

NCBITaxonomy.jl - rapid biological names finding and reconciliation

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NCBITaxonomy.jl is a package designed to facilitate the reconciliation and cleaning of taxonomic names, using a local copy of the NCBI taxonomic backbone (Federhen 2012, Schoch et al. 2020); The basic search functions are coupled with quality-of-life functions including case-insensitive search and custom fuzzy string matching to facilitate the amount of information that can be extracted automatically while allowing efficient manual curation and inspection of results. NCBITaxonomy.jl works with version 1.6 of the Julia programming language (Bezanson et al. 2017), and relies on the Apache Arrow format to store a local copy of the NCBI raw taxonomy files. The design of NCBITaxonomy.jl has been inspired by similar efforts, like the R package taxadb (Norman et al. 2020), which provides an offline alternative to packages like taxize (Chamberlain and Szöcs 2013).

1 Unambiguously identifying species is a far more challenging task than it may appear. There are a vast
2 number of reasons for this. Different databases keep different taxonomic “backbones,” *i.e.* different data
3 structures in which names are mapped to species, and organised in a hierarchy. Not all names are unique
4 identifiers to groups. For example, *Io* can either refer to a genus of plants from the aster family, or to a
5 genus of molluscs; the genus *Mus* (of which the house mouse *Mus musculus* is a species), contains a
6 sub-genus *also* named *Mus* (within which *Mus musculus* is located). Conversely, the same species can
7 have several names, which are valid synonyms: for example, the domestic cow *Bos taurus* admits *Bos*
8 *primigenius taurus* as a valid synonym. In addition to binomial names, the same species can be known by
9 many vernacular (common) names, which are language or even region-specific: *Ovis aries*, for example,
10 has valid English vernaculars including lamb, sheep, wild sheep, and domestic sheep.

11 Finally, taxonomic nomenclature changes regularly, with groups being split, merged, or moved to a new
12 position in the tree of life; this is, notably, a common occurrence with viral taxonomy, each subsequent
13 version of which can differ markedly from the last; compare, *e.g.* Lefkowitz et al. (2018) to Walker et al.
14 (2020), where entire viral sub-trees were split, re-organized, and created within just two years. These
15 taxonomic changes have profound implications for the way we perceive biodiversity at global scales
16 (Meier 2009), to the point where taxonomic revisions should sometimes be actively conducted to improve
17 *e.g.* conservation outcomes (Melville et al. 2021).

18 To add to the complexity, one must also consider that most taxa names are at some point manually typed,
19 which has the potential to introduce additional mistakes in raw data; it is likely to expect that such
20 mistakes may arise when attempting to write down the (perfectly valid) names of the bacterial isolate
21 known as *Myxococcus llanfairpwllgwyngyllgogerychwyrndrobwlllantysiliogogochensis*, or of the crowned
22 slaty flycatcher *Griseotyrannus aurantioatrocristatus*. These mistakes are more likely when dealing with
23 hyper-diverse samples (demanding to memorize more names), like plant census (Dauncey et al. 2016,
24 Wagner 2016, Conti et al. 2021); when dealing with multiple investigators with different knowledge of the
25 taxonomy; and as a result of the estimated error in any data entry exercise, which other fields estimate at
26 up to about 5% (Barchard and Pace 2011).

27 All these considerations are actually important when matching species names both within and across
28 datasets. Let us consider the following species survey of individual fishes, European chub, *Cyprinus*
29 *cephalus*, *Leuciscus cephalus*, *Squalius cephalus*: all are the same species (*S. cephalus*), referred to as one of
30 the vernacular (European chub) and two formerly accepted names now classified as synonyms. A

31 cautious estimate of diversity based on the user-supplied names would give $n = 4$ species, when there is in
32 fact only one.

33 A package with the ability to handle the sources of errors outlined above, and especially while provide an
34 authoritative classification, can accelerate the work of consuming large volumes of biodiversity data. For
35 example, this package was used in the process of developing the *CLOVER* database (Gibb et al. 2021) of
36 host-virus associations, by reconciling the names of viruses and mammals from four different sources,
37 where all of the issues described above were present.

38 Overview of functionalities

39 An up-to-date version of the documentation for `NCBITaxonomy.jl` can be found online from the EcoJulia
40 documentation hub <https://docs.ecojulia.org/>, including examples and in-line documentation of every
41 method. The package is released under the MIT license. Contributions can be made in the form of issues
42 (bug reports, questions, features suggestions) and pull requests. The package can be checked out and
43 installed anonymously from the central Julia repository:

```
using Pkg

# This line should go in the Julia configuration file - note that the path
# will be created if it doesn't exist, and will be used to store the
# raw taxonomic table
ENV["NCBITAXONOMY_PATH"] = joinpath(homedir(), "data", "NCBITaxonomy.jl")

Pkg.add("NCBITaxonomy") # Downloading the files may take a long time
```

44 The package will download the most recent version of the NCBI taxonomy database, and transform in into
45 a set of Apache Arrow files ready for use. Note that the `NCBITAXONOMY_PATH` can specified on a per-project
46 basis, and as long as the package is not re-built, the local set of tables downloaded from NCBI will not
47 change; this way, users can re-run an analysis with a guarantee that the underlying taxonomic backbone
48 has not changed.

49 Improved name matching

50 Name finding is primarily done through the `taxon` function, which admits either a unique NCBI identifier
51 (e.g. `taxon(36219)` for the bogue *Boops boops*), a string (`taxon("Boops boops")`), or a data frame with a
52 restricted list of names (see the next section). The `taxon` method has additional arguments to perform
53 fuzzy matching in order to catch possible typos (`taxon("Boops bops"; strict=false)`), to perform a
54 lowercase search (useful when alphanumeric codes are part of the taxon name, like for some viruses), and
55 to restrict the the search to a specific taxonomic rank.

56 The lowercase search can be a preferable alternative to fuzzy string matching. Consider the string
57 Adeno-associated virus 3b - it has three names with equal distance (under the Levenstein string
58 distance function):

```
julia> similarnames("Adeno-associated virus 3b"; threshold=0.95)
3-element Vector{Pair{NCBITaxon, Float64}}:
  Adeno-associated virus - 3 (ncbi:46350) => 0.96
  Adeno-associated virus 3B (ncbi:68742) => 0.96
  Adeno-associated virus 3A (ncbi:1406223) => 0.96
```

59 Depending on the operating system, either of these three names can be returned; compare to the output of
60 a case insensitive name search:

```
julia> taxon("Adeno-associated virus 3b"; casesensitive=false)
Adeno-associated virus 3B (ncbi:68742)
```

61 This returns the correct name.

62 Name matching output and error handling

63 The `taxon` function will either return a `NCBITaxon` object (made of a name and id), or throw either a
64 `NameHasNoDirectMatch` (with instructions about how to possible solve it, using the `similarnames`
65 function), or a `NameHasMultipleMatches` (listing the possible valid matches, and suggesting to use
66 `alternativetaxa` to find the correct one). Therefore, the common way to work with the `taxon` function
67 would be to wrap it in a `try/catch` statement:

```

try
  taxon(name)

  # Additional operations with the matched name
catch err
  if isa(err, NameHasNoDirectMatch)
    # What to do if no match is found
  elseif isa(err, NameHasMultipleMatches)
    # What to do if there are multiple matches
  else
    # What to do in case of another error that is not NCBITaxonomy specific
  end
end

```

68 These functions will not demand any user input in the form of key presses (though they can be wrapped in
 69 additional code to allow it), as they are intended to run on clusters without supervision. The `taxon`
 70 function has good scaling using multiple threads. For convenience in rapidly getting a taxon for
 71 demonstration purposes, we also provide a string macro, whereby e.g. `ncbi"Procyon lotor"` will return
 72 the taxon object for the raccoon.

73 **Name filtering functions**

74 As the full NCBI names table has over 3 million entries at the time of writing, we have provided a number
 75 of functions to restrict the scope of names that are searched. These are driven by the NCBI *divisions*. For
 76 example `nf = mammalfilter(true)` will return a data frame containing the names of mammals, inclusive
 77 of rodents and primates, and can be used with e.g. `taxon(nf, "Pan")`. This has the dual advantage of
 78 making search faster, but also of avoiding matching on names that are shared by another taxonomic group
 79 (which is not an issue with *Pan*, but is an issue with e.g. *Io* as mentioned in the introduction).

80 Note that the use of a restricted list of names can have significant performance consequences: compare,
 81 for example, the time taken to return the taxon *Pan* (ID 9596) in the entire database, in all mammals, and
 82 in all primates:

Names list	Fuzzy matching	Time (ms)	Allocations	Memory allocated
all	no	23	34	2 KiB
	yes	105	2580	25 MiB
mammalfilter(true)	no	0.55	32	2 KiB
	yes	1.9	551	286 KiB
primatefilter()	no	0.15	33	2 KiB
	yes	0.3	92	27 KiB

Clearly, the optimal search strategy is to (i) rely on name filters to ensure that search are conducted within the appropriate NCBI division, and (ii) only rely on fuzzy matching when the strict or lowercase match fails to return a name, as fuzzy matching can result in order of magnitude more run time and memory footprint. These numbers were obtained on a single Intel i7-8665U CPU (@ (1.90GHz). Using "chimpanzees" as the search string (the NCBI recognized vernacular for *Pan*) gave qualitatively similar results, suggesting that there is no performance cost associated with working with synonyms or vernacular input data.

Quality of life functions

In order to facilitate working with names, we provide the `authority` function (gives the full taxonomic authority for a name), `synonyms` (to get alternative valid names), `vernacular` (for English common names), and `rank` (for the taxonomic rank).

Taxonomic lineages navigation

The `children` function will return all nodes that are directly descended from a taxon; the `descendants` function will recursively apply this function to all descendants of these nodes, until only terminal leaves are reached. The `parent` function is an "upwards" equivalent, giving that taxon from which a taxon descends; the `lineage` function chains calls to `parent` until either `taxon(1)` (the taxonomy root) or an arbitrary ancestor is reached.

The `taxonomicdistance` function (and its in-place equivalent, `taxonomicdistance!`, which uses

memory-efficient re-allocation if the user needs to change the distance between taxonomic ranks) uses the Shimatani (2001) approach to reconstruct a matrix of distances based on taxonomy, which can serve as a rough proxy when no phylogenies are available.

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References

- Barchard, K. and Pace, L. 2011. Preventing human error: The impact of data entry methods on data accuracy and statistical results. - *Computers in Human Behavior* 27: 1834–1839.
- Bezanson, J. et al. 2017. Julia: A Fresh Approach to Numerical Computing. - *SIAM Review* 59: 65–98.
- Chamberlain, S. A. and Szöcs, E. 2013. Taxize: Taxonomic search and retrieval in R. - *F1000Research* 2: 191.
- Conti, M. et al. 2021. Match Algorithms for Scientific Names in FlorItaly, the Portal to the Flora of Italy. - *Plants* 10: 974.
- Dauncey, E. A. et al. 2016. Common mistakes when using plant names and how to avoid them. - *European Journal of Integrative Medicine* 8: 597–601.
- Federhen, S. 2012. The NCBI taxonomy database. - *Nucleic acids research* 40: D136–D143.
- Gibb, R. et al. 2021. Data Proliferation, Reconciliation, and Synthesis in Viral Ecology. - *BioScience in press*.
- Lefkowitz, E. J. et al. 2018. Virus taxonomy: The database of the International Committee on Taxonomy of Viruses (ICTV). - *Nucleic Acids Research* 46: D708–D717.

126 Meier, R. 2009. Biodiversity Research Based on Taxonomic Revisions - A Tale of Unrealized Opportunities
127 -. - In: pp. 323–345.

128 Melville, J. et al. 2021. A return-on-investment approach for prioritization of rigorous taxonomic research
129 needed to inform responses to the biodiversity crisis. - PLOS Biology 19: e3001210.

130 Norman, K. E. A. et al. 2020. Taxadb: A high-performance local taxonomic database interface. - Methods
131 in Ecology and Evolution 11: 1153–1159.

132 Schoch, C. L. et al. 2020. NCBI Taxonomy: A comprehensive update on curation, resources and tools. -
133 Database in press.

134 Shimatani, K. 2001. On the Measurement of Species Diversity Incorporating Species Differences. - Oikos
135 93: 135–147.

136 Wagner, V. 2016. A review of software tools for spell-checking taxon names in vegetation databases. -
137 Journal of Vegetation Science 27: 1323–1327.

138 Walker, P. J. et al. 2020. Changes to virus taxonomy and the Statutes ratified by the International
139 Committee on Taxonomy of Viruses (2020). - Archives of Virology 165: 2737–2748.