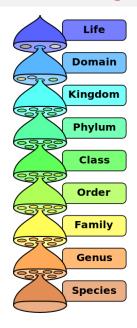
Taxa and metacoder: R packages for parsing, visualization, and manipulation of taxonomic data

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The challenges of taxonomic data



- Taxonomic data is hierarchical
- Associated with tabular data
- Can be names, classifications, or IDs
- Many different taxonomic systems
- Many different data formats
- Hierarchical visualization is difficult

Sources of taxonomic data

DNA sequence databases







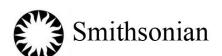
Species occurrence databases







Museum records







Sources of taxonomic data: DNA sequences

NCBI Genbank

>ACO73210.8 Homo sapiens BAC clone RP11-460N20 from 7, complete sequence AACGAACGCTGGCGGCATGCCTAACACATGCAAGTCGAACGAGACCTTCGGGTC...

UNITE

>SH099456.05FU_FJ357315_refs k__Fungi;p__Ascomycota;c__Dothideomycetes;o__Pleosporales;f__Pleosporaceae;g__Embellisia;s__Embellisia_planifunda
GCTGGCGGCGTGCCTAACACATGTAAGTCGAACGGGACTGGGGGCAACTCCAGT...

RDP

>S000448483 Sparassis crispa; MBUH-PIRJO&ILKKA94-1587/ss5 Lineage=Root;rootrank; Fungi;domain;Basidiomycota;phylum;Agaricomycetes; class;Polyporales;order;Sparassidaceae;family;Sparassis;genus AGAGTTTGATCCTGGCTCAGATTGAACGCTGGCGGAATGCTTAACACATGAAAC...

SILVA

>GCVF01000431.1.2369 Bacteria; Proteobacteria; Gammaproteobacteria; Oceanospirillales; Alcanivoraceae; Alcanivorax; Thalassiosira rotula AGAGTTTGATCCTGGCTCAGGATGAACGCTGGCGGTATGCTTAACACATGCAAG...

Sources of taxonomic data: Occurrence records

Global Biodiversity Information Facility: Archaea database

```
readr::read_tsv("datasets/gbif_archea.csv")[4:8]
```

```
# A tibble: 19,013 x 5
   kingdom phylum
                         class
                                      order
                                                        family
   <chr>
          <chr>
                         <chr>
                                                        <chr>>
                                      <chr>>
 1 Archaea Euryarchaeota Halobacteria Halobacteriales
                                                        Halobacteriaceae
 2 Archaea Euryarchaeota Thermococci Thermococcales
                                                        Thermococcaceae
 3 Archaea Euryarchaeota Thermococci Thermococcales
                                                        Thermococcaceae
 4 Archaea Crenarchaeota Thermoprotei Desulfurococcales Desulfurococcaceae
 5 Archaea Crenarchaeota Thermoprotei Desulfurococcales Pyrodictiaceae
 6 Archaea Crenarchaeota Thermoprotei Thermoproteales
                                                        Thermoproteaceae
 7 Archaea Euryarchaeota Thermococci Thermococcales
                                                        Thermococcaceae
 8 Archaea Euryarchaeota Thermococci Thermococcales
                                                        Thermococcaceae
 9 Archaea Euryarchaeota Halobacteria Halobacteriales
                                                        Halobacteriaceae
10 Archaea Euryarchaeota Halobacteria Halobacteriales
                                                        Halobacteriaceae
# ... with 19,003 more rows
```

Sources of taxonomic data: Museum records

Smithsonian Museum of Natural History: Mammal database

```
readr::read_csv("datasets/SNMNH.csv")[9]
# A tibble: 5.000 x 1
   `Name Hierarchv`
   <chr>>
 1 Abditomys latidens : Muridae : Rodentia : Mammalia : Chordata
 2 Abrawayaomys ruschii : Cricetidae : Rodentia : Mammalia : Chordata
 3 Abrawayaomys ruschii : Cricetidae : Rodentia : Mammalia : Chordata
 4 Abrocoma bennettii bennettii : Abrocomidae : Rodentia : Mammalia : Chordata
 5 Abrocoma bennettii bennettii : Abrocomidae : Rodentia : Mammalia : Chordata
 6 Abrocoma bennettii bennettii : Abrocomidae : Rodentia : Mammalia : Chordata
 7 Abrocoma bennettii bennettii : Abrocomidae : Rodentia : Mammalia : Chordata
 8 Abrocoma bennettii bennettii : Abrocomidae : Rodentia : Mammalia : Chordata
 9 Abrocoma bennettii bennettii : Abrocomidae : Rodentia : Mammalia : Chordata
10 Abrocoma bennettii bennettii : Abrocomidae : Rodentia : Mammalia : Chordata
# ... with 4,990 more rows
```

The taxa package

```
build passing codecov 87% repo status WIP downloads 311/month CRAN 0.2.1
```

The taxa package is designed to be a solid foundation for using taxonomic data in R.

- ▶ R6 classes to hold taxa, taxonomies, and associated data
- Flexible parsers to convert raw data to these classes
- Dplyr-inspired functions to manipulate these classes
- Functions to get data associated with each taxon in a taxonomy

The metacoder package: visualization of taxon data

```
readr::read tsv("datasets/gbif archea.csv") %>%
   parse_tax_data(class_cols = 4:8) %>%
   filter taxa(taxon names != "") %>%
   heat tree(node label = taxon names, node color = n obs,
                    node_size = n_obs, layout = "da")
                                                                                    Acidilobaceae
                                                                         Fervidicoccaceae
                        Halobacteriaceae
                                                                                             Thermofilaceae
                                                                             Thermoprotei
                                                                                          Thermoproteales
                                           Methanobacteriaceae
                           Halohacteriales
                                     Halorubraceae
                                                              Crenarchaeota<sub>Desulfurococcales</sub>
                                             Methanohacteriales
                           Haloarculaceae
                               Halobacteria
                                                                                 Desulfurococcaceae
                                                                           Pyrodictiaces
                                                    Archaea
                                        la loferacaceae
                             Natrialbaceae
                                           Methannhacte
                         Thermococcaceae Thermococci
                                                  Methanomassiliicoccaceae
                                        Eurvarchaeota Cuniculiplasmatacea
                                                                                                                Nodes
                  Methanocellales
                                                     Thermoplasmata
       Methanosarcinales
                                                                    Thermoplasmataceae
                   Methanomicrobia
                                                                                                           567
                                                             Thermoplasmatales
    Methermicoccaceae
                                          Methanococci
                                                                                                          2170
   Methanomicrobi
                                                                                                          4820
             lethanomicrobiales
```

Methanococcales

Methanococcaceae Methanocaldococcaceae

Methanocorpusculaceae

Methanospirillaceae

8510

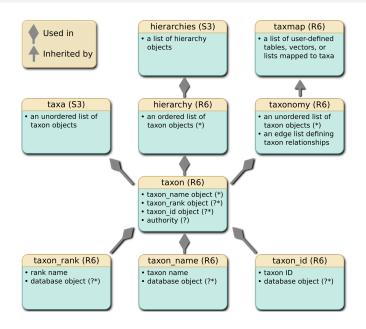
13200

19000

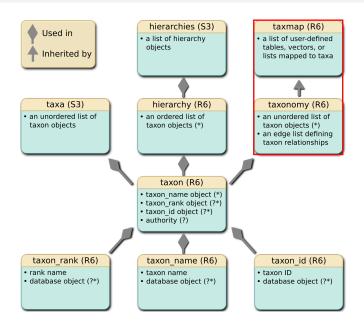
Classes defined by taxa

Classes defined by 'taxa'

Classes defined by taxa: Relationships



Classes defined by taxa: Relationships



Classes defined by taxa: The taxmap class

```
> ex_taxmap
<Taxmap>
 17 taxa: b. Mammalia, c. Plantae, d. Felidae ... p. sapiens, q. lycopersicum, r. tuberosum
 17 edges: NA->b, NA->c, b->d, b->e, b->f, c->a, d->h ... h->m, i->n, i->o, k->p, l->a, l->r
 4 data sets:
   info:
     # A tibble: 6 x 4
       taxon id name n_legs dangerous
      <chr> <chr> <dbl> <lql>
     1 m tiger 4. TRUE
     2 n cat 4. FALSE
     3 o mole 4. FALSE
     # ... with 3 more rows
   phylopic_ids: a named vector of 'character' with 6 items
      m. e148eabb-f138-43c6-b1e4-5cda2180485a ... г. 63604565-0406-460b-8cb8-1abe954b3f3a
   foods: a list of 6 items named by taxa:
      M. N. O. D. G. F
   abund:
     # A tibble: 8 x 5
       taxon id code sample id count taxon index
      <chr> <fct> <fct> <fct> <dbl>
                                          <int>
     1 m
                     Α
                                              1
                                 1.
     2 n
                     Α
                                 2.
     3 0
                                 5.
     # ... with 5 more rows
```

Parsing

Parsing

Parsing

Input data format

		Simple	Embedded	Raw string
		> print(data) [1] "input_1" "input_2" [3] "input_3"	> print(data) x	<pre>> print(data) [1] ">id:a-tax:input_1" [2] ">id:b-tax:input_2" [3] ">id:c-tax:input_3"</pre>
)) (, , , ,)	Classification Primates;Hominidae;Homo;sapiens	<pre>> print(data) [1] "Primates;Hominidae;Hom [2] "Primates;Haplorhini;Cr > parse_tax_data(data,</pre>	<pre>> print(data) x</pre>	<pre>> print(data) [1] ">id:a-tax:Primates;Hom" [2] ">id:b-tax:Primates;Hap" > extract_tax_data(data, regex = ">id:(.+)-tax:(.+)", key = c("info", "class"), class_sep = ";")</pre>
	Taxon ID	<pre>> print(data) [1] "9606" "100937" > lookup_tax_data(data,</pre>	<pre>> print(data)</pre>	> print(data) [1] ">id:a-tax:9686" [2] ">id:b-tax:100937" > extract_tax_data(data,
	Taxon name	<pre>> print(data) [1] "Homo sapiens" [2] "Primates" > lookup_tax_data(data,</pre>	> print(data) x name y 1 a Homo sapiens 100 2 b Primates 200 > lookup_tax_data(data, type = "taxon_name", column = "name")	<pre>> print(data) [1] ">id:a-tax:Homo sapiens" [2] ">id:b-tax:Primates" > extract_tax_data(data, regex = ">id:(.+)-tax:(.+)", key = c("info", "taxon_name"), database = "ncbi")</pre>
	Sequence ID AC073210	<pre>> print(data) [1] "AC073210" "KC312885" > lookup_tax_data(data, type = "seq_id")</pre>	> print(data) x ncbi_id y 1 a Ac073210 100 2 b KC312885 200 > lookup_tax_data(data, type = "seq_id", column = "ncbi_id")	> print(data) [1] ">id:a-tax:AC073210" [2] ">id:b-tax:KC312885" > extract_tax_data(data,

Parsing: vectors of classifications

Parsing: vectors of names

```
x <- c("Homo sapiens", "Macropus", "Chordata")
lookup_tax_data(x, type = "taxon_name", database = "ncbi")
<Taxmap>
 35 taxa: 131567. cellular organisms ... 9606. Homo sapiens
 35 edges: NA->131567, 131567->2759 ... 207598->9605, 9605->9606
 2 data sets:
   tax data:
     # A tibble: 35 \times 4
       taxon id ncbi name ncbi rank ncbi id
       <chr> <chr>
                                <chr>
                                           <chr>
     1 131567 cellular organisms no rank 131567
     2 2759 Eukaryota superkingdom 2759
     3 33154 Opisthokonta no rank 33154
     # ... with 32 more rows
   query data: a named vector of 'character' with 3 items
      9606. Homo sapiens, 9312. Macropus, 7711. Chordata
 0 functions:
```

Parsing: vectors of taxon or sequence IDs

Taxon IDs

```
x <- c("9606", "207598", "7711") # NCBI taxon IDs
lookup_tax_data(x, type = "taxon_id", database = "ncbi")</pre>
```

Sequence IDs

```
x <- c("AC073210", "MG014608", "AE006468") # NCBI sequence IDs
lookup_tax_data(x, type = "seq_id", database = "ncbi")</pre>
```

Parsing: tables

Global Biodiversity Information Facility: Archaea database

```
readr::read_tsv("datasets/gbif_archea.csv")[4:8]
```

```
# A tibble: 19,013 x 5
   kingdom phylum
                         class
                                      order
                                                        family
   <chr> <chr>
                         <chr>
                                                        <chr>>
                                      <chr>>
 1 Archaea Euryarchaeota Halobacteria Halobacteriales
                                                        Halobacteriaceae
 2 Archaea Euryarchaeota Thermococci Thermococcales
                                                        Thermococcaceae
 3 Archaea Euryarchaeota Thermococci Thermococcales
                                                        Thermococcaceae
 4 Archaea Crenarchaeota Thermoprotei Desulfurococcales Desulfurococcaceae
 5 Archaea Crenarchaeota Thermoprotei Desulfurococcales Pyrodictiaceae
 6 Archaea Crenarchaeota Thermoprotei Thermoproteales
                                                        Thermoproteaceae
 7 Archaea Euryarchaeota Thermococci Thermococcales
                                                        Thermococcaceae
 8 Archaea Euryarchaeota Thermococci Thermococcales
                                                        Thermococcaceae
 9 Archaea Euryarchaeota Halobacteria Halobacteriales
                                                        Halobacteriaceae
10 Archaea Euryarchaeota Halobacteria Halobacteriales
                                                        Halobacteriaceae
# ... with 19,003 more rows
```

Parsing: tables

```
x = readr::read tsv("datasets/gbif archea.csv")
parse_tax_data(x, class_cols = 4:8)
<Taxmap>
 95 taxa: ab. Archaea, ac. Euryarchaeota ... dr. Methermicoccaceae
 95 edges: NA->ab, ab->ac, ab->ad ... aw->dp, at->dq, ax->dr
 1 data sets:
   tax data:
     # A tibble: 19,013 x 45
       taxon id gbifid datasetkey occurrenceid kingdom phylum class
       1 br 1.84e9 3c6e7390-~ D7C42A39-3A~ Archaea Eurya~ Halo~
     2 bs 1.83e9 863efcc4-~ <NA> Archaea Eurya~ Ther~
     3 bs 1.83e9 863efcc4-~ <NA>
                                           Archaea Eurva~ Ther~
     # ... with 1.901e+04 more rows, and 38 more variables:
        order <chr>, family <chr>, genus <chr>, species <chr>,
        infraspecificepithet <lp>lgl>, taxonrank <chr>,
         scientificname <chr>, countrycode <chr>, locality <chr>,
        publishingorgkey <chr>, ...
 0 functions:
```

Parsing: complex strings (NCBI Genbank)

```
x = c("ACO73210.8 Homo sapiens BAC clone RP11-460N20 from 7, complete sequence"
     "AE006468.2 Salmonella enterica subsp. enterica serovar Typhimurium",
     "MG014608.1 Macropus fuliginosus Csf1r gene, enhancer")
extract_tax_data(x, database = "ncbi", regex = "([A-Z0-9.]+) (.+)",
               key = c(my ncbi id = "seq id", my desc = "info"))
<Taxmap>
 46 taxa: 131567. cellular organisms ... 9606. Homo sapiens
 46 edges: NA->131567, 131567->2759 ... 207598->9605, 9605->9606
 2 data sets:
   tax data:
     # A tibble: 46 x 4
       taxon_id ncbi_name
                               ncbi rank ncbi id
       <chr> <chr>
                                 <chr>
                                            <chr>
     1 131567 cellular organisms no rank 131567
     2 2759 Eukaryota
                             superkingdom 2759
     3 33154 Opisthokonta no rank 33154
     # ... with 43 more rows
   query_data:
     # A tibble: 3 x 4
       taxon_id my_ncbi_id my_desc
```

1 9606 AC073210.8 Homo sapiens BAC cl~ AC073210.8 Homo sap~ 0.00007 AE006460 0.001m---11- -------- AE006460 0.001m---1

<chr>

<chr> <chr>

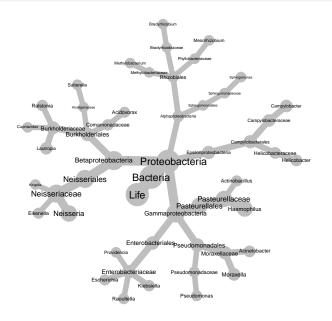
input

<chr>>

Taxon attributes

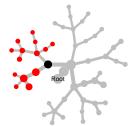
Taxon attributes

Taxon attributes: Taxonomy terminology

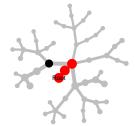


Taxon attributes: subtaxa and supertaxa

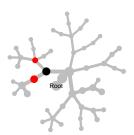
Subtaxa (recursive = T)



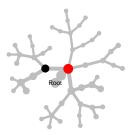
Supertaxa (recursive = T)



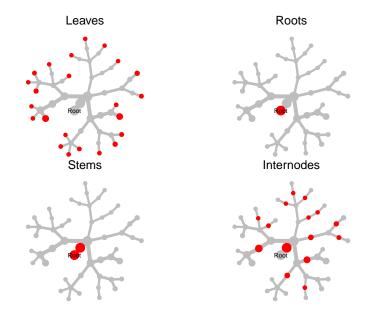
Subtaxa (recursive = F)



Supertaxa (recursive = F)



Taxon attributes: parts of a tree



Taxon attributes: functions

Ranks, names, and IDs

taxon_names, taxon_ranks, taxon_ids

Parts of the tree

branches, internodes, leaves, roots, stems, supertaxa, subtaxa

Filtering helpers

is_branch, is_internode, is_leaf, is_root, is_stem

Numbers of supertaxa/subtaxa/data

n_supertaxa, n_subtaxa, n_obs, n_supertaxa_1,
n_subtaxa_1, n_obs_1

Taxon attributes: Ranks, names, and IDs

These are derived from the list of taxon objects.

```
taxon_names(ex_taxmap) %>% head
   "Mammalia" "Plantae" "Felidae" "Notoryctidae" "Hominidae"
 "Solanaceae"
taxon_ranks(ex_taxmap) %>% head
 "class" "kingdom" "family" "family" "family" "family"
taxon_ids(ex_taxmap) %>% head
```

Taxon attributes: subtaxa

These return a list of vectors named by taxon IDs.

```
subtaxa(ex_taxmap, value = "taxon_names")[1:3]
$b
     "Felidae"
                  "Panthera"
                                   "tigris"
                                                   "Felis"
                                                                   "catus"
"Notoryctidae"
                "Notoryctes"
                                 "typhlops"
                                                "Hominidae"
                                                                    "homo"
     "sapiens"
$c
  "Solanaceae"
                   "Solanum" "lycopersicum"
                                               "tuberosum"
$d
                   m
"Panthera"
            "tigris"
                        "Felis"
                                   "catus"
```

Taxon attributes: subtaxa

These return a list of vectors named by taxon IDs.

Taxon attributes: counts

These return counts of things per taxon.

```
n_subtaxa(ex_taxmap)
n_supertaxa(ex_taxmap)
bcdefghijklmnopqr
0 0 1 1 1 1 2 2 2 2 2 3 3 3 3 3 3
n_obs(ex_taxmap, "info")
bcdefghijklmnopqr
4 2 2 1 1 2 1 1 1 1 2 1 1 1 1 1 1
n_obs(ex_taxmap, "abund")
bcdefghijklmnopqr
8 0 4 2 2 0 2 2 2 2 0 2 2 2 2 0 0
```

Manipulating

Manipulating

Manipulating: example data

reaction

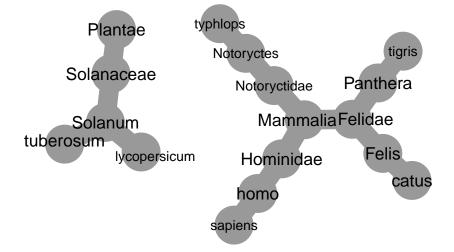
Here is the example object that will be used:

```
print(obj)
<Taxmap>
  17 taxa: b. Mammalia, c. Plantae ... q. lycopersicum, r. tuberosum
  17 edges: NA->b, NA->c, b->d, b->e ... j->o, k->p, l->q, l->r
  3 data sets:
    info:
     # A tibble: 6 x 4
       taxon_id name n_legs dangerous
       <chr> <chr> <dbl> <lgl>
     1 m tiger 4. TRUE
     2 n cat 4. FALSE
     3 o mole 4. FALSE
     # ... with 3 more rows
    phylopic_ids: a named vector of 'character' with 6 items
      m. e148eabb-f138-43[truncated] ... r. 63604565-0406-46[truncated]
   foods: a list of 6 items named by taxa:
      m, n, o, p, q, r
  1 functions:
```

Manipulating: example data

Here is the example object that will be used:

```
heat_tree(obj, node_label = taxon_names, layout = "da")
```



Subset taxonomy and user-defined data to one taxon:

```
filter_taxa(obj, taxon_names == "Plantae", subtaxa = TRUE)
<Taxmap>
  5 taxa: c. Plantae, g. Solanaceae, 1. Solanum, q. lycopersicum, r. tuberosum
  5 edges: NA->c, c->g, g->1, 1->q, 1->r
  3 data sets:
   info:
     # A tibble: 2 x 4
       taxon_id name n_legs dangerous
       <chr> <chr> <dbl> <lgl>
     1 q tomato 0. FALSE
     2 r potato 0. FALSE
   phylopic_ids: a named vector of 'character' with 2 items
      q. b6400f39-345a-47[truncated] ... r. 63604565-0406-46[truncated]
   foods: a list of 2 items named by taxa:
      q, r
  1 functions:
   reaction
```

Subset taxonomy and user-defined data to one taxon:

```
filter_taxa(obj, taxon_names == "Plantae", subtaxa = TRUE) %>%
heat_tree(node_label = taxon_names, layout = "da")
```

tuberosum

Solanum

Solanaceae

lycopersicum

Plantae

filter taxa(obj, taxon ranks == "family", supertaxa = TRUE)

Subset taxonomy to one rank:

```
<Taxmap>
 6 taxa: b. Mammalia, c. Plantae ... f. Hominidae, g. Solanaceae
 6 edges: NA->b, NA->c, b->d, b->e, b->f, c->g
 3 data sets:
   info:
     # A tibble: 6 x 4
       taxon_id name n_legs dangerous
       <chr> <chr> <dbl> <lgl>
     1 d tiger 4. TRUE
     2 d cat 4. FALSE
     3 e mole 4. FALSE
     # ... with 3 more rows
   phylopic_ids: a named vector of 'character' with 6 items
      d. e148eabb-f138-43[truncated] ... g. 63604565-0406-46[truncated]
   foods: a list of 6 items named by taxa:
      d, d, e, f, g, g
 1 functions:
   reaction
```

Subset taxonomy to one rank:

```
filter_taxa(obj, taxon_ranks == "family", supertaxa = TRUE) %>%
heat_tree(node_label = taxon_names, layout = "da")
```

Solanaceae

Plantae

Notoryctidae

Hominidae Mammalia

Felidae

Manipulating: Subsetting user data

Subset user-defined data and remove any taxa not in subset:

```
filter_obs(obj, "info", n_legs == 4, drop_taxa = TRUE)
<Taxmap>
  9 taxa: b. Mammalia, d. Felidae ... n. catus, o. typhlops
  9 edges: NA \rightarrow b, b \rightarrow d, b \rightarrow e, d \rightarrow h, d \rightarrow i, e \rightarrow j, h \rightarrow m, i \rightarrow n, j \rightarrow o
  3 data sets:
    info:
      # A tibble: 3 x 4
        taxon_id name n_legs dangerous
        <chr> <chr> <dbl> <lgl>
      1 m tiger 4. TRUE
      2 n cat 4. FALSE
      3 o
              mole 4. FALSE
    phylopic_ids: a named vector of 'character' with 3 items
       m. e148eabb-f138-43[truncated] ... o. 11b783d5-af1c-4f[truncated]
    foods: a list of 3 items named by taxa:
       m. n. o
  1 functions:
    reaction
```

Manipulating: Subsetting user data

Subset data and remove any taxa not in subset:

```
filter_obs(obj, "info", n_legs == 4, drop_taxa = TRUE) %>%
heat_tree(node_label = taxon_names, layout = "da")
```

Notoryctes

Notoryctidae

Felis Mammalia

Felidae

Panthera

tigris

Manipulating: Adding user data

Add a column to a dataset:

```
mutate obs(obj, "info", bipedal = n legs == 2)
<Taxmap>
 17 taxa: b. Mammalia, c. Plantae ... q. lycopersicum, r. tuberosum
 17 edges: NA->b, NA->c, b->d, b->e ... j->o, k->p, l->q, l->r
 3 data sets:
   info:
     # A tibble: 6 x 5
       taxon id name n legs dangerous bipedal
       <chr> <chr> <dbl> <lgl> <lgl>
     1 m tiger 4. TRUE FALSE
     2 n cat 4. FALSE FALSE
     3 o mole 4. FALSE FALSE
     # ... with 3 more rows
   phylopic_ids: a named vector of 'character' with 6 items
      m. e148eabb-f138-43[truncated] ... r. 63604565-0406-46[truncated]
   foods: a list of 6 items named by taxa:
      m, n, o, p, q, r
  1 functions:
   reaction
```

Manipulating: values accessible to NSE

The following can be used in manipulation functions as if they were independent variables using Non-Standard Evaluation (NSE):

- ► Functions that return per-taxon information
- User-defined table columns
- User-defined vectors and lists
- User-defined functions

```
unname(all_names(obj))
```

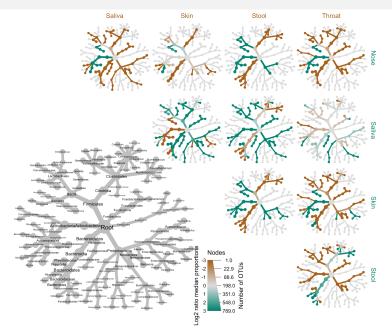
```
[1]
                                                              "classifications"
    "taxon names"
                        "taxon ids"
                                           "taxon indexes"
[5]
    "n supertaxa"
                        "n supertaxa 1"
                                           "n subtaxa"
                                                              "n subtaxa 1"
[9]
    "n leaves"
                        "n leaves 1"
                                           "taxon ranks"
                                                              "is root"
[13] "is stem"
                        "is branch"
                                           "is leaf"
                                                              "is internode"
[17] "n obs"
                        "n obs 1"
                                           "name"
                                                              "n legs"
                        "phylopic_ids"
                                                              "reaction"
[21] "dangerous"
                                           "foods"
```

Compatiblity with other packages

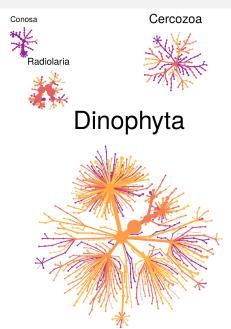
taxa is still being developed, but we hope it will become a foundation for an ecosystem of R packages that use taxonomic data.

- Flexible parsers can read most formats
- Working on making taxize compatible with taxa
- Fully compatible with metacoder

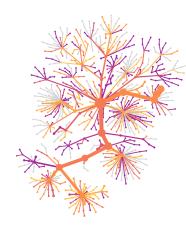
Metacoder: visulization of taxonomic data



Metacoder: visulization of taxonomic data



Metazoa



Acknowledgements













Thanks for listening!

Questions?