

¹ `ecodive`: Parallel and Memory-Efficient R Package for Ecological Diversity Analysis

³ Daniel P Smith  ^{1,2}¶, Sara J Javornik Cregeen  ^{1,2}, and Joseph F Petrosino 

⁵ 1 The Alkek Center for Metagenomics and Microbiome Research, Department of Molecular Virology and
⁶ Microbiology, Baylor College of Medicine, Houston, TX 77030, USA ² Department of Molecular Virology
⁷ and Microbiology, Baylor College of Medicine, Houston, TX, USA  ¶ Corresponding author

DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

Software

- [Review](#) ↗
- [Repository](#) ↗
- [Archive](#) ↗

Editor: [Open Journals](#) ↗

Reviewers:

- [@openjournals](#)

Submitted: 01 January 1970

Published: unpublished

License

Authors of papers retain copyright and release the work under a

Creative Commons Attribution 4.0 International License ([CC BY 4.0](#))

Statement of Need

A primary challenge in large-scale ecological analysis is the computational complexity of beta diversity calculations. These algorithms exhibit $O(n^2)$ complexity, meaning their computational cost scales quadratically with the number of samples (n). As microbiome and ecological studies grow to include thousands of samples, this quadratic scaling creates a significant bottleneck, demanding immense processing time and memory.

A second challenge is the fragmentation of diversity metrics across numerous R packages. Researchers often need to install and manage a suite of dependencies to access the full range of metrics required for a comprehensive analysis, leading to potential version conflicts and a disjointed workflow.

`ecodive` addresses both of these critical needs. First, it provides a highly optimized, parallelized C-based engine that dramatically reduces the time and memory required by these algorithms, enabling the analysis of much larger datasets. Second, it consolidates a vast collection of alpha and beta diversity metrics into a single, dependency-free package. By solving the dual problems of computational inefficiency and methodological fragmentation, `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](#)), `GUUniFrac` ([Chen et al., 2023](#)), `labdsv` ([Roberts, 2025](#)),

39 parallelDist (Eckert, 2022), philentropy (HG, 2018), phyloregion (Daru et al., 2020),
 40 phyloseq (McMurdie & Holmes, 2013), picante (Kembel et al., 2010), tabula (Frerebeau,
 41 2019), and vegan (Oksanen et al., 2025). The results, conducted using the bench R package,
 42 are summarized in Figure 1 and demonstrate ecodive's superior speed and memory efficiency
 43 for each of the metrics tested.

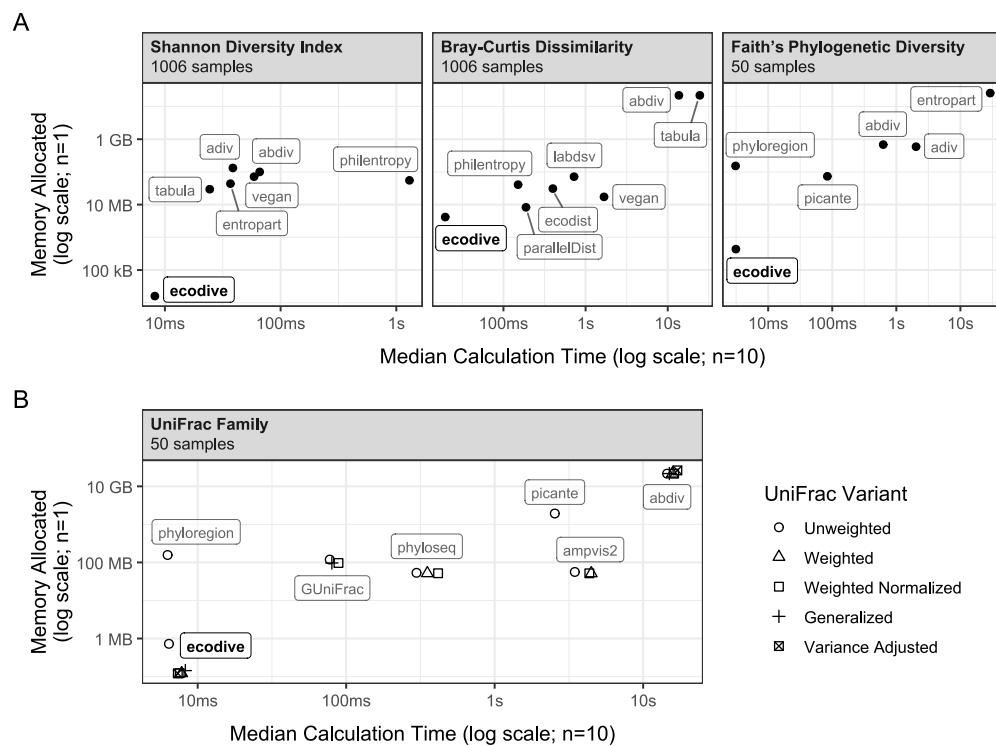


Figure 1: Figure 1: ecodive performance benchmarks. Each point represents an R package, plotted by median calculation time (x-axis) and memory consumption (y-axis) from ten trials. (A) Benchmarks for Shannon Diversity Index, Bray-Curtis Dissimilarity, and Faith's Phylogenetic Diversity. (B) Benchmarks 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.

44 Crucially, the benchmark suite also confirms these performance gains do not come at the
 45 cost of accuracy, as ecodive produces numerically identical output to the other packages.
 46 Beyond its computational advantages, ecodive has zero external R dependencies. This
 47 makes it a lightweight, stable, and secure backend, minimizing installation conflicts and
 48 simplifying long-term maintenance for developers who build upon it. The complete benchmark
 49 code and results are available in vignettes/articles/benchmark.Rmd and online at <https://cmmr.github.io/ecodive/articles/benchmark.html>.

51 Implemented Metrics

52 ecodive stands out by offering an extensive and diverse collection of 50 metrics for both alpha
 53 and beta diversity analysis, making it a uniquely comprehensive tool. It provides researchers with
 54 a wide array of both traditional and phylogeny-aware algorithms in a single, high-performance
 55 package. The suite of alpha diversity metrics includes staples like the Shannon Diversity Index
 56 (Shannon, 1948) and Chao1 (Chao, 1984), important estimators such as the Abundance-based
 57 Coverage Estimator (ACE) (Chao & Lee, 1992) and Fisher's Alpha (Fisher et al., 1943), and

58 key phylogeny-aware metrics like Faith's Phylogenetic Diversity ([Faith, 1992](#)), offering robust
59 ways to assess within-sample richness and evenness. For assessing between-sample dissimilarity,
60 ecodive implements essential beta diversity metrics widely used in microbial ecology, including
61 Bray-Curtis Dissimilarity ([Bray & Curtis, 1957](#); [Sorenson, 1948](#)), the complete UniFrac family
62 ([Q. Chang et al., 2011](#); [Chen et al., 2012](#); [C. A. Lozupone et al., 2007](#); [C. Lozupone & Knight, 2005](#)), and the Aitchison distance ([Aitchison, 1982](#)) for compositional data analysis. This
63 extensive collection allows for a thorough and multi-faceted analysis of community structure.
64
65 For the most up-to-date list and detailed descriptions, please refer to the official ecodive
66 documentation at <https://cmmr.github.io/ecodive>.

67 Programmatic Use and API

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

76 Example Usage

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

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

80 Acknowledgements

81 This study was supported by NIH/NIAD (Grant number U19 AI144297), and Baylor College
82 of Medicine and Alkek Foundation Seed. The authors also acknowledge the use of Google’s
83 Gemini for assistance in refining this manuscript.

84 References

- 85 Aitchison, J. (1982). The statistical analysis of compositional data. *Journal of the Royal Statistical Society. Series B (Methodological)*, 44(2), 139–177. <https://doi.org/10.1111/j.2517-6161.1982.tb01195.x>
- 88 Andersen, K. S., Kirkegaard, R. H., Karst, S. M., & Albertsen, M. (2018). ampvis2: An r package to analyse and visualise 16S rRNA amplicon data. *bioRxiv*. <https://doi.org/10.1101/299537>
- 91 Bittinger, K. (2020). Abdiv: Alpha and beta diversity measures. <https://doi.org/10.32614/CRAN.package.abdiv>
- 93 Bray, J. R., & Curtis, J. T. (1957). An ordination of the upland forest communities of southern Wisconsin. *Ecological Monographs*, 27(4), 325–349. <https://doi.org/10.2307/1942268>

- 95 Chang, Q., Luan, Y., & Sun, F. (2011). Variance adjusted weighted UniFrac: A powerful beta
96 diversity measure for comparing communities based on phylogeny. *BMC Bioinformatics*,
97 12(1). <https://doi.org/10.1186/1471-2105-12-118>
- 98 Chang, W., Cheng, J., Allaire, J., Sievert, C., Schloerke, B., Xie, Y., Allen, J., McPherson,
99 J., Dipert, A., & Borges, B. (2024). *Shiny: Web application framework for r*. <https://doi.org/10.32614/CRAN.package.shiny>
- 101 Chao, A. (1984). Non-parametric estimation of the number of classes in a population.
102 *Scandinavian Journal of Statistics*, 11, 265–270. <https://www.jstor.org/stable/4616294>
- 103 Chao, A., & Lee, S.-M. (1992). Estimating the number of classes via sample coverage. *Journal*
104 *of the American Statistical Association*, 87(417), 210–217. <https://doi.org/10.1080/01621459.1992.10475194>
- 106 Chen, J., Bittinger, K., Charlson, E. S., Hoffmann, C., Lewis, J., Wu, G. D., Collman,
107 R. G., Bushman, F. D., & Li, H. (2012). Associating microbiome composition with
108 environmental covariates using generalized UniFrac distances. *Bioinformatics*, 28(16),
109 2106–2113. <https://doi.org/10.1093/bioinformatics/bts342>
- 110 Chen, J., Zhang, X., Yang, L., & Zhang, L. (2023). *GUniFrac: Generalized UniFrac distances,*
111 *distance-based multivariate methods and feature-based univariate methods for microbiome*
112 *data analysis*. <https://doi.org/10.32614/CRAN.package.GUniFrac>
- 113 Daru, B. H., Karunaratne, P., & Schliep, K. (2020). Phyloregion: R package for biogeographic
114 regionalization and macroecology. *Methods in Ecology and Evolution*, 11, 1483–1491.
115 <https://doi.org/10.1111/2041-210X.13478>
- 116 Eckert, A. (2022). *parallelDist: Parallel distance matrix computation using multiple threads*.
117 <https://doi.org/10.32614/CRAN.package.parallelDist>
- 118 Faith, D. P. (1992). Conservation evaluation and phylogenetic diversity. *Biological Conservation*,
119 61, 1–10. [https://doi.org/10.1016/0006-3207\(92\)91201-3](https://doi.org/10.1016/0006-3207(92)91201-3)
- 120 Fisher, R. A., Corbet, A. S., & Williams, C. B. (1943). The relation between the number of
121 species and the number of individuals in a random sample of an animal population. *Journal*
122 *of Animal Ecology*, 12(1), 42–58. <https://doi.org/10.2307/1411>
- 123 Frerebeau, N. (2019). Tabula: An r package for analysis, seriation, and visualization of
124 archaeological count data. *Journal of Open Source Software*, 4(44), 1821. <https://doi.org/10.21105/joss.01821>
- 126 Goslee, S. C., & Urban, D. L. (2007). The ecodist package for dissimilarity-based analysis of
127 ecological data. *Journal of Statistical Software*, 22, 1–19. <https://doi.org/10.18637/jss.v022.i07>
- 129 HG, D. (2018). Philentropy: Information theory and distance quantification with r. *Journal of*
130 *Open Source Software*, 3(26), 765. <https://doi.org/10.21105/joss.00765>
- 131 Kembel, S. W., Cowan, P. D., Helmus, M. R., Cornwell, W. K., Morlon, H., Ackerly, D. D.,
132 Blomberg, S. P., & Webb, C. O. (2010). Picante: R tools for integrating phylogenies and
133 ecology. *Bioinformatics*, 26, 1463–1464. <https://doi.org/10.1093/bioinformatics/btq166>
- 134 Lozupone, C. A., Hamady, M., Kelley, S. T., & Knight, R. (2007). Quantitative and qualitative
135 beta diversity measures lead to different insights into factors that structure microbial
136 communities. *Applied and Environmental Microbiology*, 73(5), 1576–1585. <https://doi.org/10.1128/aem.01996-06>
- 138 Lozupone, C., & Knight, R. (2005). UniFrac: A new phylogenetic method for comparing
139 microbial communities. *Applied and Environmental Microbiology*, 71(12), 8228–8235.
140 <https://doi.org/10.1128/AEM.71.12.8228-8235.2005>
- 141 Marcon, E., & Herault, B. (2015). Entropart: An r package to measure and partition diversity.

- 142 *Journal of Statistical Software*, 67(8), 1–26. <https://doi.org/10.18637/jss.v067.i08>
- 143 McMurdie, P. J., & Holmes, S. (2013). Phyloseq: An r package for reproducible interactive
144 analysis and graphics of microbiome census data. *PLoS One*, 8(4), e61217. <https://doi.org/10.1371/journal.pone.0061217>
- 145 Oksanen, J., Simpson, G. L., Blanchet, F. G., Kindt, R., Legendre, P., Minchin, P. R., O'Hara,
146 R. B., Solymos, P., Stevens, M. H. H., Szoecs, E., Wagner, H., Barbour, M., Bedward, M.,
147 Bolker, B., Borcard, D., Carvalho, G., Chirico, M., De Caceres, M., Durand, S., ... Borman,
148 T. (2025). *Vegan: Community ecology package*. <https://doi.org/10.32614/CRAN.package.vegan>
- 149 Pavoine, S. (2020). Adiv: An r package to analyse biodiversity in ecology. *Methods in Ecology
150 and Evolution*, 11, 1106–1112. <https://doi.org/10.1111/2041-210X.13430>
- 151 Roberts, D. W. (2025). *Labdsv: Ordination and multivariate analysis for ecology*. <https://doi.org/10.32614/CRAN.package.labdsv>
- 152 Shannon, C. E. (1948). A mathematical theory of communication. *Bell System Technical
153 Journal*, 27(3), 379–423. <https://doi.org/10.1002/j.1538-7305.1948.tb01338.x>
- 154 Sorenson, T. (1948). A method of establishing groups of equal amplitude in plant sociology
155 based on similarity of species content. *Kongelige Danske Videnskabernes Selskab*, 5, 1–34.
- 156
- 157
- 158

DRAFT