




ecodive: Parallel and Memory-Efficient R Package for Ecological Diversity Analysis

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Summary

Characterizing the composition of biological communities is a fundamental task in ecology, but the calculations involved can be computationally prohibitive. *ecodive* is an R package that addresses this challenge by providing a highly optimized implementation of common ecological diversity metrics, including alpha-diversity (within-sample richness and evenness) and beta-diversity (between-sample dissimilarity). These metrics can incorporate species counts, relative abundances, and evolutionary relationships, providing a multi-faceted view of ecological structure. By leveraging a compiled C library with pthreads for parallelization, *ecodive* delivers substantial performance gains in both speed and memory usage, enabling researchers to analyze larger datasets more efficiently.

Statement of Need

The analysis of ecological diversity in large-scale studies is often hampered by the computational demands of calculating metrics across thousands of communities, a common requirement in modern microbiome research, where studies routinely involve analyzing thousands of samples from large cohorts. This is particularly true for phylogenetic metrics like Faith's PD (Faith, 1992) and the UniFrac distance family (Q. Chang et al., 2011; Chen et al., 2012; C. A. Lozupone et al., 2007; C. Lozupone & Knight, 2005), which integrate species abundance with evolutionary data from phylogenetic trees. The resulting high demand on processing time and memory can limit the scope and scale of scientific inquiry.

ecodive overcomes these limitations by offering a significantly faster and more memory-efficient solution. This allows researchers to analyze more samples, explore more complex questions, and obtain more robust insights from their data. By providing a high-performance, parallelized engine for these calculations, *ecodive* empowers researchers to push the boundaries of large-scale ecological analysis.

Comparison to Existing Packages

To evaluate its performance, *ecodive* was benchmarked against numerous R packages that provide their own implementations of diversity metrics, including *abdiv* (Bittinger, 2020), *adiv* (Pavoine, 2020), *ampvis2* (Andersen et al., 2018), *ecodist* (Goslee & Urban, 2007), *entropart* (Marcon & Herault, 2015), *GUniFrac* (Chen et al., 2023), *labdsv* (Roberts, 2025), *parallelDist* (Eckert, 2022), *philentropy* (HG, 2018), *phyloregion* (Daru et al., 2020), *phyloseq* (McMurdie & Holmes, 2013), *picante* (Kembel et al., 2010), *tabula* (Frerebeau, 2019), and *vegan* (Oksanen et al., 2025). The results, conducted using the *bench* package, are

summarized in Figure 1 and demonstrate ecodive's superior speed and memory efficiency for each of the metrics tested. Crucially, the benchmark suite confirms these performance gains do not come at the cost of accuracy, as ecodive produces numerically identical output to the other packages. Beyond its computational advantages, ecodive has zero external R dependencies. This makes it a lightweight, stable, and secure backend, minimizing installation conflicts and simplifying long-term maintenance for developers who build upon it. The complete benchmark code and results are available in the package vignette (`vignette('benchmark')`) and online.

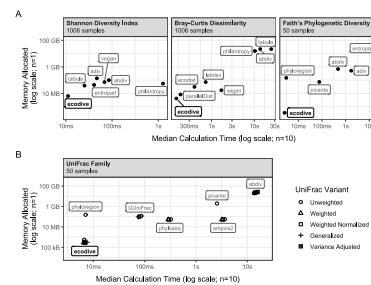


Figure 1: ecodive performance benchmarks. Each point represents an R package, plotted by median calculation time (x-axis) and memory consumption (y-axis) from ten trials. (A) Benchmarks for Shannon Diversity Index, Bray-Curtis Dissimilarity, and Faith's Phylogenetic Diversity. (B) Benchmarks for the UniFrac family of metrics, with different variants distinguished by point shape. Not all packages implement every metric, but ecodive is consistently the fastest and most memory-efficient across all tested metrics, often by several orders of magnitude.

Implemented Metrics

ecodive stands out by offering an extensive and diverse collection of over 50 metrics for both alpha and beta diversity analysis, making it a uniquely comprehensive tool. It provides researchers with a wide array of both traditional and phylogeny-aware algorithms in a single, high-performance package. The suite of alpha diversity metrics includes staples like the Shannon Diversity Index (Shannon, 1948) and Chao1 (Chao, 1984), important estimators such as the Abundance-based Coverage Estimator (ACE) (Chao & Lee, 1992) and Fisher's Alpha (Fisher et al., 1943), and key phylogeny-aware metrics like Faith's Phylogenetic Diversity, offering robust ways to assess within-sample richness and evenness. For assessing between-sample dissimilarity, ecodive implements essential beta diversity metrics widely used in microbial ecology, including Bray-Curtis Dissimilarity (Bray & Curtis, 1957; Sorenson, 1948), the complete UniFrac family, and the Aitchison distance (Aitchison, 1982) for compositional data analysis. This extensive collection allows for a thorough and multi-faceted analysis of community structure.

For the most up-to-date list and detailed descriptions, please refer to the official ecodive documentation at <https://cmmr.github.io/ecodive>.

Programmatic Use and API

Beyond interactive analysis, ecodive is engineered for programmatic use, making it an ideal backend for applications like R Shiny web apps (W. Chang et al., 2024). The package includes a `list_methods()` function that allows developers to dynamically filter and present available diversity metrics based on specific criteria. For instance, methods can be programmatically selected if they are phylogeny-aware, abundance-weighted, capable of handling non-integer counts, or are "true metrics" that satisfy the triangle inequality. This powerful API simplifies the integration of ecodive into other software, enabling developers to build sophisticated tools that offer users tailored diversity analysis options based on their dataset and analytical needs.

Example Usage

ecodive is designed for ease of use and integrates seamlessly with existing bioinformatics workflows, such as those using phyloseq objects. For example, calculating weighted UniFrac distances is straightforward:

```
data(esophagus, package = 'phyloseq')
ecodive::weighted_unifrac(esophagus)
#>           B           C
#> C 0.1050480
#> D 0.1401124 0.1422409
```

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