fundiversity: a modular R package to compute functional diversity indices

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Abstract

 $(\max 350 \text{ words})$

- 1. Functional diversity is widely used and widespread. However, the main packages used to compute functional diversity indices are not flexible and not adapted to the volume of data used in modern ecological analyses.
 - 2. We here present fundiversity, an R package that eases the computation of classical functional diversity indices. It leverages parallelization and memoization (caching results in memory) to maximize efficiency with data with thousands of columns and rows.
 - 3. We also did a performance comparison with packages that provide analog functions. In addition to being more flexible, **fundiversity** was always an order of magnitude quicker than alternatives.
 - 4. fundiversity aims to be a lightweight efficient tool to compute functional diversity indices, that can be used in a variety of contexts. Because it has been designed following clear principles, it is easy to
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 $Keywords:\;$ biodiversity, diversity facet, R package, functional biogeography, functional ecology, community ecology

extend. We hope the wider community will adopt it and we welcome all contributions.

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Authors' Contributions

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 Matthias Grenié: Conceptualization, Methodology, Software, Resources, Writing - Original Draft, Writing - Review & Editing, Supervision. Hugo Gruson: Conceptualization, Methodology, Software, Writing - Review & Editing.

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Title

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Introduction

Functional diversity, the diversity of traits across scales, is a major facet of biodiversity (Pavoine & Bonsall, 2011). It has been widely used across ecological contexts (Cadotte et al., 2011) and has been shown to relate to ecosystem functioning (Díaz & Cabido, 2001; Leps et al., 2006). Many indices exist to characterize it across its three dimensions: richness (how much?), evenness (how regular?), and divergence (how different?) (Pavoine & Bonsall, 2011). Ecologists rely on computational tools to compute these indices in a reproducible fashion, mainly in the R programming language (Lai et al., 2019; R Core Team, 2021).

- The FD package is the main tool available for functional diversity indices, having accumulated now over than 1200 citations (Laliberté et al., 2014). But FD was released in 2009 receiving only minor updates that stopped in 2015. During this time, software development practices have changed dramatically and new, higher-performance, tools have emerged in the R ecosystem. Additionally, since 2009, the size of ecological datasets has grown exponentially (Farley et al., 2018; Wüest et al., 2020) and high-performance computing
- ¹⁵ (HPC) environments have become standard. There is therefore a dire need for a modern alternative using state-of-the-art software development techniques and tools.

The main function of the FD package dbFD() lets users compute a dozen functional diversity indices in a single call from raw trait data (Laliberté et al., 2014). While great for exploratory analyses, this can increase computation time when only a single index is needed. Furthermore, it does not enforce the good

²⁰ practice of choosing beforehand the appropriate functional diversity index for the question(s) asked (Legras et al., 2018; Mason et al., 2013; Schleuter et al., 2010). It encourages the user to fish for the functional diversity index matching predicted relationships (a form of p-hacking). This can lead users to report all computed functional diversity indices even when there are no clear expectations about different functional diversity facets or to report correlated indices (Legras et al., 2018; Mason et al., 2013; McPherson et al., 2018; Schleuter et al., 2010). Computing all indices in a single function also makes long-term maintenance

and addition of new indices harder.

The average size of datasets analyzed in ecology increased several fold in the last years (Wüest et al., 2020), calling for an increase in performance of computational tools. This increase is particularly urgent considering that many diversity analyses use null models that increase the data size by two or three orders

- ³⁰ of magnitude (Gotelli & Graves, 1996). First, any improvement of the algorithmic efficiency to compute functional diversity indices could save substantial amounts of time as it is repeated many times. For example, we noted that many R packages that compute functional diversity indices do not leverage the specifically optimized matrix algebra packages included in R. Their use can cut the number of operations dramatically compared to using a loop directly in R. Second, functional diversity indices are generally computed over
- ³⁵ many mathematically independent sites. With the rise of multicore computers, parallelization, i.e. splitting independent computations between different Computing Processor Units (CPUs), is becoming the norm. Very few functional diversity R packages natively implement parallelization, leaving the burden of doing so to the user. There have been tremendous new developments in this area in R over the last few years with the release of the **future** framework (Bengtsson, 2020) that allows to seamlessly parallelize computations
- ⁴⁰ on multiple cores on a single machine, across several machines, or even on a remote cluster without changing execution code. Third, computations on the same input can be cached through a process called memoization (Wickham et al., 2021). This avoids wasting computing power on previously seen inputs. For example, many functional diversity indices rely on the computation of convex hulls across a multi-dimensional space (Cornwell et al., 2006; Villéger et al., 2008). Caching the results of this costly computation could save time

⁴⁵ and computing power when measuring the diversity across similar sets, such as sites across a given region. Increasing discussions are held regarding scientific software robustness and reliability in ecology (Mislan et al., 2016; Poisot, 2015; White, 2015; Wilson et al., 2017). Mainly because most ecologists are self-trained in programming (Farrell & Carey, 2018), these virtuous practices are rarely applied in ecology (Barraquand et al., 2014). For example, unit tests use predefined inputs to compare outputs to expectations (Poisot, ⁵⁰ 2015). Unit tests have also become standard in R packages since the release of packages streamlining this process, such as testthat and tinytest (der Loo, 2020; Wickham, 2011). Very few R functional diversity packages provide unit tests to assess that the functions behave expectedly. Automatic tests of one's code are crucial when developing a tool for a wider audience, as it may be used across different contexts.

Here, we propose a modern alternative to FD called fundiversity that benefits from modern development ⁵⁵ practices, necessary features for large-sized datasets (modularity, parallelization, and memoization), and greater flexibility. The package can be easily extended to accommodate additional diversity indices not covered by following a clear design pattern detailed in the next section. We go through a use case to show how it can be used. We then compare the performance of fundiversity against similar packages.

Main features of fundiversity

⁶⁰ To ensure the consistency of its functions and to make it user-friendly, **fundiversity** follows clear design principles. In this section, we expose its distinctive features and principles.

To give maximum flexibility to the users, we tried to build fundiversity to be as modular as possible. Each function in fundiversity computes a single functional diversity index, so that it only returns a single index and nothing more. All functions in fundiversity are prefixed with fd_ to avoid conflict with similarly named functions in other packages, as it is becoming standard practice in R packages (rOpenSci et al., 2021). In line with its modularity, we focused on making the inputs and outputs of functions coherent.

- The functions use two main inputs: a species by traits matrix and a site by species matrix; all functions accept them as first arguments. Across functions, the outputs are always structured similarly: one site column that contains the name of its sites and one column named as the computed index (such as FRic when computing functional richness). The shape of the output is predictable and easily combined with other
- data.

We designed fundiversity so it minimally modifies the input data before computing the indices (see Figure 1). When computing functional diversity indices, upstream choices regarding trait standardization and trait space construction are fully part of the scientific question (de Bello et al., 2013; Leps et al., 2006; Maire et al., 2015; Mammola et al., 2021). Several packages provide default options that automatically

⁷⁵ Maire et al., 2015; Mammola et al., 2021). Several packages provide default options that automatically build multivariate spaces or dendrograms, and choose relevant axes of variation. While useful for naive users, these abstract away part of the scientific process that should be considered when using functional diversity indices. These choices have been shown to have strong consequences on the values of downstream indices (de Bello et al., 2013; Leps et al., 2006; Maire et al., 2015; Mammola et al., 2021). fundiversity chooses to enforce better practices by leaving trait space choices to the user.

Parallelization can vastly decrease computation speed by leveraging the architecture of modern computers. Most functions in fundiversity can be parallelized out of the box. fundiversity provides parallelization through the future backend (Bengtsson, 2020). Parallelization is toggled through a single function call using future::plan() before using fundiversity functions. Thanks to the flexibility given by the

future backend, the code to use will not change whether parallelizing across several cores on a single computer, across multiple computers, or on a remote high-performance cluster. The user only needs to update the call to future::plan(). Furthermore, the future backend provides load balancing so that no cores/units stay idle for too long and the parallelized tasks are split evenly. The package contains a dedicated vignette to guide the users through transforming unparallelized to parallelized code (accessible through vignette("fundiversity_1-parallel", package = "fundiversity")).

The computation of functional diversity indices often involves null models, which require repeated operations across the same data subsets. This results in computing the same indices over the exact same assemblages over and over. Memoization can leverage the already computed indices and avoid double work. For example, to compute functional richness (FRic) the convex hull of the input data has to first be identi-

⁹⁵ fied, and then the volume of this convex hull is computed. The first step, identifying the convex hull, takes the most time and as such, storing the results of each computed convex hull can vastly cut computation time for a little memory footprint. If the set of input points is encountered a second time, the results will be taken from memory instead of being recomputed. Memoization trades a little bit of computer memory (keeping the convex hulls stored) for more computation speed. For now, fundiversity leverages memoization only for computing convex hulls (as used when computing FDiv, FRic, and FRic_intersect). It is activated by default. This behavior can be overridden by changing the fundiversity.memoise option before loading the package.

Packages depend on one another to avoid reinventing the wheel and thus reuse already developed functions. A higher number of dependencies means that a package requires more packages to be installed before ¹⁰⁵ its own installation. While having many dependencies minimizes code replication, it also comes with a high price, because if a single dependency breaks then the whole package cannot be installed anymore (Cox, 2019). Inflated dependencies have been identified as a major risk in software and especially scientific software development (Claes et al., 2014; Cox, 2019). FD has only four dependencies but other functional diversity packages have many more dependencies (up to 100 dependencies for hypervolume, see Table S3). This renders them quite brittle for the users after years of not being actively developed. fundiversity has been designed to only have minimal external dependencies, it currently depends directly on four, carefully chosen,

external packages (details on the criteria of choice in vignette("fundiversity_4-design-principles", package = "fundiversity")): future.apply which itself depends on two other packages, Matrix which is shipped with R, and geometry & vegan on which FD also depends. Considering direct and indirect dependencies, fundiversity depends on a total of 21 packages while similar packages depend on 65 packages

on average (Table S3).

Because user flexibility is key, fundiversity has minimal assumptions on the input data structure. All its functions work with data frames, matrices, or sparse matrices alike. Sparse matrices are a different formalization of matrices that do not store explicitly the cells that contain zero. They offer a reduced memory

footprint and optimized algebra library for computation (Bates & Maechler, 2021). These matrices are thus specifically relevant for occurrence/abundance matrices that contain many zeros. If the used data have a high proportion of zeros, using sparse matrices can vastly decrease computational time in fundiversity. As we underlined in the introduction, automatic software testing, while not 100% flawless, is needed to

increase the confidence in the behavior of functions. It is widespread in professional software engineering but much less in scientific software development (Kanewala & Bieman, 2014). This means that software behavior is seldom validated against known inputs to make sure that it behaves in expected ways. This fact does not mean that the software is of poor quality but rather that some simple errors could introduce unnoticed changes in the behavior of functions. Most packages that compute functional diversity indices do not include any form of automatic testing (only 3 out of 11 do it following our assessment). We do want to

point out that the lack of tests results from the lack of formal training in software development for ecologists (Farrell & Carey, 2018). We designed fundiversity with many unit tests from the beginning, executing at least every single line of code once (i.e. achieving code coverage of 100%).

fundiversity mostly computes alpha functional diversity indices, because other recent packages exist to compute other types of functional diversity indices (Hill numbers, Li, 2018; beta-diversity indices, Baselga

¹³⁵ & Orme, 2012). We focused on indices available through the dbFD() function in the FD package and on indices that could benefit from faster implementations. The included indices cover the three dimensions of functional diversity: richness (how much total diversity within the set?), evenness (how regularly are species situated along the trait space?), and divergence (how different are species compared to an average position?) (Pavoine & Bonsall, 2011). fundiversity contains the following alpha functional diversity

¹⁴⁰ indices: functional richness (FRic), functional dispersion (FDis), functional divergence (FDiv), functional evenness (FEve), and Rao's quadratic entropy (Q). We included Q as we identified the potential for important performance improvements relative to existing packages. fundiversity also contains a beta-diversity index (named FRic_intersect) as it can be useful to compare the overlap between convex hulls between sites. Thanks to its design, fundiversity can be easily extended to include more indices, we include below the

145 list of available indices in the current version of fundiversity.

| Table 1: List of functions av | vailable in fundiversity to compute |
|--------------------------------|-------------------------------------|
| functional diversity indices. | The two last columns specify which |
| functions are parallelizable a | nd memoizable. |

| Function Name | Index Name | Source | Parallelizable | Memoizable |
|----------------------|------------------------------------|--------------------------------|----------------|------------|
| fd_fdis() | Functional Dispersion (FDis) | Laliberté & Legendre (2010) | Yes | No |
| <pre>fd_fdiv()</pre> | Functional Divergence (FDiv) | Villéger et al. (2008) | Yes | Yes |
| <pre>fd_feve()</pre> | Functional Evenness (FEve) | Villéger et al. (2008) | Yes | No |
| fd_fric() | Functional Richness (FRic) | Villéger et al. (2008) | Yes | Yes |
| fd_fric_intersec | t () Functional β -diversity | Villéger et al. (2013) | Yes | Yes |
| fd_raoq() | Rao's Quadratic Entropy (Q) | Rao (1982) | No | No |

We made sure the indices were numerically exact by using the test dataset available in Villéger et al. (2008). The functions in fundiversity gave identical results to the one found in Figure 2 of Villéger et al. (2008). We summarize our comparisons in the numerical correctness vignette accessible through vignette("fundiversity_3-correctness", package = "fundiversity"). We furthermore compared the obtained results with functions in other packages and made sure to obtain similar values.

Case Study

In this section, we show how to use fundiversity in practice. As an example dataset, we included in fundiversity site-species and trait data from Nowak et al. (2019). It is accessible through calls to site_sp_birds and traits_birds when fundiversity is loaded with library() or the use of the data("site_sp_birds", package = "fundiversity") and data("traits_birds", package = "fundiversity") functions when fundiversity is not loaded. This dataset describes the presence/absence of bird species in South America at different elevations and four of their morphological traits.

[Figure 1 about here.]

The trait values show species in rows (species are specified as row names) and traits in columns with trait names as column names (Figure 1). Similarly, the site-species matrix contains sites as rows (site names are row names) and species as columns (species names are column names).

```
data("traits_birds", package = "fundiversity")
data("site_sp_birds", package = "fundiversity")
```

head(traits_birds)

| | ## | | Bill.widthmm. | Bill.lengthmm. | Kipp.s.index | Bodymassg. |
|-----|----|----------------------|---------------|----------------|--------------|------------|
| | ## | Aburria_aburri | 18.35 | 35.48 | 0.18 | 1407.5 |
| | ## | Amazona_farinosa | 26.50 | 38.81 | 0.29 | 626.0 |
| 165 | ## | Amazona_mercenaria | 17.51 | 26.30 | 0.33 | 340.0 |
| | ## | Amazona_ochrocephala | 20.17 | 31.40 | 0.26 | 440.0 |
| | ## | Ampelioides_tschudii | 16.53 | 24.58 | 0.24 | 78.4 |
| | ## | Ampelion_rufaxilla | 16.97 | 21.89 | 0.28 | 73.9 |

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| head | site | SD | birds) | Γ. | 1:3 |
|------|------|----------------|---------|----|-----|
| nouu | | _ ~ ~ _ | DII aD/ | ∟, | |

| | ## | | Aburria_aburri | Amazona_farinosa | Amazona_mercenaria |
|-----|----|-----------|----------------|------------------|--------------------|
| 170 | ## | elev_250 | 0 | 1 | 0 |
| | ## | elev_500 | 0 | 1 | 0 |
| | ## | elev_1000 | 1 | 1 | 1 |
| | ## | elev_1500 | 1 | 0 | 1 |
| | ## | elev_2000 | 0 | 0 | 1 |
| 175 | ## | elev_2500 | 0 | 0 | 1 |

Now that we have obtained trait and occurrence data we need to compute the trait dissimilarity between each pair of species. As all traits are quantitative, we first scale them to zero mean and standard deviation of one (z-score), then we compute the Euclidean distance between pairs of species.

z_traits = scale(traits_birds, center = TRUE, scale = TRUE)

```
trait_distance = as.matrix(dist(z_traits))
```

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We want to emphasize here that fundiversity does not assume anything in the upstream of the computation of functional diversity indices. Trait standardization and computation of a trait dissimilarity are left to the user's discretion. They are provided here as a full workflow example. The specific functions used in the previous chunk can vary depending on the scientific question, the nature of the traits, or the transformation needed. fundiversity does not provide any functions to deal with these upstream choices as it is the user's responsibility to carefully examine them.

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Then, we compute the functional richness at each location using the fd_fric() function. It expects quantitative trait values as the first argument and a site-species matrix as the second argument.

library("fundiversity")

birds_fric = fd_fric(z_traits, site_sp_birds)

head(birds_fric)

site FRic
1 elev_250 66.048816
2 elev_500 71.465678
3 elev_1000 43.354008
4 elev_1500 25.466685
5 elev_2000 7.725843
6 elev_2500 7.046431

If the site-species matrix is not provided, fundiversity considers that all species present in the trait matrix are all present in a single site:

fd_fric(z_traits)

site FRic
1 s1 88.9286

All other functions in fundiversity use a similar structure: the first input is trait data, the second one is a site-species matrix (Figure 1). For Rao's quadratic entropy, computed through fd_raoq(), functional dissimilarities can be specified as the third argument:

 $\mathbf{6}$

```
# With functional dissimilarity
birds_raoq = fd_raoq(traits = NULL, site_sp_birds, dist_matrix = trait_distance)
# With trait values
birds_raoq_2 = fd_raoq(z_traits, site_sp_birds)
# Both options give the same results
identical(birds_raoq, birds_raoq_2)
```

[1] TRUE

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If not all traits are quantitative, it is possible to transform them back into independent quantitative 'traits' through the use of Gower's distance (Gower, 1971; and its extensions: Podani, 1999; and Pavoine et al., 2009) then applying multivariate analysis to obtain orthogonal dimensions (Maire et al., 2015). But there are many other ways to convert qualitative traits and as such, this is out of the scope of fundiversity. We leave it to the user to decide how to proceed to obtain independent quantitative traits.

Using parallel computation

As specified above, fundiversity allows for parallel computation of functional diversity metrics through the future framework. We here demonstrate how to use it in practice with the case study. A more detailed explanation is provided in the "Parallelization" vignette of fundiversity (available through vignette("fundiversity_1-p

package = "fundiversity")).

We first have to check if the function in fundiversity is parallelizable: all functions except fd_raoq() are. Then we define the parallel setting using the future::plan() function. This allows users to define how the parallel computation should be split: across cores, across computers, across jobs of a High-

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Performing Cluster, etc. Here, we split the computation locally across the 4 cores of the computer using the future::multisession() function. We specify the number of cores to use with the workers argument in the call to the future::plan() function.

First: Setup a parallel plan future::plan(future::multisession, workers = 4)

Second: Perform the computation bird_fric = fd_fric(traits_birds, site_sp_birds)

head(bird_fric)

FRic site ## 1 elev 250 171543.73 ## 2 elev_500 185612.55 ## 3 elev_1000 112600.18 ## 4 elev_1500 66142.75 ## 5 elev_2000 20065.76 ## 6 elev_2500 18301.18

To use a different backend, you can invoke a different argument in the future::plan() function. All possible arguments are detailed in the overview vignette of the future package (accessible through vignette("future-1-overview", package = "future") once future has been installed).

The parallel computations are split across sites, so parallelization can drastically improve performance when having a large number of sites. However, given the efficiency of fundiversity functions, and the overhead costs of parallel computation, we recommend parallelizing only with matrices of at least 10.000 230 sites, or when hitting a performance limit of the default sequential execution.

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Also, parallelization should never be used in conjunction with memoization because of the risk of cache corruption if several cores access the memoized cache simultaneously (make sure to use options(fundiversity.memoise = FALSE) before loading fundiversity when using parallel computations).

235 Performance Comparison

To test the performance improvements realized by fundiversity, we compared computation time on standardized datasets across similar functions in other packages. We only compared packages that provide original functions, not wrappers that depend on other packages to compute functional diversity indices. Six packages computed similar indices to fundiversity. Most indices are also computed by the FD::dbFD() function, but the comparison would be unfair as it computes many indices in a single call, while functions

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original functions, not wrappers that depend on other packages to compute functional diversity indices. Six packages computed similar indices to fundiversity. Most indices are also computed by the FD::dbFD() function, but the comparison would be unfair as it computes many indices in a single call, while functions in fundiversity only compute single indices. We considered functions from: adiv (Pavoine, 2020), BAT (Cardoso et al., 2015), betapart (Baselga & Orme, 2012), hillR (Li, 2018), mFD (Magneville et al., 2022), and FD (Laliberté et al., 2014) (see Table 2 for the correspondence between packages). A continuously updated version of this section can be found in the performance comparison vignette within the fundiversity package with vignette("fundiversity_2-performance", package = "fundiversity").

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| Index Name | fundiversity Functions | Equivalent Functions |
|-------------------------------|--------------------------------|---|
| Functional Dispersion (FDis) | fd_fdis() | FD::fdisp() |
| | | <pre>mFD::alpha.fd.multidim(,</pre> |
| | | <pre>ind_vect = "fdis")</pre> |
| Functional Divergence (FDiv) | fd_fdiv() | mFD::alpha.fd.multidim(, |
| | | <pre>ind_vect = "fdiv")</pre> |
| Functional Evenness (FEve) | fd_feve() | mFD::alpha.fd.multidim(, |
| | | <pre>ind_vect = "feve")</pre> |
| Functional Richness (FRic) | <pre>fd_fric()</pre> | BAT::alpha() (tree) |
| | | BAT::hull.alpha() (hull) |
| | | mFD::alpha.fd.multidim(, |
| | | <pre>ind_vect = "fric")</pre> |
| Rao's Quadratic Entropy (Q) | fd_raoq() | adiv::QE() |
| | | BAT::rao() |
| | | hillR::hill_func() |
| | | mFD::alpha.fd.hill(, q = |
| | | 2, tau = "max") |
| Functional β -diversity | <pre>fd_fric_intersect()</pre> | <pre>betapart::functional.beta.pair()</pre> |
| | | hillR::hill_func_parti_pairwise() |

Table: List of fundiversity functions with corresponding functions in other packages. The name of the package is indicated before the :: while the name of the functions (including specified arguments) follows. For testing purposes, we used datasets of increasing size with the number of species being 200, 500, or

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For testing purposes, we used datasets of increasing size with the number of species being 200, 500, or 1000; the number of traits 2, 4, or 10; and the number of sites 50, 100, or 500. For each set of parameters, we generated a fictional site-species matrix and species-trait matrix containing only continuous traits. We used these simulated data to perform benchmarks across comparable functions (Table d). The benchmark was run 30 times through the **bench** package (Hester & Vaughan, 2021). A summary of the results of the benchmark can be seen in Fig. 2. The full results detailing the timings for each combination of parameters and functions are available in the Supplementary Material (Fig. S4).

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[Figure 2 about here.]

For all the indices and functions tested, fundiversity is at least one order of magnitude faster than alternative packages. For functional dispersion (FDis), fundiversity is two orders of magnitude faster

compared to BAT and mFD. For functional divergence (FDiv), fundiversity is one order of magnitude faster than mFD. For functional evenness (FEve), fundiversity is two orders of magnitude faster than mFD

with sequential and parallelized versions having similar performances. For Rao's quadratic entropy (Q), fundiversity is one order of magnitude faster than hillR and mFD, two orders faster than adiv, and three orders of magnitude faster than BAT. For functional richness (FRic), fundiversity is half an order of magnitude faster than the hull version of BAT, as well as one and a half orders of magnitude faster than its tree version and mFD. For functional richness intersection (beta functional diversity), fundiversity is two orders of magnitude faster than betapart and hillR. 265

[Figure 3 about here.]

As shown in Fig. 2, the parallelized versions of fundiversity functions executed on average one order of magnitude faster than the sequential versions. For functional richness we even observed a difference of two orders of magnitude. However, for functional dispersion, parallelization increased the overall computation

time. This may be due to inherent parallelization issues: there is an overhead cost when splitting tasks across multiple cores of a computer. The efficiency of parallelization depends on the difficulty of the tasks that are split between cores. In the case of functional richness, the main task is computing the convex hull, which is computationally costly, which is why parallelization increases performance in this case. However, computing functional dispersion is simpler, and as such, does not benefit from being split across different

cores. Different values for the number of cores, species, traits, or sites produce qualitatively the same results 275 (full results in Fig. S5).

One important note regarding parallelization in fundiversity is that it is important to avoid doing both memoization and parallelization simultaneously. Memoization creates a cache to avoid recomputing results and the cache may be corrupted if several cores access the same results at the same time. We noticed that toggling memoization while performing parallelization severely increases total computational time compared

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to sequential performance.

Note that these benchmarks only assess the packages' computation speed and in no way any package's intrinsic quality or usefulness. We are comparing fundiversity, a package whose main goal is performance, with other packages that may have other primary goals and offer other benefits. For example, several

packages offer nice default visualization functions to plot the different diversity indices, while we explicitly considered that visualization functions were not part of fundiversity and let the users decide how they want to plot their indices.

Conclusion

We proposed a modern alternative R package to compute functional diversity indices. This package follows current best development practices and leverages modern features like parallelization and memoization 290 to increase its performance. This is only made possible by recent developments that were, for the most part, not available at the time when alternative packages came out. fundiversity does not propose to replace the entire toolkit for the researcher interested in functional diversity (including the upstream selection of the traits and the building of a functional space), but instead focuses on improving the most computationally costing step: computing functional diversity indices. We hope it will be a useful contribution to this toolkit.

To ensure its long-term maintainability, we made the package available on GitHub, it is perennially archived on Zenodo, sits in an independent GitHub organization, and is written following clear design principles. This package aims to always be a work in progress, as such we welcome contributions from interested users and developers.

Data Availability 300

fundiversity is available on CRAN through install.packages("fundiversity") as well as on GitHub at https://github.com/funecology/fundiversity, for archival all releases are available on Zenodo at https://doi.org/10.5281/zenodo.4761754. The data used in this article are available from the package, through data(package = "fundiversity") call.

305 Supplementary Information

[Figure 4 about here.]

[Figure 5 about here.]

Table 3: Table S1. Number of dependencies for functional diversity packages

| Package Name | Number of Hard Dependencies | Number of Total Dependencies |
|--------------|-----------------------------|------------------------------|
| vegan | 7 | 19 |
| FD | 18 | 18 |
| fundiversity | 21 | 68 |
| betapart | 24 | 24 |
| TPD | 41 | 75 |
| hillR | 54 | 92 |
| entropart | 76 | 118 |
| adiv | 85 | 85 |
| hypervolume | 100 | 137 |
| BAT | 107 | 107 |
| hilldiv | 126 | 126 |
| mFD | 128 | 136 |

References

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Barraquand, F., Ezard, T. H. G., Jørgensen, P. S., Zimmerman, N., Chamberlain, S., Salguero-Gómez, R.,
 ³¹⁰ Curran, T. J., & Poisot, T. (2014). Lack of quantitative training among early-career ecologists: A survey

of the problem and potential solutions. *PeerJ*, 2, e285. https://doi.org/10.7717/peerj.285 Baselga, A., & Orme, C. D. L. (2012). Betapart: An R package for the study of beta diversity. *Methods in Ecology and Evolution*, 3(5), 808-812. https://doi.org/10.1111/j.2041-210X.2012.00224.x

Bates, D., & Maechler, M. (2021). Matrix: Sparse and dense matrix classes and methods [Manual].

Cadotte, M. W., Carscadden, K., & Mirotchnick, N. (2011). Beyond species: Functional diversity and the maintenance of ecological processes and services. *Journal of Applied Ecology*, 48(5), 1079–1087. https://doi.org/10.1111/j.1365-2664.2011.02048.x

³²⁰ Cardoso, P., Rigal, F., & Carvalho, J. C. (2015). BAT – Biodiversity Assessment Tools, an R package for the measurement and estimation of alpha and beta taxon, phylogenetic and functional diversity. *Methods* in Ecology and Evolution, 6(2), 232–236. https://doi.org/10.1111/2041-210X.12310

Claes, M., Mens, T., & Grosjean, P. (2014). On the maintainability of CRAN packages. 2014 Software Evolution Week - IEEE Conference on Software Maintenance, Reengineering, and Reverse Engineering (CSMR-WCRE), 308-312. https://doi.org/10.1109/CSMR-WCRE.2014.6747183

- Cornwell, W. K., Schwilk, D. W., & Ackerly, D. D. (2006). A Trait-Based Test for Habitat Filtering: Convex Hull Volume. *Ecology*, 87(6), 1465–1471. https://doi.org/10.1890/0012-9658(2006)87%5B1465: ATTFHF%5D2.0.C0;2
 - Cox, R. (2019). Surviving software dependencies. Communications of the ACM, 62(9), 36-43. https://doi.org/10.1145/3347446
- de Bello, F., Carmona, C. P., Mason, N. W. H., Sebastià, M.-T., & Lepš, J. (2013). Which trait dissimilarity for functional diversity: Trait means or trait overlap? *Journal of Vegetation Science*, 24(5), 807–819. https://doi.org/10.1111/jvs.12008

Bengtsson, H. (2020). A unifying framework for parallel and distributed processing in r using futures. https://arxiv.org/abs/2008.00553

der Loo, M. van. (2020). A method for deriving information from running R code. *The R Journal*, Accepted for publication.

- Díaz, S., & Cabido, M. (2001). Vive la différence: Plant functional diversity matters to ecosystem processes. Trends in Ecology & Evolution, 16(11), 646–655. https://doi.org/10.1016/S0169-5347(01)02283-2
 Farley, S. S., Dawson, A., Goring, S. J., & Williams, J. W. (2018). Situating Ecology as a Big-Data Science:
- Current Advances, Challenges, and Solutions. *BioScience*, 68(8), 563-576. https://doi.org/10.1093/ ³⁴⁰ biosci/biy068
- Farrell, K. J., & Carey, C. C. (2018). Power, pitfalls, and potential for integrating computational literacy into undergraduate ecology courses. *Ecology and Evolution*, 8(16), 7744-7751. https://doi.org/10. 1002/ece3.4363

Gotelli, N. J., & Graves, G. R. (1996). Null models in ecology. Smithsonian Institution Press.

- Gower, J. C. (1971). A general coefficient of similarity and some of its properties. Biometrics, 857–871.
 Hester, J., & Vaughan, D. (2021). Bench: High precision timing of r expressions. https://CRAN.R
 - project.org/package=bench Kanewala, U., & Bieman, J. M. (2014). Testing scientific software: A systematic literature review. Information and Software Technology, 56(10), 1219-1232. https://doi.org/10.1016/j.infsof.2014.05.006
- Lai, J., Lortie, C. J., Muenchen, R. A., Yang, J., & Ma, K. (2019). Evaluating the popularity of R in ecology. *Ecosphere*, 10(1), e02567. http://esajournals-onlinelibrary-wiley-com/doi/abs/10.1002/ecs2. 2567
 - Laliberté, E., & Legendre, P. (2010). A distance-based framework for measuring functional diversity from multiple traits. *Ecology*, 91(1), 299–305. https://doi.org/10.1890/08-2244.1
- ³⁵⁵ Laliberté, E., Legendre, P., & Shipley, B. (2014). FD: Measuring functional diversity from multiple traits, and other tools for functional ecology.
 - Legras, G., Loiseau, N., & Gaertner, J. -C. (2018). Functional richness: Overview of indices and underlying concepts. Acta Oecologica, 87, 34–44. https://doi.org/10.1016/j.actao.2018.02.007
- Leps, J., Bello, F., Lavorel, S., & Berman, S. (2006). Quantifying and interpreting functional diversity of natural communities: Practical considerations matter. *Preslia*, 78, 481–501.
 - Li, D. (2018). hillR: Taxonomic, functional, and phylogenetic diversity and similarity through Hill Numbers. Journal of Open Source Software, 3(31), 1041. https://doi.org/10.21105/joss.01041
 - Magneville, C., Loiseau, N., Albouy, C., Casajus, N., Claverie, T., Escalas, A., Leprieur, F., Maire, E., Mouillot, D., & Villéger, S. (2022). mFD: An R package to compute and illustrate the multiple facets of functional diversity. *Ecography*, 2022(1). https://doi.org/10.1111/ecog.05904
- Maire, E., Grenouillet, G., Brosse, S., & Villéger, S. (2015). How many dimensions are needed to accurately assess functional diversity? A pragmatic approach for assessing the quality of functional spaces. *Global Ecology and Biogeography*, 24(6), 728–740. https://doi.org/10.1111/geb.12299
- Mammola, S., Carmona, C. P., Guillerme, T., & Cardoso, P. (2021). Concepts and applications in functional diversity. *Functional Ecology*, 35(9), 1869–1885. https://doi.org/10.1111/1365-2435.13882
- Mason, N. W. H., de Bello, F., Mouillot, D., Pavoine, S., & Dray, S. (2013). A guide for using functional diversity indices to reveal changes in assembly processes along ecological gradients. *Journal of Vegetation Science*, 24(5), 794–806. https://doi.org/10.1111/jvs.12013
- McPherson, J. M., Yeager, L. A., & Baum, J. K. (2018). A simulation tool to scrutinise the behaviour of functional diversity metrics. *Methods in Ecology and Evolution*, 9(1), 200–206. https://doi.org/10.
 - 1111/2041-210X.12855
 Mislan, K. A. S., Heer, J. M., & White, E. P. (2016). Elevating The Status of Code in Ecology. Trends in Ecology & Evolution, 31(1), 4-7. https://doi.org/10.1016/j.tree.2015.11.006
 - Nowak, L., Kissling, W. D., Bender, I. M. A., Dehling, D. M., Töpfer, T., Böhning-Gaese, K., & Schleuning, M. (2019). Data from: Projecting consequences of global warming for the functional diversity of fleshy-fruited plants and frugivorous birds along a tropical elevational gradient. In *Data Dryad Digital*
 - Repository (pp. 264849 bytes). https://doi.org/10.5061/DRYAD.CON737B Pavoine, S. (2020). Adiv: An r package to analyse biodiversity in ecology. Methods in Ecology and Evolution, 11(9), 1106-1112. https://doi.org/10.1111/2041-210X.13430

365

380

335

Pavoine, S., & Bonsall, M. B. (2011). Measuring biodiversity to explain community assembly: A unified

approach. *Biological Reviews*, 86(4), 792-812. https://doi.org/10.1111/j.1469-185X.2010.00171. x

- Pavoine, S., Vallet, J., Dufour, A.-B., Gachet, S., & Daniel, H. (2009). On the challenge of treating various types of variables: Application for improving the measurement of functional diversity. *Oikos*, 118(3), 391-402. https://doi.org/10.1111/j.1600-0706.2008.16668.x
- Podani, J. (1999). Extending Gower's general coefficient of similarity to ordinal characters. Taxon, 331-340.
 Poisot, T. (2015). Best publishing practices to improve user confidence in scientific software. Ideas in Ecology and Evolution, 8. https://doi.org/10.4033/iee.2015.8.8.f

390

- R Core Team. (2021). R: A language and environment for statistical computing [Manual]. R Foundation for Statistical Computing. https://www.R-project.org/
- Rao, C. R. (1982). Diversity and dissimilarity coefficients: A unified approach. Theoretical Population Biology, 21(1), 24–43. https://doi.org/10.1016/0040-5809(82)90004-1
 - rOpenSci, Anderson, B., Chamberlain, S., DeCicco, L., Gustavsen, J., Krystalli, A., Lepore, M., Mullen, L., Ram, K., Ross, N., Salmon, M., & Vidoni, M. (2021). *rOpenSci packages: Development, maintenance*,
- and peer review (Version 0.6.0) [Computer software]. Zenodo. https://doi.org/10.5281/zenodo. 4554776
 - Schleuter, D., Daufresne, M., Massol, F., & Argillier, C. (2010). A user's guide to functional diversity indices. *Ecological Monographs*, 80(3), 469–484. https://doi.org/10.1890/08-2225.1
- Villéger, S., Grenouillet, G., & Brosse, S. (2013). Decomposing functional β-diversity reveals that low
 functional β-diversity is driven by low functional turnover in European fish assemblages. *Global Ecology* and Biogeography, 22(6), 671–681. https://doi.org/10.1111/geb.12021
 - Villéger, S., Mason, N. W. H., & Mouillot, D. (2008). New Multidimensional Functional Diversity Indices for a Multifaceted Framework in Functional Ecology. *Ecology*, 89(8), 2290–2301. https://doi.org/10. 1890/07-1206.1
- White, E. (2015). Some thoughts on best publishing practices for scientific software. Ideas in Ecology and Evolution, 8. https://doi.org/10.4033/iee.2015.8.9.c
 - Wickham, H. (2011). Testthat: Get started with testing. The R Journal, 3, 5–10.
 - Wickham, H., Hester, J., Chang, W., Müller, K., & Cook, D. (2021). *Memoise: Memoisation of functions* [Manual]. https://CRAN.R-project.org/package=memoise
- ⁴¹⁵ Wilson, G., Bryan, J., Cranston, K., Kitzes, J., Nederbragt, L., & Teal, T. K. (2017). Good enough practices in scientific computing. *PLOS Computational Biology*, 13(6), e1005510. https://doi.org/10.1371/ journal.pcbi.1005510
 - Wüest, R. O., Zimmermann, N. E., Zurell, D., Alexander, J. M., Fritz, S. A., Hof, C., Kreft, H., Normand, S., Cabral, J. S., Szekely, E., Thuiller, W., Wikelski, M., & Karger, D. N. (2020). Macroecology in the
- 420 age of Big Data Where to go from here? Journal of Biogeography, 47(1), 1–12. https://doi.org/10. 1111/jbi.13633

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Figure 1: Conceptual diagram showing the input and typical ouput data from 'fundiversity' functions. Input data are generally a site-species table and a species-traits table, and the output gives back a table of functional diversity index per site.



Figure 2: Timing comparison across functional diversity indices between packages. Each point represents the execution time of one run using a simulated dataset, the points are transparent and jittered to avoid overplotting. We here show the performance results considering only a single set of parameters with 4 traits, 500 species, and 100 sites, repeated 30 times.



Figure 3: Timing comparison between parallel and sequential version of fundiversity functions across functional diversity indices. Each point represents the execution time of one run using simulated datasets with fixed properties (4 traits, 100 sites, 500 species), the points are transparent and jittered to avoid overplotting. The parallel version ran across 6 cores.

Functional Dispersion



Functional Divergence



Functional Evenness



Number of traits

→ 2

-▲· 3

-∎· 4

| +- | 10 |
|----|----|
| | |

Rao's Quadratic Entropy



 Number of species

 ←
 200

 ←
 500

 ←
 1000

Functional Richness



Functional Richness intersect



Figure 4: Performance comparison across functions of different packages over a range of parameters (number of traits, species, and sites). Note that each combination of parameters ran 30 iterations. The lines show trends of execution time in function of number of sites of the input dataset.



Figure 5: Performance comparison across internal functions over a range of parameters (number of traits, species, and sites) and different parallelization parameters. Note that each combination of parameters ran 20 iterations. The lines show trends of execution time in function of number of sites of the input dataset.