













# 1 phylo2vec: a library for vector-based phylogenetic tree 2 manipulation

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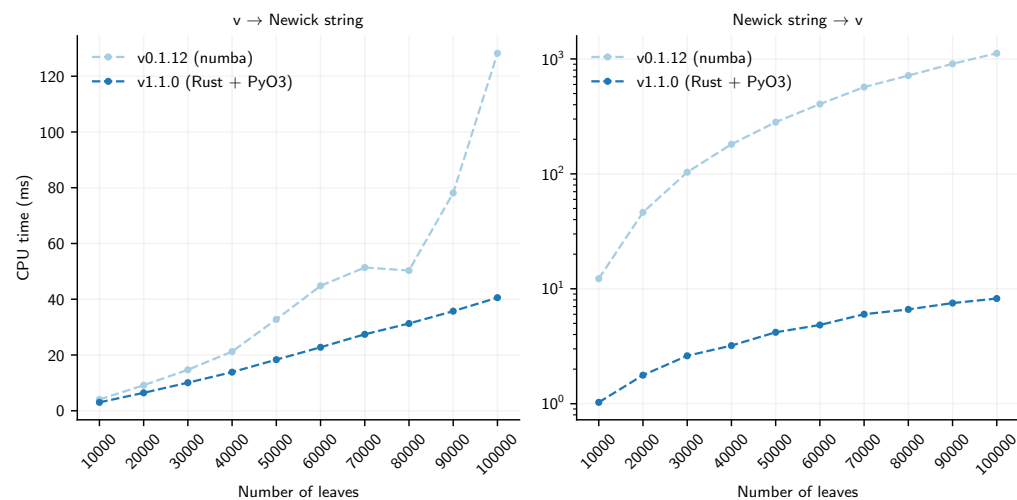
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## 11 Summary

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

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



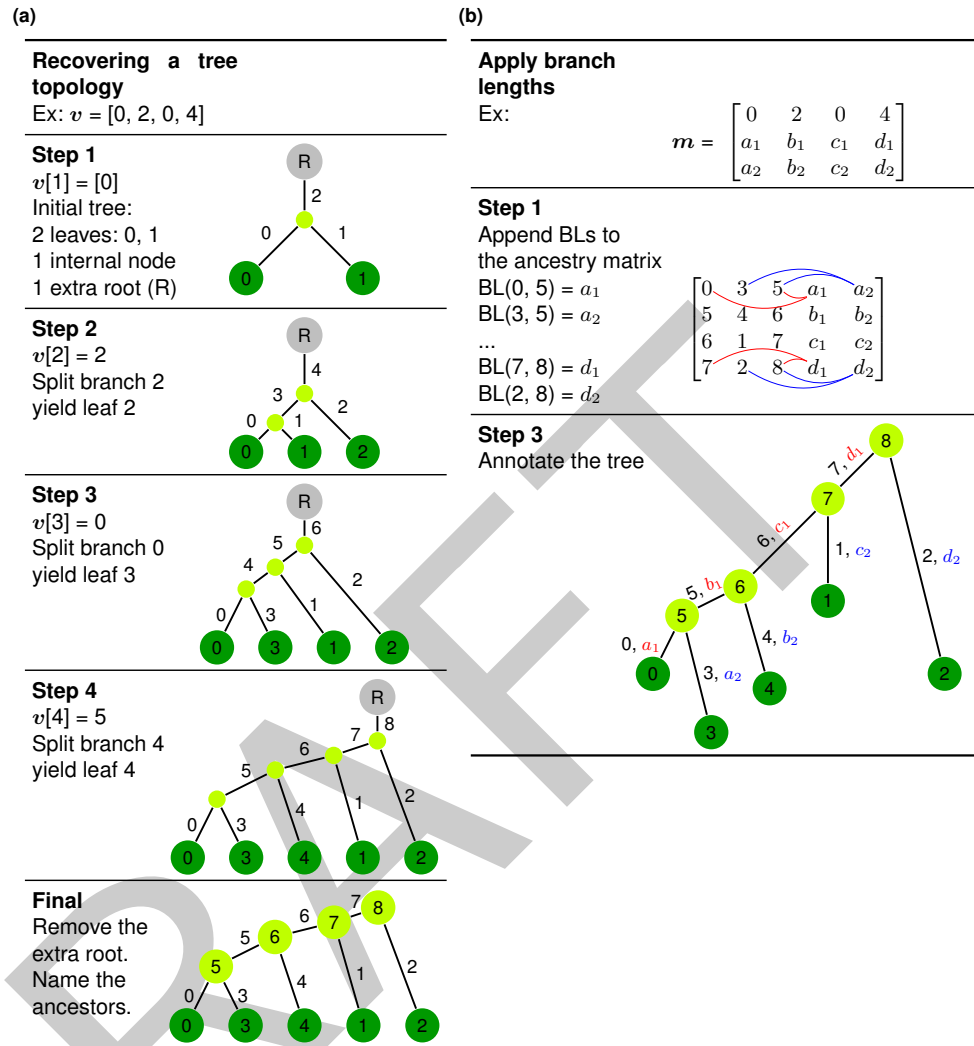
**Figure 1:** Benchmark times for converting a phylo2vec vector to a Newick string (left) and vice versa (right). For each size, we evaluated the execution time for a minimum of 20 rounds using pytest-benchmark. We compare the execution time of the Python functions in the latest release, which rely on 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)

## 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 optimization 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). In particular, it allows for branch length annotations, 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), a  $\mathcal{O}(n \log n)$  implementation of vector-to-Newick conversion based on Adelson-Velsky and Landis (AVL; (Adelson-Velsky & Landis, 1962)) trees, and a  $\mathcal{O}(n \log n)$  implementation of Newick-to-vector conversion making use of Fenwick trees (Fenwick, 1994) during the vector construction. Moreover, the current release features several new additions, including several leaf-level operations (pruning, placement, MRCA finding), fast cophenetic distance matrix calculation, and a skeleton for Bayesian phylogenetic inference using Markov Chain Monte Carlo (MCMC) in the highly optimised Beagle library that underpins a number of phylogenetic software (Ayres et al., 2012; Suchard & Rambaut, 2009). The inference framework leverages similarities between phylo2vec and BEAGLE's inner representation of post-order traversal. Lastly, user-friendliness is enhanced by step-by-step demos of the inner workings of phylo2vec's vector representation.



**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. These columns denote the length of the branch connecting each parent and their two children nodes, respectively.

## Maintenance

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