References

Bailey, N. T. (1964). The elements of stochastic processes with applications to the natural sciences. New York, London, Sydney: John Wiley & Soins.

Bouckaert, R., Lemey, P., Dunn, M., Greenhill, S. J., Alekseyenko, A. V., Drummond, A. J., Gray, R. D., et al. (2012). Mapping the origins and expansion of the indo-european language family. *Science*, *337*(6097), 957–960.

Foote, M., Hunter, J. P., Janis, C. M., & Sepkoski, J. J. (1999). Evolutionary and preservational constraints on origins of biologic groups: Divergence times of eutherian mammals. *Science*, 283(5406), 1310–1314. doi:10.1126/science.283.5406.1310

Harmon, L. J. (2019). Phylogenetic comparative methods. University of Idaho.

Huerta-Cepas, J., Serra, F., & Bork, P. (2016). ETE 3: Reconstruction, Analysis, and Visualization of Phylogenomic Data. *Molecular Biology and Evolution*, 33(6), 1635-1638. doi:10.1093/molbev/msw046

Maurits, L., Forkel, R., Kaiping, G. A., & Atkinson, Q. D. (2017). BEASTling: A software tool for linguistic phylogenetics using beast 2. *PloS One*, *12*(8).

Noutahi, M.-R. (2017). How to simulate a phylogenetic tree? Retrieved from https://mrnoutahi.com/2017/12/05/How-to-simulate-a-tree/

Paradis, E., & Schliep, K. (2018). Ape 5.0: An environment for modern phylogenetics and evolutionary analyses in R. *Bioinformatics*, *35*, 526–528.

Pennell, M., Eastman, J., Slater, G., Brown, J., Uyeda, J., FitzJohn, R., Alfaro, M., et al. (2014). Geiger v2.0: An expanded suite of methods for fitting macroevolutionary models to phylogenetic trees. *Bioinformatics*, *30*, 2216–2218.

Robinson, P. (2016). The digital revolution in scholarly editing. *Ars Edendi Lecture Series*, *4*, 181–207.

Stadler, T. (2011). Simulating trees with a fixed number of extant species. *Systematic Biology*, 60(5), 676–684. doi:10.1093/sysbio/syr029