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. This is particularly true for phylogenetic metrics like Faith’s PD (Faith 1992) and the UniFrac distance family (C. Lozupone and 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

While numerous R packages can calculate diversity metrics, our comparison focuses on those that provide their own implementations: abdiv (Bittinger 2020), adiv (Pavoine 2020), ampvis2 (Andersen et al. 2018), ecodist (Goslee and Urban 2007), entropart (Marcon and Herault 2015), GUniFrac (Chen et al. 2023), phyloregion (Daru, Karunarathne, and Schliep 2020), phyloseq (McMurdie and Holmes 2013), picante (Kembel et al. 2010), and vegan (Oksanen et al. 2025). ecodive sets itself apart from these packages through its superior performance. Furthermore, ecodive has zero external R dependencies. This makes it a lightweight, stable, and secure computational backend, minimizing installation conflicts and simplifying long-term maintenance for developers who build upon it.

Comprehensive benchmarks, conducted using the bench package (Hester and Vaughan 2025), demonstrate these advantages across a range of metrics (Figures 1-3). The complete benchmark code and results are available in the package vignette (vignette('benchmark')) and online.

Figure 1: UniFrac benchmarks. ecodive demonstrates substantial performance gains for UniFrac, being 2 to 3,900x faster and using 50 - 32,000x less memory, which helps overcome computational bottlenecks in large-scale analyses.

Figure 2: Classic beta diversity benchmarks. ecodive is 6 to 2,300x faster and uses 1 to 1,800x less memory, enabling more efficient analysis of community dissimilarities.

Figure 3: Alpha diversity benchmarks. ecodive is 2 to 43,000x faster and uses 1 to 33,000x less memory, significantly accelerating the analysis of diversity within single samples.

# Implemented Metrics

ecodive provides a comprehensive suite of alpha and beta diversity metrics. The current implementation includes:

### Alpha Diversity

* Classic: Shannon Index (Shannon 1948), Simpson Index (Simpson 1949; Gini 1912), Inverse Simpson Index (Simpson 1949), and Chao1 (Chao 1984).
* Phylogenetic: Faith’s Phylogenetic Diversity (Faith 1992).

### Beta Diversity

* Classic: Bray-Curtis (Bray and Curtis 1957; Sorenson 1948), Canberra (Lance and Williams 1967), Euclidean (Gower and Legendre 1986; Legendre and Caceres 2013), Gower (Gower 1971; Gower and Legendre 1986), Jaccard (Jaccard 1908), Kulczynski (Kulczynski 1927), and Manhattan (Kaufman and Rousseeuw 1990).
* Phylogenetic: Unweighted UniFrac (C. Lozupone and Knight 2005), Weighted UniFrac (C. A. Lozupone et al. 2007), Normalized Weighted UniFrac (C. A. Lozupone et al. 2007), Generalized UniFrac (Chen et al. 2012), and Variance Adjusted Weighted UniFrac (Chang, Luan, and Sun 2011).

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

# 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:

library(phyloseq)  
data(esophagus)  
  
ecodive::weighted\_unifrac(esophagus)  
#> B C  
#> C 0.1050480   
#> D 0.1401124 0.1422409

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