taxize - taxonomic search and retrieval in R

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Abstract

All species are hierarchically related to one another, and we use taxonomic names to label the nodes in this hierarchy. Taxonomic data is becoming increasingly available on the web, but scientists need a way to access it in a programmatic fashion that's easy and reproducible. We have developed taxize, an open-source software package (freely available from http://cran.r-project.org/web/packages/taxize/index.html) for the R language. taxize provides simple, programmatic access to taxonomic data for 13 data sources around the web. We discuss the need for a taxonomic toolbelt in R, and outline a suite of use cases for which taxize is ideally suited (including a full workflow as an appendix). The taxize package facilitates open and reproducible science by allowing taxonomic data collection to be done in the open-source R platform.

Author Summary

Introduction

Evolution by natural selection has led to a hierarchical relationship among all living organisms. Thus, species are categorized using a taxonomic hierarchy, starting with the binomial species name (e.g, *Homo sapiens*), moving up to genus (*Homo*), then family (*Hominidae*), and on up to Domain (*Eukarya*). Biologists, whether studying organisms at the cell, organismal, or community level, can put their study taxa into taxonomic context, allowing them to know close and distant relatives, find relevant literature, and more.

The use of taxonomic names is, unfortunately, not straightforward. Taxonomic names often vary due to name changes at the generic or specific levels, lumping or splitting lower taxa (genera, species) among higher taxa (families), and name spelling changes. For example, a study found that a compilation of 308,000 plant observations from 51 digitized herbarium records had 22,100 unique taxon names, of which only 13,000 were accepted names [1,2]. In addition, there is no one authoritative taxonomic names source for all taxa - although, there are taxon specific sources that are used by many scientists. Different sources (e.g., uBio, Tropicos, ITIS) may use different accepted names for the same taxon. For example, while the Integrated Taxonomic Information Service (ITIS) has Helianthus x glaucus as an accepted name, The Plant List [3] has that name as unresolved. But Helianthus glaucus is an accepted name in The Plant List, while ITIS does not list this name.

One attempt to help inconsistencies in taxonomy is the use of numeric codes. For example, ITIS assigns a Taxonomic Serial Number (TSN) to each taxon, while the Universal Biological Indexer and Organizer (uBio) assigns each taxon a NameBank identifier (namebankID), and Tropicos assigns their own identifier to each taxon. Codes are helpful within a database as they can easily refer to, for example, Helianthus annuus with a code like 123456 instead of its whole name. However, each database uses their own code; in this case for Helianthus annuus, ITIS uses 36616, uBio uses 2658020, and Tropicos uses 40022652. Yet, there are no universal codes for taxa across databases, leading to additional confusion. Last, name comparisons across databases have to be done with the actual names, not the codes.

Taxonomic data is getting easier to obtain through the web (e.g., [4]). However, there are a number of good reasons to obtain taxonomic information programatically rather than through a web interface. First, if you have more than a few names to lookup on a website, it can take quite a long time to enter each name, get data, and repeat for each species. Programatically getting taxonomic names solves the problem by looping over a list of names. In addition, doing taxonomic searching, etc. becomes reproducible. With increasing reports of irreproducibility in science [5,6], it is extremely important to make science workflows repeatable. Science workflows can now easily incorporate text, code, and images in a single executable document [7].

The R language is a widely used language by biologists, and now has over 4,000 packages on the Comprehensive R Archive Network (CRAN) and more than 2,500 packages on other repositories to extend R. R is great for manipulating, visualizing and fitting statistical models to data. [8] gives a detailed discussion of advantages of R in computational biology. Getting data from the web will be increasingly common as more and more data gets moved to the cloud. Therefore there is a need to get data from the web directly into R. Increasingly, data is available from the web via application programming interfaces (API). These allow computers to talk to one another using code that is not human readable, but is machine readable. Web APIs often define a number of methods that allow users to search for a species name, or retrieve the synonyms for a species name, for example. A further advantage of APIs is that they are language agnostic, meaning that data can be consumed in almost any computing context, allowing users to interact with the web API without having to know the details of the code. Moreover data can be accessed from every computer, whereas for example an Excel file can only be opened in a few programs.

The goal of taxize, an R package in development, is to make many use cases having to do with retrieving and resolving taxonomic names easy and reproducible. In taxize, we have written a suite of R functions that interact with many taxonomic data sources via their web APIs (Table 1). The interface to each function is usually a simple list of species names, just as a user would do with a web API. Therefore, we hope moving from a web to R interface for taxonomic names will be relatively seamless (if one is already nominally familiar with R).

Here, we justify the need for taxize, discuss our data sources, and run through a suite of use cases to demonstrate the variety of ways that users can interact with taxize.

Why we need taxize?

There are a large suite of applications developed around the problem of searching for, resolving, and getting higher taxonomy for species names. For example, Linnaeus [9] provides the ability to search for taxonomic names in documents and normalize those names found. In addition, there are many web interfaces to search for and normalize names such as Encyclopedia of Life's Global Names Resolver [10], uBio tools [11], and iPlant's Taxonomic Name Resolution Service [12].

All of these data repositories provide ways to search for taxonomic names and resolve them in some cases. However, scientists ideally need a tool that can be used programmatically, and thereby facilitate reproducible research. The goal of taxize is to make it easy to create reproducible and easy to use workflows for searching for taxonomic names, resolving them, getting higher taxonomic names, and other tasks related to research dealing with species.

Data sources and package details

taxize uses many data sources (Table 1), and more can easily be added. There are two common tasks provided by the data sources: name search and name resolution. Other functionality in taxize includes retrieving a classification tree for a species, or retrieving child taxa of a focal taxon. One of the data sources (Phylomatic) returns phylogenies, while another (NCBI) returns genetic sequence data. However,

there are other R packages that are focused solely on sequence data, such as rsnps [13], rentrez [14], BoSSA [15], and ape [16], so taxize will not venture deeply into these other domains.

Some of the data sources taxize interacts with require authentication. That is, in addition to the search terms the user provides (e.g., *Homo sapiens*), the data provider requires an alphanumeric identification key so that they can better manage their servers, collect analytics, and shut down users that abuse the API. The services that do require an API key in taxize are: Encyclopedia of Life (EOL) [4], the Universal Biological Indexer and Organizer (uBio) [11], Tropicos [17], and Plantminer [18]. One can easily obtain API keys by visiting the website of each service (see Table 1 for links to each site). There are two typical ways of using API keys. First, you can pass in your API key in a function call (e.g., ubio_namebank(srchName='Ursus americanus', key='your_alphanumeric_key')). Second, you can store your key in the .Rprofile file, which is a common place to store settings. We recommend the second option as it simplifies function calls as taxize detects the stored keys.

One available data source in taxize is The Plant List [3]. The connection in taxize is done via the taxonstand package [19] that solely interacts with that The Plant List. We provide a few convenience functions that wrap taxonstand into taxize.

taxize would not have been possible without the work of others. taxize uses httr [20] and RCurl [21] for doing calls to web APIs, XML [22] for parsing XML, RJSONIO [23] for parsing JSON, and stringr [?] and plyr [24] for manipulating data.

New data sources can be added; we plan to add the following sources: Wikispecies and The Tree of Life. A connection to freshwaterecology.info [25] (a database with autecological characteristics, ecological preferences and biological traits as well as distribution patterns of more than 12.000 European freshwater organisms belonging to fish, macro-invertebrates, macrophytes, diatoms and phytoplankton) will be finished when their new API will be released. In addition, the authors may be contacted for further suggestions of data sources to be added.

Use cases

There are a variety of use cases for which taxize is ideally suited. We discuss here several ideal use cases for taxize. Moreover a complete reproducible workflow from a species list to a phylogeny and a distribution map can be found in the supplement.

First, install taxize

First, one must install and load taxize into the R session.

```
install.packages("taxize")
library(taxize)
```

Advanced users can also download and install the latest development copy from GitHub [26].

Resolve taxonomic names

This is a common task in biology. We often have a list of species names and we want to know a) if we have the most up to date names, b) if our names are spelled correctly, and c) the scientific name for a common name. One way to resolve names is via the Global Names Resolver (GNR) service provided by the Encyclopedia of Life [10]. Here, we are searching for two misspelled names:

```
temp <- gnr_resolve(names = c("Helianthos annus", "Homo saapiens"), returndf = TRUE)
temp[, -c(1, 4)]</pre>
```

The correct spellings are *Helianthus annuus* and *Homo sapiens*. Another approach uses the Taxonomic Name Resolution Service via the Taxosaurus API [27] developed by iPLant and the Phylotastic organization. In this example, we provide a list of species names, some of which are misspelled, and we'll call the API with the *tnrs* function.

```
mynames <- c("Helianthus annuus", "Pinus contort", "Poa anua", "Abis magnifica",
    "Rosa california", "Festuca arundinace", "Sorbus occidentalos", "Madia sateva")
tnrs(query = mynames)[, -c(5:7)]
        submittedName
                            acceptedName
                                             sourceId score
7
    Helianthus annuus
                       Helianthus annuus iPlant_TNRS
                                                      1.00
4
       Pinus contort
                          Pinus contorta iPlant_TNRS 0.98
5
             Poa anua
                                Poa annua iPlant_TNRS
                                                       0.96
3
       Abis magnifica
                         Abies magnifica iPlant_TNRS
8
      Rosa california
                         Rosa californica iPlant_TNRS
                                                       0.99
  Festuca arundinace Festuca arundinacea iPlant_TNRS
1 Sorbus occidentalos Sorbus occidentalis iPlant_TNRS
                                                       0.99
                             Madia sativa iPlant_TNRS
         Madia sateva
```

It turns out there are a few corrections: e.g., *Madia sateva* should be *Madia sativa*, and *Rosa california* should be *Rosa californica*. Note that this search worked because fuzzy matching was employed to retrieve names that were close, but not exact matches. Fuzzy matching is only available for plants in the TNRS service, so we advise using EOL's Global Names Resolver if you need to resolve animal names.

taxize takes the approach that the user should be able to make decisions about what resource to trust, rather than making the decision. Both the EOL GNR and the TNRS services provide data from a variety of data sources. The user may trust a specific data source, thus may want to use the names from that data source. In the future, we may provide the ability for taxize to suggest the best match from a variety of sources.

Retrieve higher taxonomic names

Another task biologists often face is getting higher taxonomic names for a taxa list. Having the higher taxonomy allows you to put into context the relationships of your species list. For example, you may find out that species A and species B are in Family C, which may lead to some interesting insight, as opposed to not knowing that Species A and B are closely related. This also makes it easy to aggregate/standardize data to a specific taxonomic level (e.g., family level) or to match data to other databases with different taxonomic resolution (e.g., trait databases).

A number of data sources in taxize provide the capability to retrieve higher taxonomic names, but we will highlight two of the more useful ones: Integrated Taxonomic Information System (ITIS) [28] and National Center for Biotechnology Information (NCBI) [29]. First, we'll search for two species, *Abies procera* and *Pinus contorta* within ITIS.

```
Division
                     Tracheophyta 846496
5
     Subdivision Spermatophytina 846504
6
   Infradivision
                     Gymnospermae 846506
7
                        Pinopsida 500009
           Class
8
           Order
                          Pinales 500028
9
          Family
                         Pinaceae 18030
10
           Genus
                            Abies 18031
11
         Species
                    Abies procera 181835
$`Pinus contorta`
        rankName
                        taxonName
                                     tsn
1
         Kingdom
                          Plantae 202422
2
      Subkingdom
                  Viridaeplantae 846492
3
    Infrakingdom
                     Streptophyta 846494
4
        Division
                     Tracheophyta 846496
5
     Subdivision Spermatophytina 846504
6
   Infradivision
                     Gymnospermae 846506
7
                        Pinopsida 500009
           Class
8
           Order
                          Pinales 500028
9
          Family
                         Pinaceae
                                  18030
10
                            Pinus
                                   18035
           Genus
11
         Species
                  Pinus contorta 183327
```

It turns out both species are in the family Pinaceae. You can also get this type of information from the NCBI by doing classification(specieslist, db = 'ncbi').

Instead of a full classification, you may only want a single name, say a family name for your species of interest. The function tax_name is built just for this purpose. As with the classification-function you can specify the data source with the db argument, either ITIS or NCBI.

```
tax_name(query = "Helianthus annuus", get = "family", db = "itis")
    family
1 Asteraceae
tax_name(query = "Helianthus annuus", get = "family", db = "ncbi")
    family
1 Asteraceae
```

I may happen that a data source does not provide information on the querried species, than one could take the result from another source and union the results from the different sources.

Interactive name selection

As mentioned most databases use a numeric code to reference a species. A general workflow in taxize is: Retrieve Code for the queried species and then use this code to query more data/information. Below are a few examples. When you run these examples in R, you are presented with a command prompt asking for the row that contains the name you would like back; that output is not printed below for brevity. In this example, the search term has many matches. The function returns a data frame of the matches, and asks for the user to input what row number to accept.

```
get_tsn(searchterm = "Heliastes", searchtype = "sciname")
           combinedname
                           tsn
1
     Heliastes bicolor 615238
2
  Heliastes chrysurus 615250
3
    Heliastes cinctus 615573
4 Heliastes dimidiatus 615257
5 Heliastes hypsilepis 615273
6 Heliastes immaculatus 615639
7 Heliastes opercularis 615300
8
       Heliastes ovalis 615301
1
NA
attr(,"class")
[1] "tsn"
```

In another example, you can pass in a long list of taxonomic names:

In another example, note that no match at all returns an NA:

```
get_uid(sciname = c("Chironomus riparius", "aaa vva"))
[1] "315576" NA
attr(,"class")
[1] "uid"
```

Retrieve a phylogeny

Ecologists are increasingly taking a phylogenetic approach to ecology, applying phylogenies to topics such as the study of community structure [30], ecological networks [31], functional trait ecology [32]. Yet, Many biologists are not adequately trained in reconstructing phylogenies. Fortunately, there are some sources for getting a phylogeny without having to know how to build one; one of these is for angiosperms, called Phylomatic [33]. We have created a workflow in taxize that accepts a species list, and taxize works behind the scenes to get higher taxonomic names, which are required by Phylomatic to get a phylogeny. Here is a short example, producing the tree in figure 1.

```
taxa <- c("Poa annua", "Abies procera", "Helianthus annuus")
tree <- phylomatic_tree(taxa = taxa)
tree$tip.label <- capwords(tree$tip.label)
plot(tree, cex = 1)</pre>
```

Behind the scenes the function *phylomatic_tree* retrieves a Taxonomic Serial Number (TSN) from ITIS for each species name, then a string is created for each species like this *poaceae/oryza/oryza_sativa* (with format 'family/genus/genus_epithet'). These strings are submitted to the Phylomatic API, and if no errors occur, a phylogeny in newick format is returned. The *phylomatic_tree()* function also cleans up the newick string and converts it to an **ape** *phylo* object. The output from *phylomatic_tree()* is a *phylo* object, which can be used for plotting and phylogenetic analyses. Be aware that Phylomatic has certain limitations - refer to the paper describing Phylomatic [33] and the website http://phylodiversity.net/phylomatic/.

There are currently no resources for getting a phylogeny of animals simply from species names. However, a few projects are working on this problem, including the Open Tree of Life [34]. We will incorporate these resources when the appropriate APIs are available.

What taxa are the children of my taxon of interest?

If someone is not a taxonomic specialist on a particular taxon he likely does not know what children taxa are within a family, or within a genus. This task becomes especially unwieldy when there are a large number of taxa downstream. You can of course go to a website like Wikispecies [35] or Encyclopedia of Life [4] to get downstream names. However, taxize provides an easy way to programatically search for downstream taxa, both for the Catalogue of Life (CoL) [36] and the Integrated Taxonomic Information System [28]. Here is a short example using the CoL in which we want to find all the species within the genus *Apis* (honey bees).

```
col_downstream(name = "Apis", downto = "Species")[[1]]
                    childtaxa_name childtaxa_rank
  childtaxa_id
1
       6971712 Apis andreniformis
                                           Species
2
       6971713
                       Apis cerana
                                           Species
3
       6971714
                      Apis dorsata
                                           Species
4
       6971715
                       Apis florea
                                           Species
5
       6971716 Apis koschevnikovi
                                           Species
6
       6845885
                    Apis mellifera
                                           Species
7
       6971717
                  Apis nigrocincta
                                           Species
```

The result from the above call to $col_downstream()$ is a data.frame that gives a number of columns of different information.

IUCN Status

There are a number of things we can do once we have the correct taxonomic names. One thing we can do is ask about the conservation status of a species (IUCN Red List of Threatened Species [37]). We have provided a set of functions, *iucn_summary* and *iucn_status*, to search for species names, and extract the status information, respectively. Here, we search for the Panther and Lynx.

It turns out that the panther has a status of endangered (EN) and the lynx has a status of least concern (LC).

Search for available genes in GenBank

Another use case available in taxize deals with genetic sequences. taxize has three functions to interact with GenBank to search for available genes (get_genes_avail), download genes by GenBank ID (get_genes), and download genes via taxonomic name search, including retrieving a congeneric if the searched taxon does not exist in the database (get_segs). In this example, we search for gene sequences for $Umbra\ limi$.

```
out <- get_genes_avail(taxon_name = "Umbra limi", seqrange = "1:2000", getrelated = FALSE)
```

Then we can ask if 'RAG1' exists in any of the gene names.

```
out[grep("RAG1", out$genesavail, ignore.case = TRUE), ]
        spused length
413 Umbra limi
427 Umbra limi
                  959
434 Umbra limi
                 1631
                                                                              genesavail
413 isolate UlimA recombinase activating protein 1 (rag1) gene, exon 3 and partial cds
427
              recombination-activating protein 1 (RAG1) gene, intron 2 and partial cds
434
                           recombination-activating protein 1 (RAG1) gene, partial cds
   access_num
                     ids
413
      JX190826 394772608
427
      AY459526 45479841
434
      AY380548 38858304
```

It turns out that there are XX different unique records found. However, this doesn't mean that there are XX different genes found as the API does not provide metadata to classify genes. However, at the end of the example, we showed that you can use regular expressions (e.g., via *grep*) to search for the gene of interest.

Matching species tables with different taxonomic resolution

Biologist often need to match different sets of data tied to species. For example, trait-based approaches are a promising tool in ecology [38]. One problem is that abundance data must be matched with trait databases like [39]. These two data tables may contain species information on different taxonomic levels and possibly data must be aggregated to a joint taxomic level, so that the data can be merged. taxize can help in this data-cleaning step, providing a reproducible workflow:

We can use the mentioned *classification*-function to retrieve the taxonomic hierarchy and then search the hierarchies up- and downwards for matches. Here is an example to match a species with names on three different taxonomic levels.

```
A <- "gammarus roeseli"

B1 <- "gammarus roeseli"

B2 <- "gammarus"

B3 <- "gammaridae"

A_clas <- classification(A, db = 'ncbi')

B1_clas <- classification(B1, db = 'ncbi')
```

```
B2_clas <- classification(B2, db = 'ncbi')
B3_clas <- classification(B3, db = 'ncbi')

B1[match(A, B1)]
[1] "gammarus roeseli"
A_clas[[1]]$Rank[tolower(A_clas[[1]]$ScientificName) %in% B2]
[1] "genus"
A_clas[[1]]$Rank[tolower(A_clas[[1]]$ScientificName) %in% B3]
[1] "family"</pre>
```

If we find a direct match (here *Gammarus roeseli*), we are lucky. But we can also match Gammaridae with *Gammarus roeseli*, but on a lower taxonomic level. A more comprehensive and realistic example (matching a trait table with an abundance table) is given in Appendix B.

Aggregating data to a specific taxonomic rank

In biology, one can asks questions at varying taxonomic levels. One may perform analyses on different taxonomic levels. This use case is easily handled in taxize. A function called $tax_{-}agg$ will aggregate community data to a specific taxonomic level. In this example, we take data of 5 species and aggregate them to family level. Again we can specify if we want to use data from ITIS or NCBI.

```
data(dune, package = 'vegan')
df <- dune[ , 1:5]</pre>
colnames(df) <- c("Bellis perennis", "Empetrum nigrum", "Juncus bufonius",</pre>
                  "Juncus articulatus", "xxx")
head(df)
   Bellis perennis Empetrum nigrum Juncus bufonius Juncus articulatus xxx
2
                                  0
                                                   0
                                                                          0
                 0
                                  0
                                                   3
                                                                       0
                                                                          0
13
                 2
                                                  0
4
                                  0
                                                                       0 0
16
                 0
                                  0
                                                  0
                                                                       3 0
6
                 0
                                  0
                                                   0
                                                                      0 0
1
                                                   0
agg <- tax_agg(df, rank = 'family', db = 'ncbi')</pre>
agg
Aggregated community data
Level of Aggregation: FAMILY
No. taxa before aggregation: 5
No. taxa after aggregation: 4
No. taxa not found: 1
```

he	ad(agg\$x)			
	Asteraceae	Ericaceae	Juncaceae	XXX
2	3	0	0	0
13	0	0	3	0
4	2	0	0	0
16	0	0	3	0
6	0	0	0	0
1	0	0	0	0

We see that the two Juncus species are aggregated to Juncaceae and their abundances are summed up. If a taxon is one lower taxonomic resolution then the querried or the taxon is not found in the database (like in the example taxon xxx) then these are not aggregated and returned as is.

Conclusions

Taxonomic information is increasingly sought out by biologists as we take phylogenetic and taxonomic approaches to science. Taxonomic data is becoming more widely available on the web, yet scientists require programmatic access to this data for developing reproducible workflows. taxize was created to bridge this gap - to bring taxonomic data on the web into R, where the data can be easily manipulated, visualized, and analyzed in a reproducible workflow.

We have outlined a suite of use cases in taxize that will likely fit real use cases of many biologists. Of course we have not thought of all possible use cases, so we hope that the biology community can give us feedback on what use cases they want to see available in taxize. One thing we could change in the future is to make functions that fit use cases, and then allow users to select the data source as a parameter in the function. This could possibly make the user interface easier to understand.

taxize is currently under development and will be for some time given the large number of data sources kitted together in the package, and the fact that APIs for each data source can change, requiring changes in taxize code. Contributions to taxize are strongly encouraged, and can be easily done using GitHub here [26]. We hope taxize will be taking up by the community and developed collaboratively, making it progressively better through time as new use cases arise, bug reports squashed, and contributions merged.

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Figure Legends

Figure 1. A Phylogeny for the three species.

Tables

Table 1. Some key functions in taxize, what they do, and their data sources

Function name	What it does	Source
apg_lookup	Changes names to match the	Angiosperm Phylogeny
apg_100kup	APGIII list	Group [40]
classification	Upstream classification	Various
col_children	Direct children	Catalogue of Life [36]
$col_downstream$	Downstream taxa to specified rank	Catalogue of Life [36]
eol_hierarchy	Upstream classification	Encyclopedia of Life [4]
eol_search	Search EOL taxon information	Encyclopedia of Life [4]
get_seqs	Get NCBI sequences	National Center for Biotechnology Information [29]
get_tsn	Get ITIS TSN	Integrated Taxonomic Information System [28]
$\operatorname{get_uid}$	Get NCBI UID	National Center for Biotechnology Information [29]
searchbycommonname	Search ITIS by common name	Integrated Taxonomic Information System [28]
searchbyscientificname	Search ITIS by scientific name	Integrated Taxonomic Information System [28]
gisd_isinvasive	Inasiveness status	Global Invasive Species Database [41]
gni_parse	Parse scientific names into components	Global Names Index [4,42]
gni_search	Search EOL's global names index	Global Names Index [4,42]
gnr_resolve	Resolve names using EOL's global names index	Global Names Resolver [4, 10]
$itis_downstream$	Downstream taxa to specified rank	Integrated Taxonomic Information System [28]
iucn_status	IUCN status	IUCN Red List [37]
$phylomatic_tree$	Get a plant Phylogeny	Phylomatic [33]
plantminer	Search Plantminer	Plantminer [18]
tax_name	Get taxonomic name for specific rank	Various
tax_rank	Get rank of a taxonomic name	Various
tnrs	Resolve names using iPlant	iPlant Taxonomic Name Resolution Service [12]
$tp_acceptednames$	Check for accepted names using Tropicos	Tropicos [17]
tpl_search	Search the Plant List	The Plant List [3]
ubio_namebank	Search uBio	uBio [11]