

phylo2vec: a library for vector-based phylogenetic tree manipulation

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Summary

Phylogenetics is a fundamental component of many analysis frameworks in computational and evolutionary biology (Yang, 2014) as well as linguistics (Atkinson & Gray, 2005). Recently, the advent of large-scale genomics and the SARS-CoV-2 pandemic has underscored the necessity to scale phylogenetic software to handle large datasets of genomes or phylogenetic trees (Attwood et al., 2022; Kapli et al., 2020; Khurana et al., 2024; Kraemer et al., 2025). While significant efforts have focused on scaling phylogenetic inference (De Maio et al., 2023; Sanderson, 2021; Turakhia et al., 2021), visualization (Sanderson, 2022), and lineage identification (McBroome et al., 2024), an emerging body of research has been dedicated to efficient representations of data for genomes (Deorowicz et al., 2023) and phylogenetic trees such as phylo2vec (Penn et al., 2024), HOP (Chauve et al., 2025), and OLA (Richman et al., 2025). Compared to traditional tree representations such as the Newick format (Felsenstein, 2004), which describes a phylogenetic tree as a string of nested parentheses enclosing pairs of leaves or subtrees, these modern representations utilize integer vectors to define the tree topology traversal. This approach offers several advantages, including easier manipulability, increased memory efficiency, and applicability to downstream tasks such as machine learning (Penn et al., 2024).

Here, we present the new release of phylo2vec (or Phylo2Vec), a high-performance software package for encoding, manipulating, and analysing binary phylogenetic trees. At its core, the package is based on the phylo2vec (Penn et al., 2024) representation of binary trees, which defines a bijection from any tree topology with n leaves into an integer vector of size $n - 1$. Compared to the traditional Newick format, phylo2vec was designed with fast sampling and rapid tree comparison in mind. This release features a core implementation in Rust, providing significant performance improvements and memory efficiency (Figure 1), while remaining available in Python (superseding the release described in the original paper (Penn et al., 2024)) and R via dedicated wrappers, making it accessible to a broad audience in the bioinformatics community.

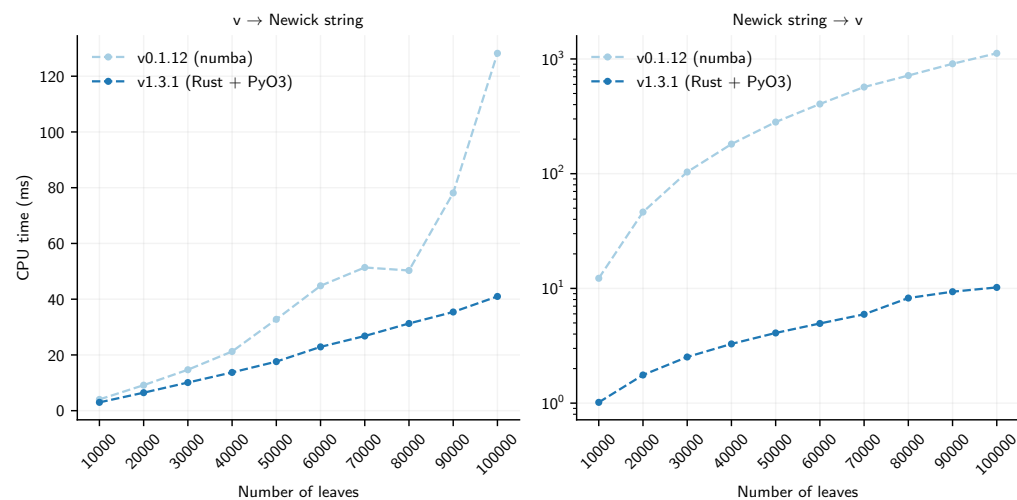


Figure 1: Benchmark times for converting a phylo2vec vector to a Newick string (left) and vice versa (right). For each size, we evaluated the execution time for a minimum of 20 rounds using pytest-benchmark. We compare the execution time of the Python functions in the latest release, which rely on Rust bindings via PyO3, with the previous release (Penn et al., 2024), which make use of just-in-time (JIT) compilation of Python functions using Numba (Lam et al., 2015). Execution times were benchmarked on an AMD Ryzen Threadripper PRO 5995WX with a 64-core CPU @ 7 GHz and 256 GB of RAM.

Statement of need

The purpose of the phylo2vec library is threefold. First, the core of the library aims at providing a robust phylogenetic tree manipulation library in Rust, complementing other efforts such as light_phylogeny (Duchemin et al., 2018), which focuses on tree visualization and manipulation of reconciled phylogenies (Nakhleh, 2013), and rust-bio (Köster, 2016), a comprehensive bioinformatics library which does not yet cover phylogenetics. Second, phylo2vec aims at complementing existing phylogenetic libraries such as ape (Paradis & Schliep, 2019) in R, and ete3 (Huerta-Cepas et al., 2016) and DendroPy (Moreno et al., 2024) in Python, by providing fast tree sampling, fast tree comparison and efficient tree data compression (Penn et al., 2024). Third, the inherent tree representation of phylo2vec offers a pathway to gradient-based optimisation frameworks for phylogenetic inference. A notable example is GradME (Penn et al., 2023), which relaxes the vector representation of phylo2vec into a continuous space.

Features

The presented release of phylo2vec addresses several limitations of (Penn et al., 2024). From an optimisation perspective, it introduces efficient $\mathcal{O}(n \log n)$ implementations for both vector-to-Newick and Newick-to-vector conversions, leveraging Adelson-Velsky and Landis (AVL) trees (Adelson-Velsky & Landis, 1962) and Fenwick trees (Fenwick, 1994), respectively.

In terms of new features, it supports branch length annotations by extending the vector representation of size $n - 1$ to a matrix of size $(n - 1) \times 3$, where n denotes the number of leaves (or taxa) in a tree (Figure 2). Further enhancements include several leaf-level operations (pruning, placement, MRCA identification), fast cophenetic distance matrix calculation, and various optimisation schemes based on phylo2vec tree representations, notably hill-climbing and GradME (Penn et al., 2023). Bayesian phylogenetic inference via Markov Chain Monte Carlo (MCMC) with phylo2vec matrices is also made possible by a likelihood function that leverages tree representation similarities between phylo2vec and BEAGLE, a highly optimised library that underpins a number of phylogenetic software (Ayres et al., 2012; Suchard & Rambaut, 2009).

63 Finally, user-friendliness is enhanced by step-by-step demos of the inner workings of phylo2vec's
64 representations and their conversion to commonly used phylogenetic tree formats (e.g., Newick
65 string, list of edges).

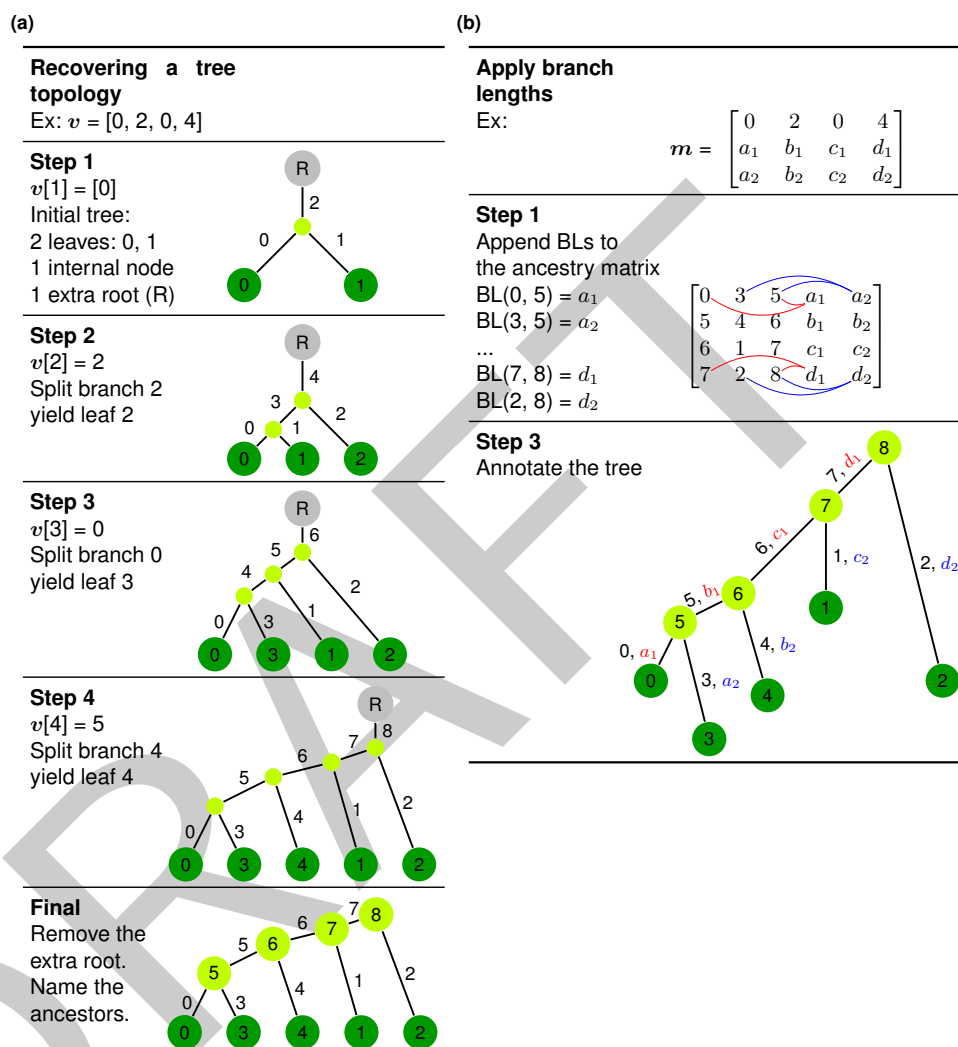


Figure 2: Recovering a tree from a phylo2vec vector: example for $v = [0, 2, 0, 4]$. (a) Main algorithm for leaf placement described in (Penn et al., 2024). (b) Augmenting the phylo2vec vector into a matrix m with branch lengths. We use an intermediary ancestry matrix whereby each row describes a cherry (two children nodes and the parent node), which we augment with two columns of branch lengths. The node with the smallest descendant will have the branch length in the 2nd column, and the other the branch length in the 3rd column.

66 Maintenance

67 With Phylo2Vec, we aim to support long-term maintenance through implementing recommended
68 software practices explicitly into the structure of the project and development workflow, rather
69 than leaving them implied. This avoids human error as the repo's structure itself enforces good
70 practices, rather than placing the responsibility solely on code contributors. More specifically,
71 we have structured the project such that the Rust API contains the core algorithms, and
72 all other language components are APIs that bind to the Rust functions. This avoids tight
73 coupling, as it allows for the possibility of adding new languages to bind to the Rust API's,

without needing to change anything in the Rust project itself. Additionally, we have established a robust continuous integration (CI) pipeline using GitHub Actions, which features:

- Unit test frameworks for Rust ([cargo](#)), Python ([pytest](#)), and R (testthat ([Wickham, 2011](#)))
- Benchmarking on the Rust code ([criterion](#)) and its Python bindings ([pytest-benchmark](#))

Lastly, to complement Jupyter Notebook demos, comprehensive documentation is provided using [Jupyter Book](#) and [Read The Docs](#).

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