

Neotoma paper

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neotoma: A Programmatic Interface to the Neotoma Paleoecological Database

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Abstract:

Paleoecological data are integral to ecological analyses. First, they provide an opportunity to study ecological and evolutionary interactions between communities and abiotic environments over long time scales. Second, they allow us to study processes that occur infrequently, such as megadroughts, hurricanes, and rapid climate change. Third, the past allows us to study ecological processes in the absence of widespread anthropogenic influence.

The R package *neotoma*, described here, obtains and manipulates data from the Neotoma Paleoecological Database (Neotoma Database: <http://www.neotomadb.org>). The Neotoma Database is a public-domain searchable repository for multiproxy paleoecological records spanning the past 5 million years. The Neotoma Database provides the cyberinfrastructure to study spatiotemporal dynamics of species and communities from the Pliocene to the present; *neotoma* provides a user interface to enable these studies. *neotoma* searches the Neotoma Database using terms that can include location, taxon name, or dataset type (e.g., pollen, vertebrate fauna, ostracode) using the Database's Application Programming Interface (API). The package returns a set of nested metadata associated with the site, including the full assemblage record, geochronological data to enable the rebuilding of age models, dataset metadata (e.g. age range of samples, date of accession into Neotoma, principal investigator), and site metadata (e.g. location, site name and description). *neotoma* also provides tools to allow cross-site analysis, including the ability to standardize taxonomies using built-in taxonomies derived from the published literature or user-provided taxonomies.

To demonstrate the use of the *neotoma* package we provide examples of key functions based on the published literature, for both plant and mammal taxa.

Keywords: R software, *neotoma*, paleoecology, database, pollen, mammal

Introduction

Paleoecological data are fundamental to understanding the patterns and drivers of biogeographical, climatic, and evolutionary change, ranging from the recent past to the dawn of life. Although individual site-level studies have provided significant insights into past ecological dynamics, the true power of paleoecological data emerges from networks of data assembled to study broad-scale ecological and evolutionary phenomena, e.g. the responses of speciation rates to the five major extinction events in geological history (Peters & Foote 2001; Raup & Sepkoski 1984; Sepkoski 1997) and the rapid and individualistic responses of species to the climate changes accompanying recent glacial-interglacial cycles (Davis 1981; Schroeder et al. 1996; Huntley & Webb 1988; Tzedakis 1994; Williams et al. 2004). Paleoeoinformatics (Brewer et al. 2012; Uhen et al. 2013) is dedicated to providing tools to researchers across disciplines to access and use large paleoecological datasets spanning thousands of years. These datasets may be used to provide better insight into regional vegetation change (Blois et al. 2013; Blarquez, Carcaillet, et al. 2014), patterns of biomass burning (Marlon et al. 2013), or changing rates

of geophysical processes through time (Goring et al. 2012). The increasing interest in uniting ecological and paleoecological data in order to better understand responses to a rapidly changing world (Fritz et al. 2013; Behrensmeyer & Miller 2012; Dietl & Flessa 2011) will require more robust tools to access and synthesize data from the modern and paleo time domains.

The Neotoma Paleoecological Database represents a consortium of paleoecological databases, with distributed scientific governance and expertise, but sharing a common database infrastructure. Constituent databases include, among others, the European, Latin American, and North American Pollen Databases; the North American Plant Macrofossil Database; FAUNMAP (Pliocene to Quaternary mammal fossils in the United States and Canada); the North Dakota State University Fossil Insect Database; the North American Non-Marine Ostrocode Database; and the Diatom Paleolimnology Data Cooperative. Neotoma is the outgrowth of a longstanding collaboration between the European Pollen Database and the North American Pollen Database (Grimm et al. 2013) and the desire to integrate these data with faunal and other paleo data. The database framework was generalized from the pollen databases (which had identical structures) and the FAUNMAP database to accommodate both macro- and microfossil data as well as other kinds of data such as geochemical, isotopic, and loss-on-ignition. Work is underway to include other taxonomic groups and depositional contexts (e.g. testate amoeba records, packrat midden data), thus further expanding the data that can be accommodated by Neotoma. Crucially, Neotoma is a vetted database. Through the use of data stewards --- domain experts distributed among constituent bases who can check for inaccuracies, upload and manage data records --- Neotoma can support high quality control assurance for each of the constituent data types, and receive feedback from research communities involved with each specific data type (Grimm et al. 2013).

The Neotoma Database has also developed an Application Programming Interface (API) that allow users to query the database via web services, which return data using properly formed URL requests. For example, the URL:
<http://api.neotomadb.org/v1/apps/geochronologies/?datasetid=8> will return all geochronological data for the record associated with the dataset ID 8.

The analysis of paleoecological data is often performed using the statistical software R (R Core Team 2014). There are several R packages designed specifically for paleoecological data analysis, including *analogue* (Simpson & Oksanen 2014; Simpson 2007) and *rioja* (Juggins 2013) for paleoenvironmental reconstruction, *Bchron* (Parnell 2014) for radiocarbon dating and age-depth modeling and *paleofire* to access and analyse charcoal data (Blarquez, Vannière, et al. 2014). Given the rapid proliferation and availability of these analytical tools in R, the rate-limiting step for analysis has become the difficulty of obtaining and importing data into R. This bottleneck has meant reliance on static datasets that are available as published, and rarely updated, and on more *ad hoc* methods such as the distribution of individual datasets from author to analyst.

With an increasing push on the ecological community to perform and publish reproducible research that include numerically reproducible results (Goring et al. 2013; Goring et al. 2012; Wolkovich et al. 2012; Reichman et al. 2011) it is important to provide tools that

allow analysts to directly access dynamic datasets, and to provide tools to support reproducible workflows. The rOpenSci project (<http://ropensci.org/>) is dedicated to developing tools that use R to facilitate a culture shift toward reproducible science in the ecology community. As part of this effort, rOpenSci provides a number of tools that can directly interact with APIs to access data from a number of databases including `rfishbase` for FishBase (Boettiger et al. 2012), and `taxize` for the Encyclopedia of Life, iPlant/Taxosaurus and others (Chamberlain & Szöcs 2013) among others.

The `neotoma` package addresses concerns regarding data access and workflow reproducibility by providing users with tools that allow paleoecologists to query, download, organize, and summarize data from the Neotoma database using R. Here we describe the `neotoma` package, then we present use cases for the package, using examples drawn from the ecological literature, with the general objective of illustrating how `neotoma` provides tools to perform paleoecological research in an open and reproducible manner.

The `neotoma` package

The `neotoma` R package is an interface between the Neotoma Paleoecological Database (<http://neotomadb.org>) and statistical tools in R. `neotoma` uses an API to send data requests to the Neotoma Database, and then forms data objects that are compatible for use with existing packages such as `analogue` (Simpson & Oksanen 2014) and `rioja` (Juggins 2013), which are used for environmental reconstruction, manipulation, and presentation of paleoecological data. The `neotoma` package also includes tools to standardize pollen taxon names across sample sites using a set of published pollen taxonomies for North America, or user defined taxonomies.

Data in the `neotoma` package is represented in three main classes (Figure 1): "`site`"s, "`dataset`"s (grouped into "`dataset_list`"s), and "`download`"s (grouped into "`download_list`"s). A "`site`" is the most basic form of spatial information representing the spatial locations of datasets along with site names, descriptions and a unique `site.id`. "`site`"s are "`data.frame`"s with columns `siteid`, `sitename`, `lat`, `long`, `elev`, `description`, `long_acc`, and `lat_acc`. These column headings are generally self explanatory; `long_acc` and `lat_acc` are used to indicate the width of the bounding box for a sample site (with a midpoint of `long` and `lat`). In the Neotoma Database, examples of sites include a lake from which one or more cores are collected, a cave from which one or more faunal assemblages are collected, an archaeological dig with one or more excavation pits, and so forth. Each unique site returned by the `get_site()` search is placed in a row, providing enough descriptive data to plot locations and understand the spatial context of a site.

Although `get_site()` is useful for first-pass surveys of data availability, analysts more commonly will want to search for and retrieve datasets stored in the Neotoma Database. The function `get_dataset()` uses search terms almost identical to those used in `get_site()`, and it returns a more complete description of the datasets available. However, at this time only `get_site()` has the ability to search for sites based on site names.

"`dataset`"s associated with individual sites can be obtained using `get_dataset()`. Each search using `get_dataset()` returns a "`dataset_list`", a list of one or more "`dataset`"s,

equal to the number of datasets returned by the function. `get_dataset()` returns the metadata associated with a dataset in the Neotoma Database. Neotoma's datasets are the containers for a set of samples of the same type from a single collection unit within a site. Examples of datasets in Neotoma include 1) all the pollen counts from a single core from a lake, 2) all the geochronological measurements (e.g radiocarbon dates) from a sediment core, 3) all the faunal data from an excavation in a cave, 4) all the plant macrofossil data from a packrat midden. In neotoma, a "dataset" includes the "site" for each "dataset" (as "site.data", Figure 1), along with the "dataset" specific metadata ("dataset.meta" in Figure 1). The dataset also includes the principal investigator, submission date to Neotoma, and the date that the information was accessed via the Neotoma API using the R package. "dataset_list"s and "dataset"s can be used to access the full "download" using the `get_download()` method.

`get_download()` returns an object of class "download_list" containing one or more objects of class "download" (Figure 1). `get_download()` will also return a confirmation message for each individual API call as the function proceeds that can be turned off using the argument `verbose = FALSE`. Each "download" contains the associated "dataset" (Figure 1). The "sample.meta" component is where the core depth and age information is stored. The actual chronologies are stored in "chronologies". If a core has a single age model then "chronologies" has a length of one. Some cores have multiple chronologies and these are also included in the "chronologies" list. The default chronology is stored in "sample.meta" and is always the first chronology in "chronologies".

To build a new chronology with the same chronological controls as an existing chronology, perhaps using a different algorithm, `get_chroncontrol()` can be used to return the chronological controls and the "chronology.id" in either "sample.meta" or any one of the "chronologies" objects. While the chronological controls used to build a chronology may vary across chronologies for a single site, the default model contains the "best" chronological control data, as determined at the time the chronologies for the collection unit were last reviewed. It is important to note, however, that the "best" chronologies for most collection units in the database were based on "classical" age models (Blaauw 2010) that do not include estimates of uncertainty. Moreover, these default age models that are in calibrated radiocarbon years utilize radiocarbon dates that are calibrated *a priori*. Bayesian age modeling programs, such as Bacon (Blaauw & Christen 2011), which provides estimates of uncertainty, as well as the classical age modeling program `clam` (Blaauw 2010), which also returns estimates of uncertainty, utilize uncalibrated radiocarbon dates as input. Thus, the calibrated ages of many existing age models in Neotoma will not be appropriate for these programs, and the age controls may have to be obtained from the geochronology table using `get_geochron()`.

The age controls of existing default radiocarbon-year chronologies may sometimes be appropriate for programs such as Bacon and `clam`; however, many of these chronologies rejected radiocarbon dates *a priori*, which could be included when using Bacon. The neotoma package has a function to interface directly with Bacon or `clam`, called `write_agefile()`, which will output a correctly formatted age file for either of these applications using a "download" object.

The "taxon.list" component lists taxa found in the dataset samples ("counts") and any laboratory data ("lab.data"), along with the units of measurement and taxonomic grouping (Figure 1). The "counts" are the actual count, presence or percentage data recorded for the dataset. The "lab.data" component contains information about any spike used to determine concentrations, sample quantities and, in some cases, charcoal counts.

Each of these objects, "site", "dataset" and "download" can be obtained using direct calls to the API, or using functions defined in the neotoma package (Figure 2).

Examples

Here we present several examples that both introduce users to the neotoma package, and highlight how neotoma can be used in a paleoecological workflow. We begin with a simple example in which we compare change in *Alnus* pollen between two sites during the late Quaternary, followed by two more involved examples where we look at *Pinus* migration and changes in late-Quaternary mammal distributions in the United States.

A simple example

A researcher is interested in finding the pollen record for Marion Lake, in British Columbia (Mathewes 1973), and comparing changes in *Alnus* pollen to the Louise Pond record (Pellatt & Mathewes 1997) from Haida G'Waii, further north. We search for specific sites by name using `get_site()`, making use of the wildcard "%" to catch sites whose site names begin with the strings "Marion Lake" or "Louise Pond":

```
library("neotoma")
marion <- get_site(sitename = 'Marion Lake%')

The API call was successful, you have returned 1 records.

louise <- get_site(sitename = 'Louise Pond%')

The API call was successful, you have returned 1 records.

louise
```

	siteid	long	lat	elev
Louise Pond	1618	-131.8	53.42	650

```
description
Louise Pond Glacial scour lake. Physiography: Queen Charlotte Ranges, Louis
e Island. Surrounding vegetation: Tsuga mertensiana, Pinus contorta.
long.acc lat.acc
Louise Pond 0 0
```

In each case `get_site()` returns a single "site" (Figures 1 & 2). Here we queried the Neotoma database for site based on sitename, but alternately we could have queried for sites within a geographical bounding box, or by geopolitical region.

To get "dataset"s for these records we can bind the two records together by rows using `rbind()`, and pass the result directly to `get_dataset()` (Figure 2):

```

224 western.sites <- rbind(marion, louise)
225 western.data <- get_dataset(western.sites)

```

226 western.data is a "dataset_list", containing two "dataset"s (Figure 1). The "dataset"
 227 for a site will be nested within a "dataset_list", even if only a single site is returned, so
 228 that methods can be consistent across classes and functions. This means that a single
 229 "dataset" must be retrieved as *e.g.*, western.data[[1]] (this is also the case for
 230 "download" and "download_list" objects). The use of "dataset" and "dataset_list"
 231 classes allow us to easily move between get_dataset(), get_site() and get_download().
 232 We can see the special print() method for both "dataset"s and "dataset_list"s:

```

233 western.data
234   A dataset_list containing 2 objects:
235   Accessed from 2014-10-06 09:16h to 2014-10-06 09:16h.
236   Datasets:
237   dataset.id           site.name    long   lat   type
238       1705 Marion Lake (CA:British Columbia) -122.5 49.31 pollen
239       1670 Louise Pond                      -131.8 53.42 pollen

```

```

240 western.data[[1]]
241   A dataset for Marion Lake (CA:British Columbia)
242   Accessed 2014-10-06 09:16h.
243   dataset.id           site.name    long   lat   type
244       1705 Marion Lake (CA:British Columbia) -122.5 49.31 pollen

```

245 before we download the full records and print them:

```

246 western.dl <- get_download(western.data)
247   API call was successful. Returned record for Marion Lake(CA:British Columbi
248 a)
249   API call was successful. Returned record for Louise Pond
250   Warning:
251   Modifiers are absent from the lab objects Lycopodium tablets, Lycopodium sp
252 ike, Sample quantity.
253   get_download will use uniqueidentifiers to resolve the problem.

```

```

254 western.dl
255   A download_list containing 2 objects:
256   Accessed from 2014-10-07 20:38h to 2014-10-07 20:38h.
257   Datasets:
258   dataset.id           site.name    long   lat   age.younger
259       1705 Marion Lake (CA:British Columbia) -122.5 49.31      58
260       1670 Louise Pond                      -131.8 53.42      62
261   age.older   type
262       13051 pollen
263       10065 pollen

```

```

264 western.dl[[1]]

```



```

265 A download object for Marion Lake (CA:British Columbia)
266 Accessed 2014-10-07 20:38h.
267   dataset.id           site.name    long   lat age.young
268       1705 Marion Lake (CA:British Columbia) -122.5 49.31      58
269   age.old   type
270      13051 pollen

```

271 Pollen taxonomy can vary substantially across cores depending on the level taxonomic
 272 resolution used by a pollen analyst, or as a result of changes to taxonomies over time. One
 273 analyst might discriminate subgenera of *Pinus*, another might simply identify *Pinus* to the
 274 genus level. Gramineae - a common pollen type in earlier pollen records - has now been
 275 renamed Poaceae. This variable and shifting taxonomy is a first-order challenge for
 276 analysts seeking to analyze the dynamics of taxa across multiple groups. neotoma provides
 277 several options for standardized taxonomic list, corresponding to three published
 278 taxonomies for the United States and Canada (Gavin et al. 2003; Whitmore et al. 2005;
 279 Williams & Shuman 2008). This function can be helpful, but should be used with care. The
 280 aggregation table is accessible using the command `data(pollen.equiv)` and the function
 281 to compile the data is called `compile_taxa()`. It can accomodate either the internal
 282 translation table provided with the package, or a user-defined table with the same
 283 structure as `pollen.equiv`.

284 We are interested in comparing the relative pollen abundances of *Alnus* between two sites.
 285 We compile the pollen data using the 'P25' taxonomy from Gavin et al. (2003). The first
 286 record downloaded is Marion Lake. We can see the "download" for Marion Lake the
 287 `taxon.table` has 5 columns:

```

288 head(western.dl[[1]]$taxon.list)

```

taxon.name	variable.units	variable.element	variable.context	taxon.group
Tsuga heterophylla	NISP	pollen		Vascular plants
Poaceae	NISP	pollen		Vascular plants
Tsuga mertensiana	NISP	pollen		Vascular plants
Rosaceae	NISP	pollen		Vascular plants
Pteridium	NISP	spore		Vascular plants
Acer circinatum	NISP	pollen		Vascular plants

289 Once we apply `compile_taxa()` to the dataset using the 'P25' compiler:

```

290 western.comp <- compile_taxa(western.dl, list.name = 'P25')
291 names(western.comp) <- c("marion", "louise")

```


292 The `taxon.table` for Marion Lake now has an extra column (note that several columns
 293 were removed to improve readability).

294 `head(western.comp[[1]]$taxon.list[,c(1, 5, 6)])`

	taxon.name	taxon.group	compressed
2	Tsuga heterophylla	Vascular plants	Tsuga
29	Poaceae	Vascular plants	Poaceae
3	Tsuga mertensiana	Vascular plants	Tsuga
4	Rosaceae	Vascular plants	Other
5	Pteridium	Vascular plants	Other
6	Acer circinatum	Vascular plants	Acer

295 `compile_taxa()` returns a "download_list" or "download", for which `taxon.list` gains a
 296 column named `compressed` to link the original taxonomy to the revised taxonomy. This
 297 linkage is an important reference for researchers who choose to use this package for large-
 298 scale analysis, but who might need to later check the aggregated taxonomic groups against
 299 the original data. In this example we see that spore-types have been lumped into a single
 300 taxon *Other* along with other taxa such as Rosaceae.

301 The sample data ("counts") contained in each "download" in the "download_list"
 302 `western.d1` are converted into percentages using `tran()` from the `analogue` package
 303 (Simpson 2007). We can then compare *Alnus* pollen percentages from these two locations
 304 to learn about vegetation changes on the west coast of North America during the Holocene:

```
305 library("analogue")
306
307 marion.alnus <- tran(x = western.comp$marion$counts, method = 'percent')[, 'Alnus']
308
309 louise.alnus <- tran(x = western.comp$louise$counts, method = 'percent')[, 'Alnus']
310
311
312 alnus.df <- data.frame(alnus = c(marion.alnus, louise.alnus),
313                        ages = c(western.comp$marion$sample.meta$age,
314                                western.comp$louise$sample.meta$age),
315                        site = c(rep('Marion', length(marion.alnus)),
316                                rep('Louise', length(louise.alnus))))
317
318 plot(alnus ~ ages, data = alnus.df, col = alnus.df$site, pch = 19,
319      xlab = 'Years Before Present', ylab = 'Percent Alnus')
```

320 Marion Lake (red, Figure 3) maintains much higher proportions of *Alnus* throughout its
 321 history, and has a rapid increase in *Alnus* pollen during the historical period. This rapid
 322 shift in the last 200 years is likely as a result of rapid colonization by pioneer *Alnus rubra*
 323 following forest clearance and fire in the lower mainland of British Columbia (Mathewes
 324 1973).

It is also possible to plot the pollen stratigraphy (Figure 4) at any one site using the analogue package for R (Simpson 2007). Here we plot Marion Lake:

```
core.pct <- data.frame(tran(western.comp[[1]]$counts, method = "percent"))
core.pct$age <- western.comp[[1]]$sample.meta$age
# Eliminate taxa with no samples greater than 4%.
core.pct <- chooseTaxa(core.pct, max.abun = 4)
Stratiplot(age ~ ., core.pct, sort = 'wa', type = 'poly',
           ylab = "Years Before Present")
```

Pinus migration following the last Glacial Maximum

Macdonald and Cwynar (1991) used *Pinus* pollen percentages to map the northward migration of lodgepole pine (*Pinus contorta* var *latifolia*) following the retreat of the Laurentide Ice Sheet and the accompanying rise of temperatures in the late-Glacial and early Holocene. In their study a cutoff of 15% *Pinus* pollen was defined as the indicator of *Pinus* presence. Strong and Hills (2013) have remapped the migration front using a lower pollen proportion (5%) and more sites. Here, the analysis is partially replicated. Note that additional R packages must be installed and loaded for the following examples.

A spatial bounding box delimiting sites is defined for the search. Strong and Hills (2013) use a region approximately bounded by 54°N and 65°N, and from 110°W to 130°W. The function `get_site()` can return all sites within a slightly expanded bounding box:

```
#install.packages('ggmap', 'ggplot2', 'reshape2', 'Bchron', 'gridExtra')
library("ggmap")
library("ggplot2")
library("reshape2")
library("Bchron")
library("gridExtra")

all.sites <- get_site(loc = c(-140, 45, -110, 65))
```

The API call was successful, you have returned 444 records.

The code above returned 444 sites. To narrow down the search we will use `get_dataset()` to search for all *Pinus* taxa within the same bounding box as above. `get_dataset()` can also limit the type of dataset, either by looking for specific taxa, or by describing the dataset type (e.g., `datasettype = 'pollen'` or `datasettype = 'mammal'`). The % wildcard indicates that any characters may follow a string starting with "Pinus":

```
all.datasets <- get_dataset(loc = c(-140, 45, -110, 65),
                           datasettype = 'pollen',
                           taxonname = 'Pinus%')
```

The API returned 69 datasets. Many dropped sites were pollen surface samples, or sites with datasets for other taxonomic groups. The distribution of the 69 fossil pollen sites can be plotted over the original 444 sites. We use the `ggplot2` package (Wickham 2009) to make the figures:

```

365 map <- map_data('world')
366 ggplot(data = data.frame(map), aes(long, lat)) +
367   geom_polygon(aes(group=group), color = 'steelblue', alpha = 0.2) +
368   geom_point(data = all.sites, aes(x = long, y = lat)) +
369   geom_point(data = get_site(all.datasets),
370     aes(x = long, y = lat), color = 2) +
371   xlab('Longitude West') +
372   ylab('Latitude North') +
373   coord_map(projection = 'albers', lat0 = 40, lat1 = 65,
374     xlim = c(-140, -110), ylim = c(45, 70))

```

375 The map (Figure 5) shows a number of sites in the interior of British Columbia that have no
 376 fossil pollen. There are also other sites not shown here that may have relevant data but
 377 have yet to be entered into the database. This highlights a common challenge in
 378 paleoecoinformatics --- the import of individual records into data repositories takes some
 379 time and is an on-going process that is aided by the collective contributions of the original
 380 analysts, data stewards, and large-scale research initiatives (e.g. PAGES 2K, PaleON).
 381 Fortunately, new software tools are speeding up the process of uploading and vetting data.
 382 The Tilia software (<http://www.neotomadb.org/data/category/tilia>) has been updated to
 383 allow direct upload to the Neotoma Database and includes a large number of automated
 384 data quality checks and standardized look-up tables for variable names. Because neotoma
 385 directly links to the Neotoma Database via APIs, analyses using neotoma can be updated
 386 continuously as new sites are added.

387 To obtain the data for the 69 sites we use `get_download()`:

```

388 all.downloads <- get_download(all.datasets, verbose = FALSE)

```

389 Only the percentage of *Pinus* is of interest, so we can again compile the taxa across the
 390 "download_list" using the 'P25' taxonomy (Gavin et al. 2003):

```

391 compiled.cores <- compile_taxa(all.downloads, 'P25')

```

392 We want to determine which sample has the first local *Pinus* presence in each core using a
 393 cutoff of 5% (Strong & Hills 2013). We can find which rows in the *Pinus* column in each
 394 "download"'s "count" data frame have presence over 5% and then find the highest row
 395 number since the samples in a dataset are ordered stratigraphically, with the youngest
 396 sample in the top row and the oldest sample in the bottom row. This is a more complicated
 397 example:

```

398 top.pinus <- function(x) {
399   x.pct <- tran(x$counts, method = "proportion")
400   # Cores must span at least the last 5000 years (and have no missing dates)
401   :
402   old.enough <- max(x$sample.meta$age) > 5000 & !all(is.na(x$sample.meta$age))
403 }
404 # Find the highest row index associated with Pinus presence over 5%
405 oldest.row <- ifelse(any(x.pct[, 'Pinus'] > .05 & old.enough),
406   max(which(x.pct[, 'Pinus'] > .05)),
407   0)

```

```

408 # return a data.frame with site name & Location, and the age and date type
409 # (since some records have ages in radiocarbon years) for the oldest Pinus
410 .
411 out <- if (oldest.row > 0) {
412   data.frame(site = x$dataset$site.data$site.name,
413             lat = x$dataset$site.data$lat,
414             long = x$dataset$site.data$long,
415             age = x$sample.meta$age[oldest.row],
416             date = x$sample.meta$age.type[oldest.row])
417 } else {
418   NULL
419 }
420 out
421 }
422
423 # Apply the function 'top.pinus' to each core using lapply and rbind:
424 summary.pinus <- do.call("rbind.data.frame", lapply(compiled.cores, top.pinus
425 ))

```

426 We need to calibrate dates that are recorded in radiocarbon years using the Bchron
 427 package (Parnell 2014). In most cases the original uncertainty for individual ages is not
 428 recorded in "sample.meta" so we assume a 100 year standard deviation. Note that direct
 429 recalibration of radiocarbon dates from interpolated age models is not the best approach,
 430 but is sufficient for our purposes here:

```

431 radio.years <- summary.pinus$date %in% 'Radiocarbon years BP'
432 sryears <- sum(radio.years, na.rm = TRUE)
433 # BChronCalibrate is in the BChron package:
434 calibrated <- BChronCalibrate(summary.pinus$age[radio.years],
435                               ageSds = rep(100, sryears),
436                               calCurves = rep('intcal13', sryears))
437
438 # we want the weighted means from 'calibrated'
439 wmean.date <- function(x) sum(x$ageGrid*x$densities / sum(x$densities))
440
441 summary.pinus$age[radio.years] <- sapply(calibrated, wmean.date)
442 summary.pinus <- na.omit(summary.pinus)
443 summary.pinus <- subset(summary.pinus, subset=!(age < 2000 & long < -130))
444
445 # A loess curve is straightforward, but not the best model:
446 regress <- ggplot(summary.pinus, aes(x = lat, y = age)) +
447   geom_point(aes(color = age), size = 2) +
448   scale_y_reverse(expand = c(0, 100)) +
449   xlab('Latitude North') +
450   ylab('Years Before Present') +
451   geom_smooth(n = 40, method = 'loess') +
452   geom_rect(aes(xmin = 59, xmax = 60, ymin = 7000, ymax = 100
453 00),
454             color = 2, fill = 'blue', alpha = 0.01)

```

```

455 mapped <- ggplot(data = data.frame(map), aes(long, lat)) +
456             geom_polygon(aes(group = group), color = 'steelblue', alpha
457 = 0.2) +
458             geom_point(data = summary.pinus,
459             aes(x = long, y = lat, colour = age), size = 3) +
460             coord_map(projection = 'albers', lat0 = 40, lat1 = 65,
461             xlim = c(-140, -110), ylim = c(40, 70)) +
462             theme(legend.position = 'none')
464
465 grid.arrange(mapped, regress, nrow=1)

```

The results show a clear pattern of northward expansion for *Pinus* in northwestern North America (Figure 6). These results broadly agree with the findings of Strong and Hills (2013) who suggest that *Pinus* reached a northern extent between 59°N and 60°N at approximately 10--7 ka cal BP as a result of geographic barriers before continuing northward after 7 ka cal BP.

Mammal Distributions in the Pleistocene

Graham et al. (1996) built and applied the FAUNMAP dataset (<http://www.ucmp.berkeley.edu/faunmap/>) of fossil assemblages to elucidate patterns of change in mammal distributions through the Pleistocene to the present. The paper uses various multivariate analyses to show, in part, that mammal species have responded in a Gleasonian manner to climate change since the late-Pleistocene. Graham et al. (1996) show some species migrating northward in response to warming climates, others staying relatively stable, and some moving southward. FAUNMAP has been incorporated into Neotoma (and expanded with new records), and this example performs some simple analyses that show how different species responded to the changing climate of the last deglaciation.

First, all vertebrate fauna datasets are obtained from Neotoma:

```

483 # Bounding box is effectively the continental USA, excluding Alaska
484 mam.set <- get_dataset(datasettype= 'vertebrate fauna',
485                       loc = c(-125, 24, -66, 49.5))
486 # Retrieving this many sites can be very time consuming
487 mam.d1 <- get_download(mam.set)

```

Sites are assigned to time-period bins as in Graham et al. (1996); Modern (< 0.5 ka cal BP), Late Holocene (0.5-- 4 ka cal BP), Early-Mid Holocene (4--10 ka cal BP), Late Glacial (10--15 ka cal BP), Full Glacial (15--20 ka cal BP) and Late Pleistocene (> 20 ka cal BP). The first step is to build a large table with time and xy coordinates for each site. Time data in "sample.meta" for the mammal data is not the same as for pollen where age is commonly found in the sample.meta\$age component. Most vertebrate fauna samples are assigned only younger (sample.meta\$age.younger) and older (sample.meta\$age.older, Figure 1) bounds with no estimates of mean or median age. In this example we average the younger and older ages to determine sample age. We recognize that this averaging of ages is likely to be methodologically indefensible in the scientific literature, but is sufficient for

498 illustrative purposes here. Here we make use of the reshape2 package (Wickham 2007) to
499 help manipulate data structures.

```
500 compiled.mam <- compile_downloads(mam.d1)
501 time.bins <- c(500, 4000, 10000, 15000, 20000)
502 mean.age <- rowMeans(compiled.mam[,c('age.old', 'age.young', 'age')],
503                       na.rm = TRUE)
504 interval <- findInterval(mean.age, time.bins)
505 periods <- c('Modern',
506              'Late Holocene',
507              'Early-Mid Holocene',
508              'Late Glacial',
509              'Full Glacial',
510              'Late Pleistocene')
511 compiled.mam$ageInterval <- periods[interval + 1]
512 mam.melt <- melt(compiled.mam,
513                 measure.vars = 10:(ncol(compiled.mam)-1),
514                 na.rm = TRUE,
515                 factorsAsStrings = TRUE)
516 mam.melt <- transform(mam.melt, ageInterval = factor(ageInterval, levels = pe
517 riods))
518 mam.lat <- dcast(data = mam.melt, variable ~ ageInterval, value.var = 'lat',
519                 fun.aggregate = mean, drop = TRUE)[,c(1, 3, 5, 6)]
520 # We only want taxa that appear at all time periods:
521 mam.lat <- mam.lat[rowSums(is.na(mam.lat)) == 0, ]
522 # Group the samples based on the range & direction (N vs S) of migration.
523 # A shift of only 1 degree is considered stationary.
524 mam.lat$grouping <- factor(findInterval(mam.lat[,2] - mam.lat[, 4],
525                                         c(-11, -1, 1, 20)),
526                            labels = c('Southward', 'Stationary', 'Northward')
527 )
528 mam.lat.melt <- melt(mam.lat)
529 colnames(mam.lat.melt)[2:3] <- c('cluster', 'Era')
```

530 The output of the above manipulations is displayed via a ggplot2 plot using

```
531 ggplot(mam.lat.melt, aes(x = Era, y = value)) +
532   geom_path(aes(group = variable, color = cluster)) +
533   facet_wrap(~ cluster) +
534   scale_x_discrete(expand = c(.1, 0)) +
535   ylab('Mean Latitude of Occurrence') +
536   theme(axis.text.x = element_text(angle = 90, hjust = 1))
```

537 Even with this fairly simple set of analyses we see that species did not respond uniformly to
538 climatic warming following deglaciation (Figure 7), consistent with the prior work of
539 Graham *et al.* (1996). Although most range shifts were northward, a number of taxa show
540 little change in their ranges and a number show southward range shifts (Figure 7). This
541 example does not examine east-west movement and ignores the issues that may be
542 associated with the complex topography of the mountainous west, or possible confounding
543 effects introduced by temporal variations in the available set of sites. The broader point

here is that the use of neotoma can support research that is synchronized with the data holdings of large repositories such as Neotoma and reproducible.

Conclusion

The whole of the fossil record is much greater than the sum of its parts. Many of our discipline's most important advances were made possible only by the synthesis of many individual fossil occurrences into regional- to global-scale databases of species occurrences, *e.g.*, the Neotoma Paleoecology Database and the Paleobiological Database. Current frontiers in paleoecological informatics include 1) facilitating the input of data into these databases, 2) improved sophistication of the data models employed by these databases, enabling them to handle increasingly complex arrays of paleobiological and associated geochronological data, and 3) enabling the frictionless integration of these resources with other cyberinfrastructure (Uhen et al. 2013; Brewer et al. 2012; Committee 2014).

Here we present the neotoma package for R and show how it can be used to directly transfer data from the Neotoma Paleoecology Database into the R statistical computing environment. The broader goals of this effort are 1) to ease the transfer of data from Neotoma into an environment widely used for paleoecological analyses (Simpson & Oksanen 2014; Simpson 2007; Juggins 2013) and 2) to enable transparent and reproducible scientific workflows. The neotoma package itself is available either from the CRAN repository, or from GitHub (<http://github.com/ropensci/neotoma>) where ongoing open-source development continues. Suggestions for improvement and new code contributions by readers and users are welcome.

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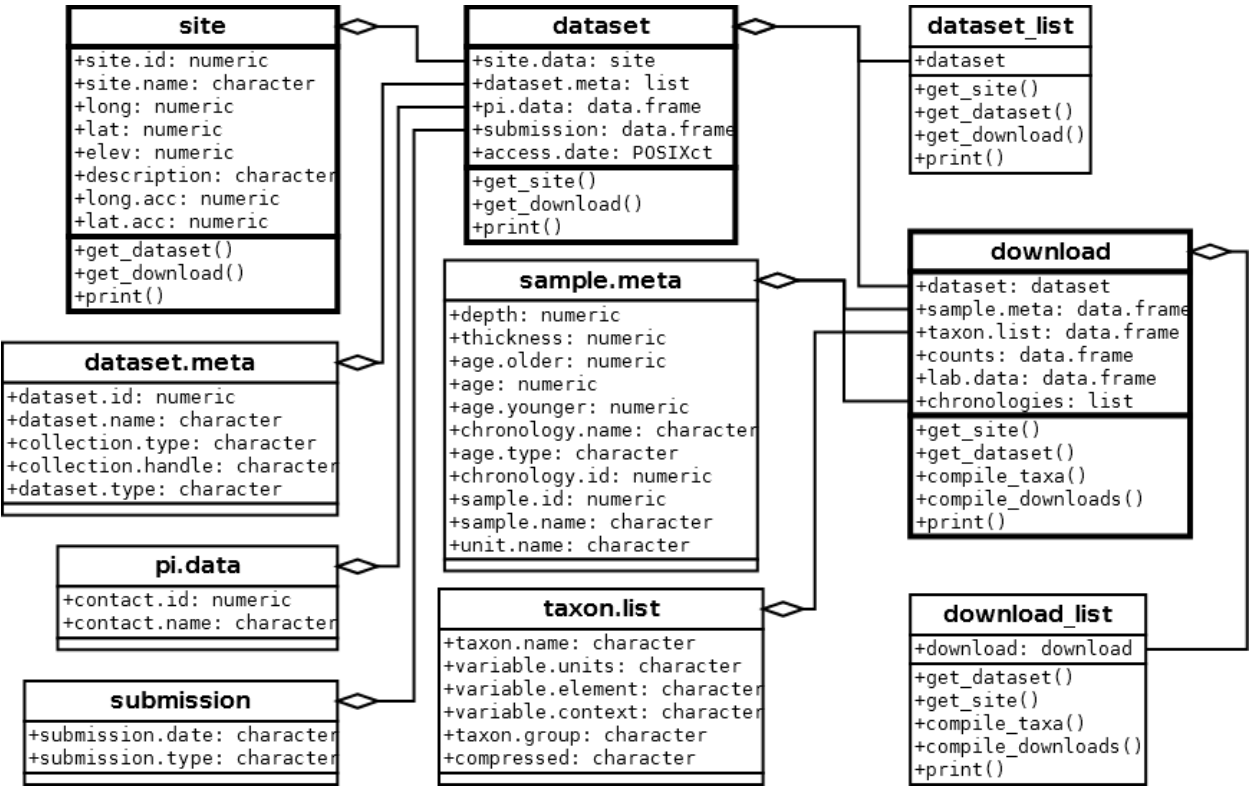
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685

686 **Figures**

687

688



689

690 **Figure 1.** Major classes in neotoma, their relations to one another and the associated methods
691 (functions). The classes described below have a heavier outline than their associated
692 variables.

693

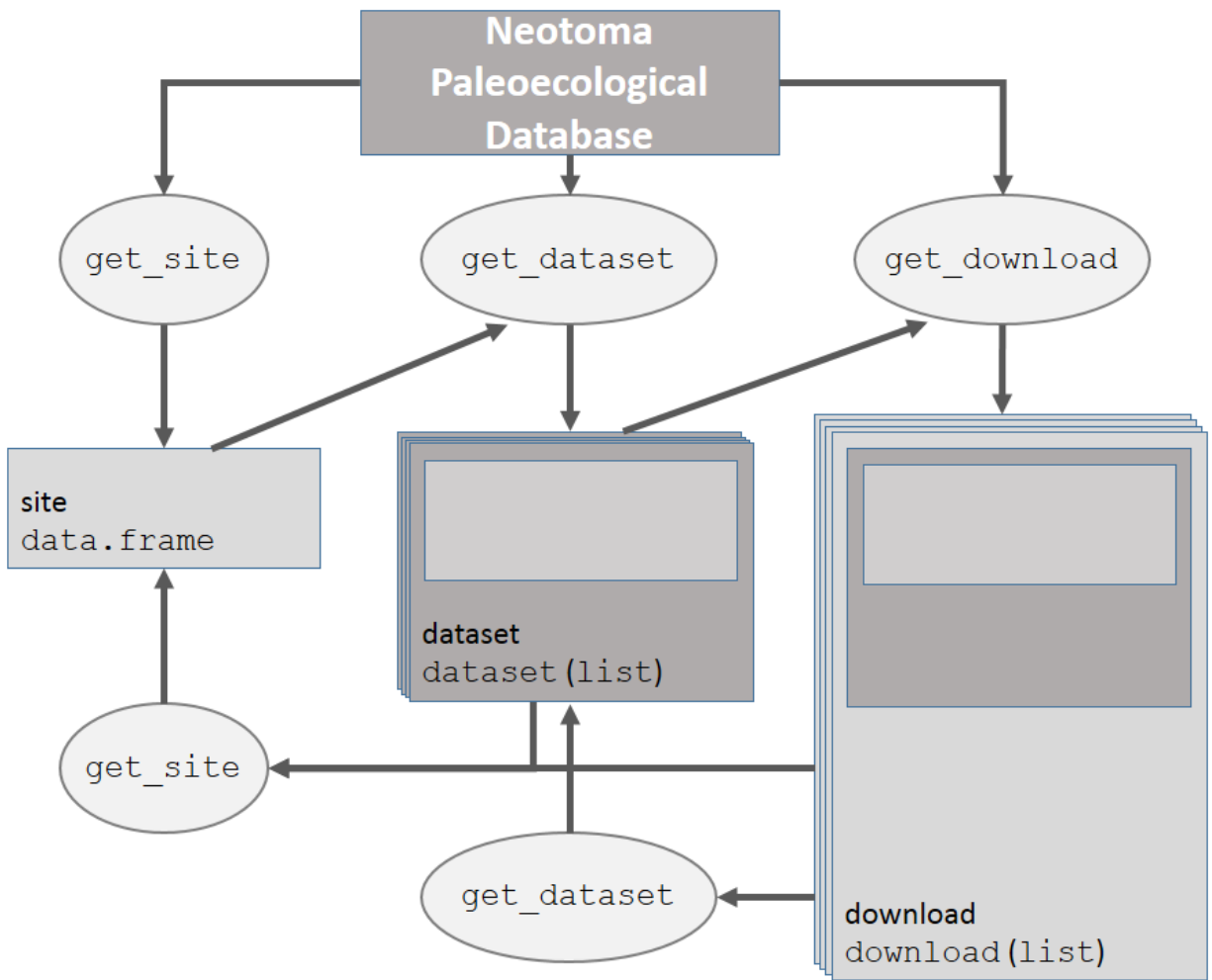


Figure 2. How the main data objects relate to one another in the *neotoma* package, and the helper functions used to move from one data type to another.

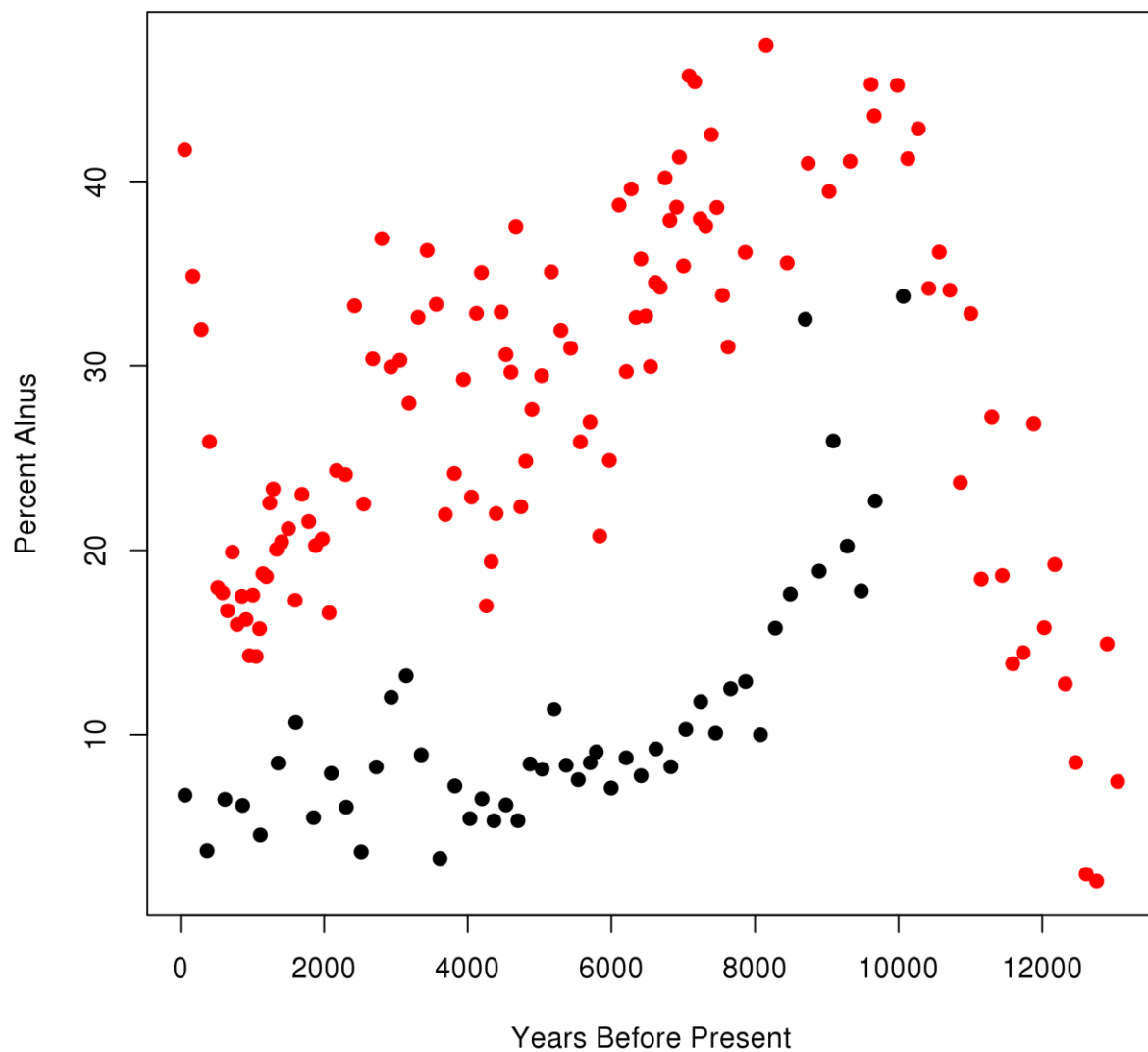


Figure 3. Plots of *Alnus* pollen percentages at two sites, one in the lower mainland of British Columbia (Marion Lake, red) and the other on Haida G'waii (Louise Pond, black). Axis labels are presented as if the code was run directly, but represent calibrated radiocarbon years before present on the x-axis and *Alnus* pollen percentages on the y-axis.

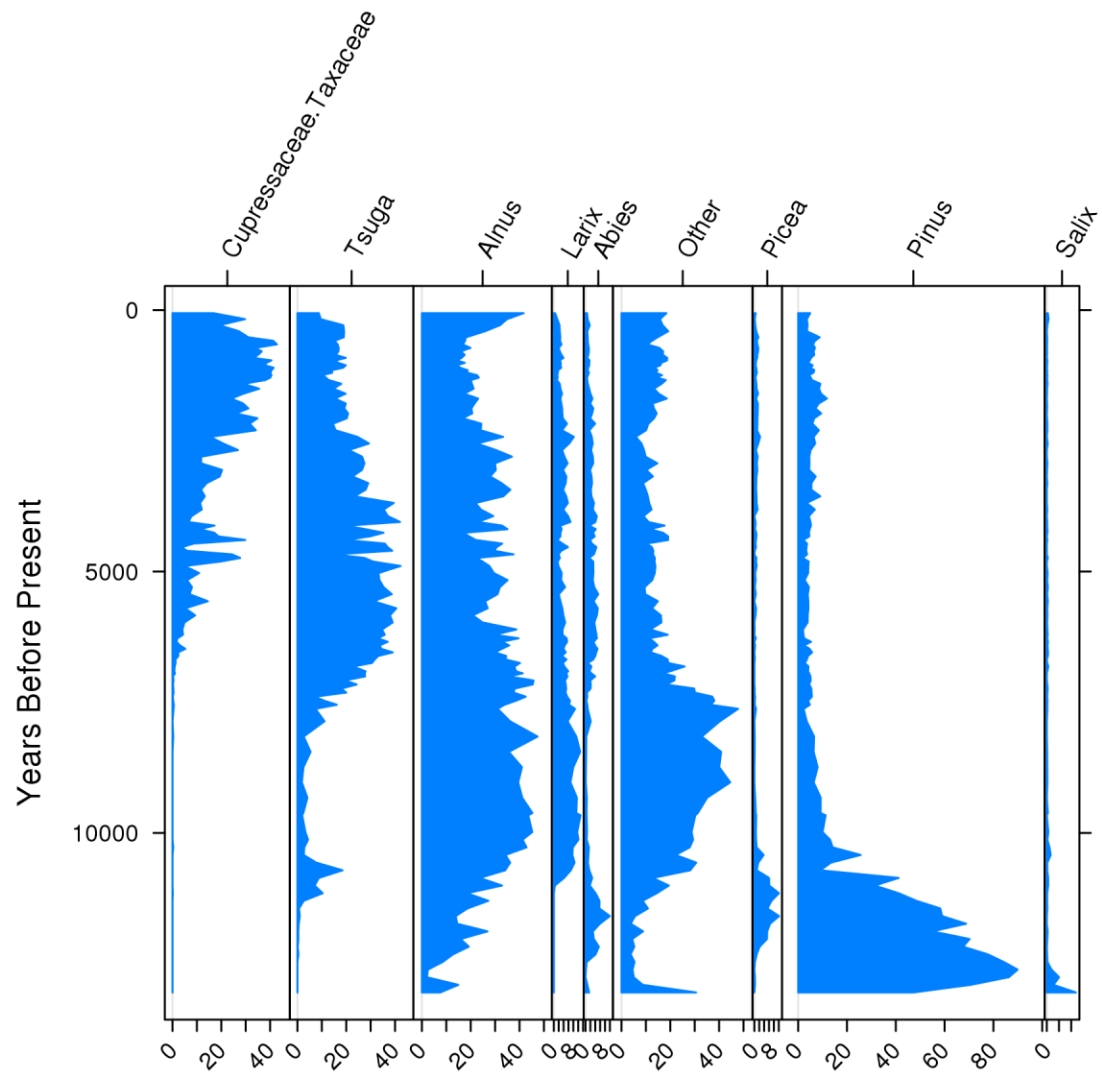


Figure 4. Stratigraphic plot for Marion Lake. Age is plotted on the y-axis in calibrated radiocarbon years before present. The *anaLogue* package provides the opportunity for users to further customize the stratigraphic plot if so desired.

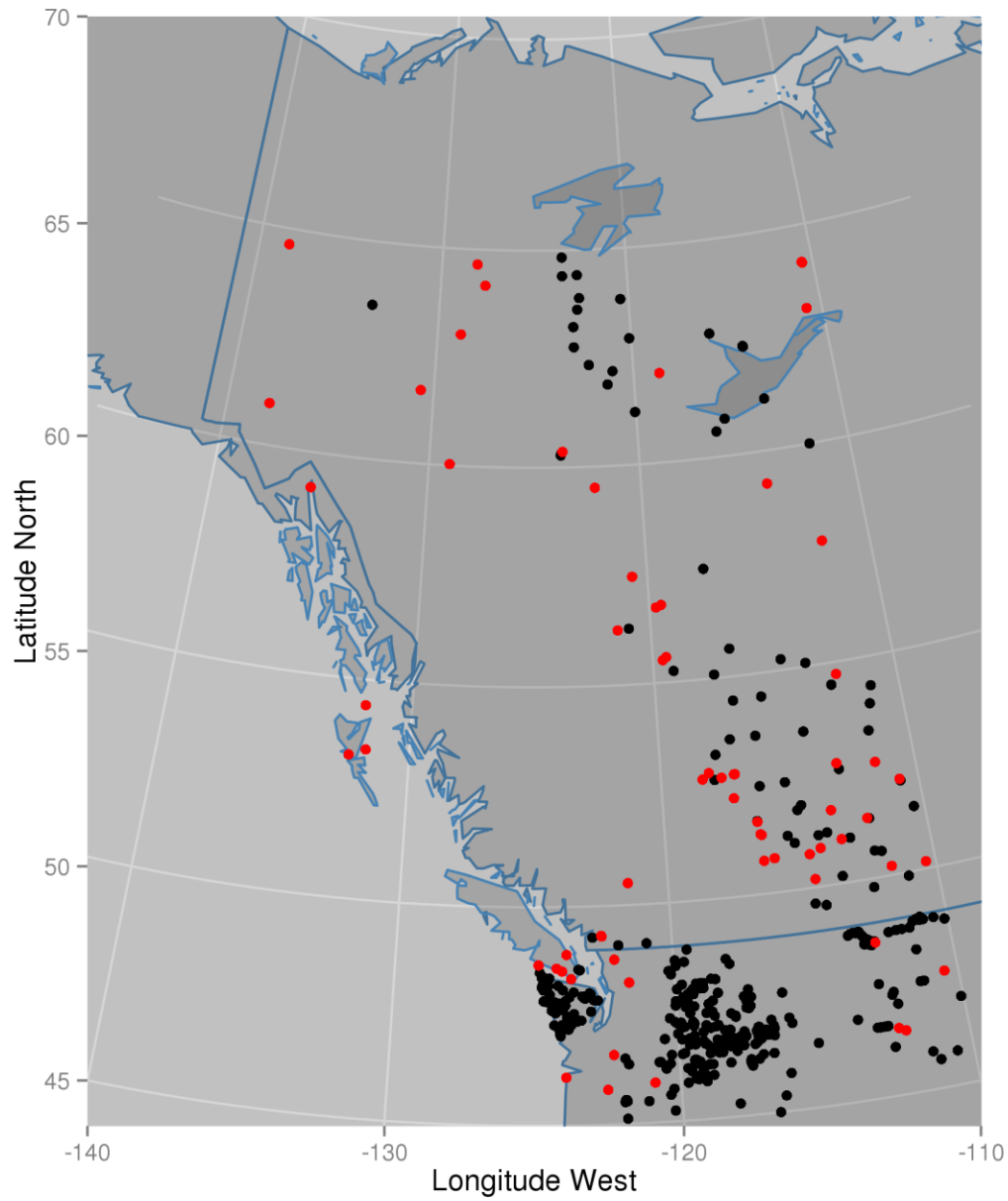


Figure 5 Mapped sites with pollen cores in British Columbia, Alberta and the Yukon Territory of Canada (red), including other Neotoma sites without stratigraphic pollen data (black).

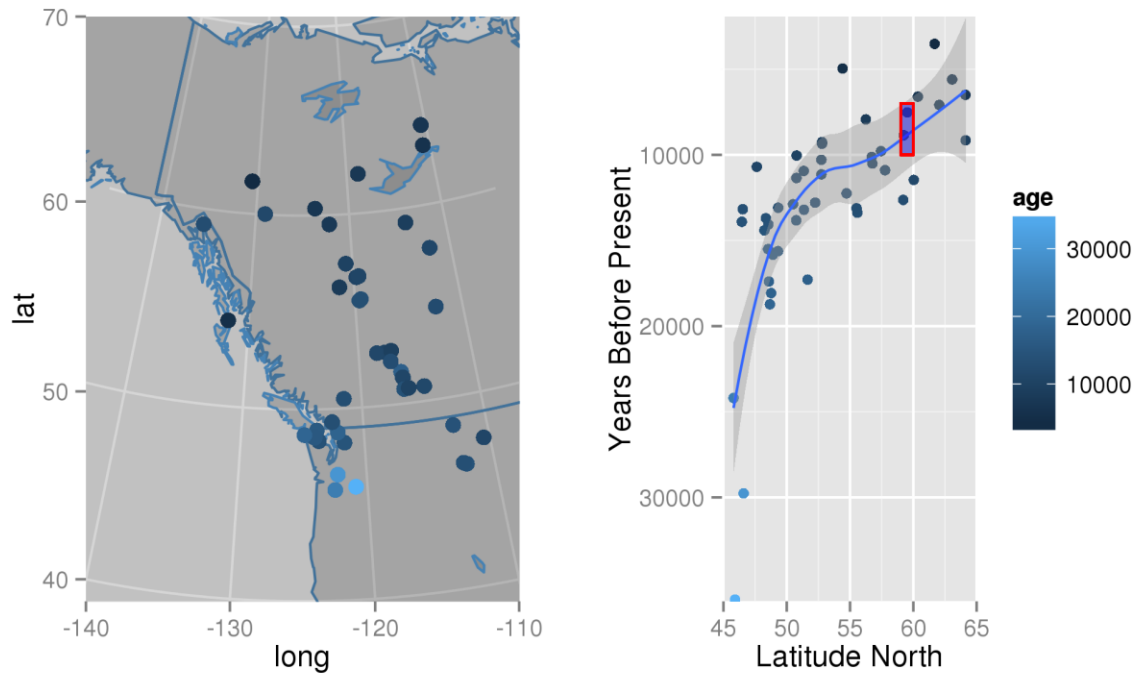
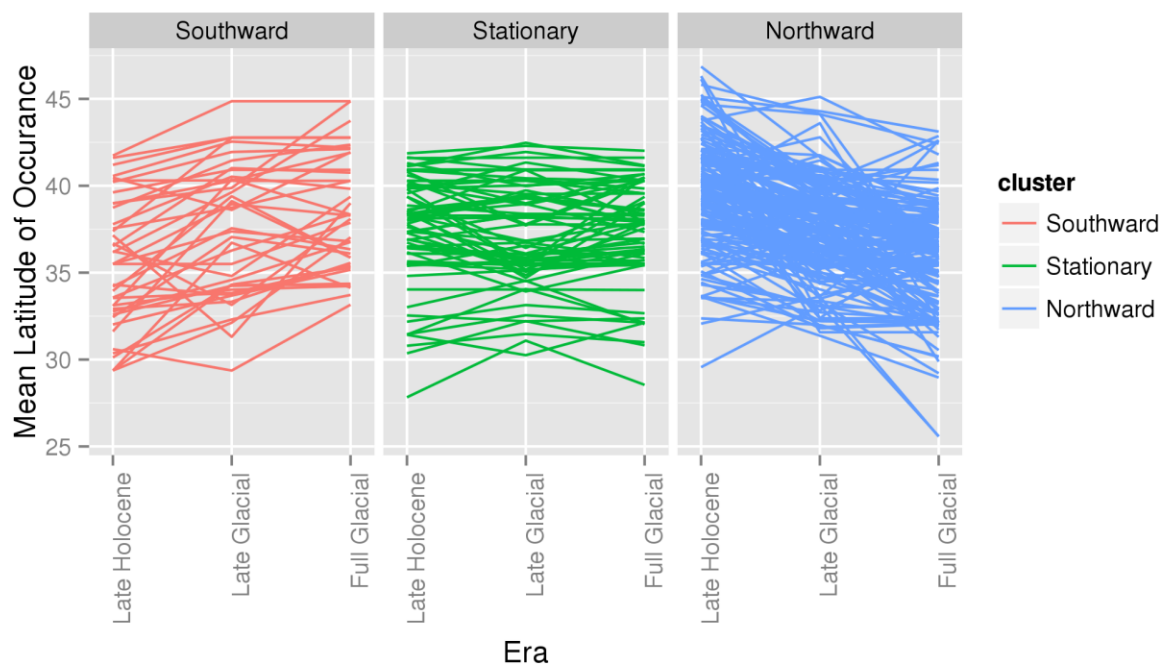


Figure 6. Mapped ages of first *Pinus* establishment in the interior of British Columbia and the Yukon Territory based on a 5% pollen cut-off. The age of first appearance is also plotted and smoothed with a loess curve.



718

719 **Figure 7.** Mean latitudinal distribution of fossil mammal taxa during the late-Pleistocene
 720 show that while there appears to be a net northward migratory pattern, a number of taxa
 721 appear not to shift their ranges, or move southward following deglaciation.