Paleo superstatistics notebook

Getting the data

PBDB API

To obtain the PBDB data we make use of the API in script `data/pbdb_data_get.R`, which accesses the API and cleans the data by:

- removing poorly lithified specimens
- removing collections at the basin scale
- including only fine-scale stratigraphy (below the "group" level)
- resolving taxonomy to the genus or subgenus level where availible (storing genus or subgenus as `otu`)
- combining multiple records of the same OTU per collection
- importing standardized timebins from fossilworks.org (timebins are scraped with script `data/fossilworks_tbins_intervals.R`)

The data gathering script `data/pbdb_data_get.R` is shown below:

```
setwd('data')

# call to the API
show <- paste0(c('ident', 'phylo', 'lith', 'loc', 'time', 'geo', 'stratext',
                 'ecospace'),
               collapse = ',')
version <- '1.2'
base_name <- 'Animalia^Craniata'
min_ma <- 0
max_ma <- 560
timerule <- 'contain'
envtype <- 'marine'

# break-up backbone URI just so it can be nicely displayed
bbURI <- paste0('https://paleobiodb.org/data%s/occs/list.csv?',
                'base_name=%s&show=%s&limit=all&min_ma=%s&max_ma=%s&',
                'timerule=%s&envtype=%s')

# the actual call to the URI
uri <- sprintf(bbURI,
               version,
               base_name,
               show,
               min_ma,
               max_ma,
               timerule,
               envtype)

# get pbdb occurences
x <- read.csv(uri, as.is = TRUE)

# write out raw data
write.csv(x, 'pbdb_data_raw.csv', row.names = FALSE)
```

```
# clean up

# remove unnecceary columns
c2rm <- c('record_type', 'reid_no', 'flags', 'identified_name',
          'identified_rank', 'identified_no', 'difference', 'species_name',
          'species_reso', 'lithdescript', 'lithology1', 'minor_lithology1',
          'lithology2', 'lithification2', 'minor_lithology2', 'cc', 'state',
          'county', 'latlng_basis', 'geogcomments', 'geology_comments',
          'zone', 'localsection', 'localbed', 'localorder',
          'regionalsection', 'regionalbed', 'regionalorder',
          'stratcomments')
x <- x[, !(names(x) %in% c2rm)]

# only well lithified specimens
x <- x[x$lithification1 %in% c('', 'lithified'), ]


# no basin-scale collections
x <- x[x$geogscale != 'basin', ]

# fine scale stratigraphy only
x <- x[!(x$stratscale %in% c('group', 'supergroup')), ]

# resolve taxonomy to genus or subgenus where availible
otu <- x$genus
otu[x$subgenus_name != ''] <- ifelse(x$subgenus_reso[x$subgenus_name != ''] == '',
                                     x$subgenus_name[x$subgenus_name != ''],
                                     otu[x$subgenus_name != ''])
otu[x$primary_reso != ''] <- ''
x$otu <- otu
x <- x[x$otu != '', ]


# combine multiple records of same otu per collection
x <- x[!duplicated(x[, c('collection_no', 'otu')]), ]


# standard time bins
stages <- read.csv('tbins_stages.csv', as.is = TRUE)
earlyTbin <- stages$tbin[match(x$early_interval, stages$name)]
lateTbin <- stages$tbin[match(x$late_interval, stages$name)]
lateTbin[is.na(lateTbin)] <- earlyTbin[is.na(lateTbin)]
earlyTbin[earlyTbin != lateTbin] <- NA

x$tbin <- earlyTbin
x <- x[!is.na(x$tbin), ]


# write out fully processed data
write.csv(x, 'pbdb_data.csv', row.names = FALSE)
```

Scraping fossilworks

The script to pull Alory's time bins (`data/fossilworks_tbins_intervals.R`) is below:

```
# **script to scrape time bins from fossilworks.org**

options(stringsAsFactors = FALSE)

setwd('data')

# loop through interval info on fossilworks.org
coreURI <- 'http://fossilworks.org/bridge.pl?a=displayInterval&interval_no='

tbinInfo <- lapply(1:1108, function(i) {
    print(i)
    linfo <- try(readLines(paste0(coreURI, i), n = 150))

    if('try-error' %in% class(linfo))
        linfo <- try(readLines(paste0(coreURI, i), n = 150))

    if('try-error' %in% class(linfo)) {
        thisTbin <- thisMax <- thisMin <- thisName <- NA
    } else {
        thisTbin <- gsub('^.*10 million year bin: |<br>.*$', '',
                         linfo[grep('10 million year bin', linfo)])
        thisMax <- as.numeric(gsub('^.*Lower boundary: equal to | Ma.*$|[^0-9\\.]', '',
                                   linfo[grep('Lower boundary: equal to', linfo)]))
        thisMin <- as.numeric(gsub('^.*Upper boundary: equal to | Ma.*$|[^0-9\\.]', '',
                                   linfo[grep('Upper boundary: equal to', linfo)]))
        thisName <- gsub('^.*<p class="pageTitle">|</p>.*$', '',
                         linfo[grep('class="pageTitle"', linfo)])
    }

    return(data.frame(name = ifelse(length(thisName) == 0, NA, thisName),
                      tbin = ifelse(length(thisTbin) == 0, NA, thisTbin),
                      ma_min = ifelse(length(thisMin) == 0, NA, thisMin),
                      ma_max = ifelse(length(thisMax) == 0, NA, thisMax)))
})

tbinInfo <- do.call(rbind, tbinInfo)


# clean up
# --------

tbinInfo <- tbinInfo[!is.na(tbinInfo$name), ]

# remove 'stage' and equivilant from name
tbinInfo$name <- gsub(' [[:lower:]].*', '', tbinInfo$name)

# split up stages with a '/' into both names
temp <- tbinInfo[grep('/', tbinInfo$name), ]
tbinInfo$name <- gsub('.*/', '', tbinInfo$name)
temp$name <- gsub('/.* ', ' ', temp$name)
```

```
tbinInfo <- rbind(tbinInfo, temp)

# fix random typo
tbinInfo$name[tbinInfo$name == 'Cazenovia'] <- 'Cazenovian'


# write out
write.csv(tbinInfo, 'tbins_stages.csv', row.names = FALSE)


# also write out summary of each time bin, most importantly (for plottin)
# its midpoint

tbinmid <- sapply(unique(tbinInfo$tbin[!is.na(tbinInfo$tbin)]), function(tbin) {
    tt <- unlist(tbinInfo[tbinInfo$tbin == tbin, c('ma_min', 'ma_max')])
    return(mean(range(tt, na.rm = TRUE)))
})

tbinmid <- sort(tbinmid, decreasing = TRUE)

write.csv(data.frame(tbin = names(tbinmid), ma_mid = as.numeric(tbinmid)), 'data/tbinsMid.csv',
          row.names = FALSE)
```

Three timer and publication bias correction

Once the data have been downloaded and cleaned, we correct for incomplete and biased sampling with the script `data/pbdb_3TPub_make.R` which sources the function `R/make3TPub.R` to generate the main output: a matrix with time bins as rows, taxa (families in this case) as columns and bias-corrected richness as cells.

```
# **this script produces diversity estimates per family per time bin from PBDB data
# corrected by the '3 timers method' and for possible publication bias**

# source function to produce a matrix of time by taxon with cells
# of corrected diversity
source('R/make3TPub.R')

# load other needed funcitons

# source('code/sstat_comp.R')
# source('code/sstat_methods.R')
# source('code/Px_gam.R')

# load and prepare data
# ---------------------

pbdbDat <- read.csv('data/pbdb_data.csv', as.is = TRUE)

# make column for midpoint ma
pbdbDat$ma_mid <- (pbdbDat$max_ma + pbdbDat$min_ma) / 2

# get rid of poor temporal resolution
pbdbDat <- pbdbDat[pbdbDat$tbin != '', ]
```

```r
# get rid of bad taxonomy
pbdbDat <- pbdbDat[pbdbDat$family != '', ]
pbdbDat <- pbdbDat[pbdbDat$otu != '', ]

# get bin times
pbdbDat$mid_ma <- (pbdbDat$min_ma + pbdbDat$max_ma) / 2
pbdbTime <- sort(tapply(pbdbDat$mid_ma, pbdbDat$tbin, mean))
pbdbDat$tbin <- factor(pbdbDat$tbin, levels = names(pbdbTime))


# data.frame to hold publication, diversity and 3T stat
famTbinBias <- aggregate(list(div = pbdbDat$otu), list(fam = pbdbDat$family,
                                                       tbin = pbdbDat$tbin),
                         function(x) length(unique(x)))


# three timer stat and publication bias
# -------------------------------------

# matrix to determine three timers and part timers (sensu alroy 2008)
mt <- matrix(0, nrow = nlevels(pbdbDat$tbin),
             ncol = nlevels(pbdbDat$tbin))
diag(mt) <- -10
mt[abs(row(mt) - col(mt)) == 1] <- 1

# loop through and compute three timers and part timers
timers <- lapply(split(pbdbDat$tbin, pbdbDat$otu),
                 function(x) {
                     # browser()
                     tbins <- integer(nlevels(x))
                     tbins[as.integer(unique(x))] <- 1
                     t3 <- as.integer(mt %*% tbins == 2)
                     tp <- as.integer(mt %*% tbins == -8)

                     return(cbind(t3, tp))
                 })

# compute 3 timer stat from 3 timers and part timers
timers <- array(unlist(timers), dim = c(nrow(timers[[1]]), 2, length(timers)))
t3stat <- 1 - rowSums(timers[, 1, ]) / (rowSums(timers[, 1, ]) + rowSums(timers[, 2, ]))

# add to data.frame holding all info to be saved
famTbinBias$T3Stat <- t3stat[match(famTbinBias$tbin,
                                   levels(pbdbDat$tbin))]
famTbinBias$T3Div <- famTbinBias$div / famTbinBias$T3Stat

# record pubs per tbin
tbinPub <- tapply(pbdbDat$reference_no, pbdbDat$tbin,
                  function(x) length(unique(x)))
famTbinBias$tbinPub <- tbinPub[famTbinBias$tbin]

# calculate corrected diversity
pdf('ms/figSupp_divByPub_foo.pdf', width = 4, height = 4)
```

```
pbdbFamDiv <- with(famTbinBias,
                  make3TPub(div, T3Stat, tbinPub, fam, tbin, pbdbTime,
                            minPub = 10, plotit = TRUE))
dev.off()

# write out corrected diversity
write.csv(pbdbFamDiv, 'data/pbdb_3TPub-corrected.csv')
```

Here is the guts of the `make3TPub` function

```
#' @description function to produce a matrix of time by taxa with cells of corrected diversity
#' @param rawDiv the raw diversity of each taxon in each time interval
#' @param t3stat the 3 timer stat for each diversity record
#' @param pub the number of publications associated with each diversity record
#' @param taxa the taxon names for each diversity record
#' @param tbin the time interval of each diversity record
#' @param tbinTime times associated with each `tbin`
#' @param minPub minimum number of publications for inclusion in regression analysis
#' @param plotit logical, should plot of taxon richness versus number of publications be made
#' @return a matrix with rows corresponding to time intervals and columns to the given taxa
#' each cell in the matrix represents corrected taxon richness


make3TPub <- function(rawDiv,  t3stat,  pub,  taxa,  tbin,  tbinTime,
                      minPub = 10,  plotit = FALSE) {
    #   put data together so can be universally manipulated
    x <- data.frame(rawDiv = rawDiv, t3stat = t3stat, pub = pub, taxa = taxa, tbin = tbin)
    x$tbin <- as.character(x$tbin)
    x$taxa <- as.character(x$taxa)

    x <- x[!is.na(t3stat) & pub >=  minPub, ]

    tbinTime <- tbinTime[names(tbinTime) %in% x$tbin]

    #   3-timer correction
    t3cor <- x$rawDiv/x$t3stat

    #   publication correction
    logPub <- log(x$pub)
    pubLM <- lm(log(t3cor)~logPub)
    pbdbPubLM <<- pubLM # save regression to global env

    pubResid <- exp(pubLM$residuals)

    #   plot so you can verify cuttoff etc.
    if(plotit) {
        plot(log(x$pub), log(t3cor),
             xlab = 'log(Number of publications)',
             ylab = 'log(3T-corrected number of genera)')
        abline(pubLM, col = 'red')
    }

    tbinTaxa <- socorro::tidy2mat(x$tbin, x$taxa, pubResid)
```

```
    return(tbinTaxa[names(sort(tbinTime, decreasing = TRUE)), ])
}
```

Super statistical analysis of 3TPub-corrected PBDB data

Once data have been bias-corrected we can complete their super-statistical analysis. We do that in the script `analysis/pbdb_sstat.R` shown here:

```
# **script to run super stat analysis on PBDB data and make plots**

# source needed functions
R.utils::sourceDirectory('R', modifiedOnly = FALSE)
library(socorro) # for plotting

# load and prepare data
# ---------------------

pbdbFamDiv <- read.csv('data/pbdb_3TPub-corrected.csv', row.names = 1)


# coarsen to higher taxonomic groupings

pbdbTax <- read.csv('data/pbdb_taxa.csv', as.is = TRUE)

#' helper function to coarsen taxonomic resolution of `pbdbFamDiv` object
#' @param level a character string specifying the taxonomic level (from order through phylum)

coarsenTaxa <- function(level) {
    m <- tidy2mat(pbdbTax$family[match(colnames(pbdbFamDiv), pbdbTax$family)],
                  pbdbTax[match(colnames(pbdbFamDiv), pbdbTax$family), level],
                  rep(1, ncol(pbdbFamDiv)))
    m <- m[colnames(pbdbFamDiv), ]

    out <- as.matrix(pbdbFamDiv) %*% m
    out <- out[, colnames(out) != '']

    return(out)
}

pbdbOrdDiv <- coarsenTaxa('order')
pbdbClsDiv <- coarsenTaxa('class')
pbdbPhyDiv <- coarsenTaxa('phylum')


# tbin midpoints
tbinMid <- read.csv('data/tbinsMid.csv', as.is = TRUE)
tbinNames <- tbinMid$tbin
tbinMid <- as.numeric(tbinMid[, 2])
names(tbinMid) <- tbinNames

tbinMid <- tbinMid[rownames(pbdbFamDiv)]
```

```r
# super stat analysis
# -------------------

#' helper function to calculate corrected flux
#' @param x the matrix of corrected diversities over which to calculate fluxes

calcFlux <- function(x) {
    apply(x, 2, function(X) {
        flux <- diff(c(0, X))
        return(flux[flux != 0])
    })
}


# calculate flux for families
pbdbFamFlux <- calcFlux(pbdbFamDiv)

# make sstat object for families
sstatPBDBfam3TP <- sstatComp(pbdbFamFlux, minN = 10, plotit = FALSE)

# likelihood CI for family-level sstat analysis
sstatPBDBfam3TPCI <- bootMLE.sstat(sstatPBDBfam3TP, B = 1000, useAll = FALSE)


# do the same for higher taxo levels
pbdbOrdFlux <- calcFlux(pbdbOrdDiv)
sstatPBDBOrd <- sstatComp(pbdbOrdFlux, minN = 10, plotit = FALSE)

pbdbClsFlux <- calcFlux(pbdbClsDiv)
sstatPBDBCls <- sstatComp(pbdbClsFlux, minN = 10, plotit = FALSE)

pbdbPhyFlux <- calcFlux(pbdbPhyDiv)
sstatPBDBPhy <- sstatComp(pbdbPhyFlux, minN = 10, plotit = FALSE)


# plot all sstat analyses
pdf('ms/fig_Px.pdf', width = 4.25 * 1.25, height = 4 * 1.25)

layout(matrix(1:4, nrow = 2, byrow = TRUE))
par(oma = c(3, 3, 0, 0) + 0.5, mar = c(0.1, 0.1, 1.51, 0.1),
    mgp = c(2, 0.5, 0), cex.lab = 1.4)

plot(sstatPBDBfam3TP, xlim = c(1e-04, 5e+02), ylim = c(8e-05, 1),
     xaxt = 'n', yaxt = 'n',
     panel.first = quote(mlePoly(sstatPBDBfam3TPCI$sstat, PPx.gam,
                                 col = hsv(alpha = 0.25), border = NA)))
mtext('Families', side = 3, line = 0)
logAxis(2, expLab = TRUE)

plot(sstatPBDBOrd, xlim = c(1e-04, 5e+02), ylim = c(8e-05, 1), xaxt = 'n', yaxt = 'n',
     addLegend = FALSE)
mtext('Orders', side = 3, line = 0)
```

```r
plot(sstatPBDBCls, xlim = c(1e-04, 5e+02), ylim = c(8e-05, 1), xaxt = 'n', yaxt = 'n',
     addLegend = FALSE)
mtext('Classes', side = 3, line = 0)
logAxis(1:2, expLab = TRUE)

plot(sstatPBDBPhy, xlim = c(1e-04, 5e+02), ylim = c(8e-05, 1), xaxt = 'n', yaxt = 'n',
     addLegend = FALSE)
mtext('Phyla', side = 3, line = 0)
logAxis(1, expLab = TRUE)

mtext('|Fluctuations|', side = 1, outer = TRUE, line = 2)
mtext('Cumulative density', side = 2, outer = TRUE, line = 2)
dev.off()




# plot p_k(x|b) and f(beta) for families
# --------------------------------------

# idea for normality test: sample 1 from each order and do ks test on that subsampled set

# highlight individual trajectories
loFam <- 'Tainoceratidae' # nautiloid
miFam <- 'Lophospiridae' # sea snails
hiFam <- 'Spondylidae' # bivalve
lo <- pbdbFamDiv[, loFam]
mi <- pbdbFamDiv[, miFam]
hi <- pbdbFamDiv[, hiFam]
cols <- hsv(h = c(0.7, 0.45, 0.12), s = c(0.7, 1, 1), v = c(0.8, 0.8, 1))
names(cols) <- c('hi', 'mi', 'lo')

# make CDF for all scale family-level fluctuations
pAll <- lapply(sstatPBDBfam3TP$raw.pk,
               function(x) simpECDF(scale(x)[, 1], complement = TRUE))

pHighlight <- pAll[c(loFam, miFam, hiFam)]

pAll <- do.call(rbind, pAll)

# function to help with individual trajectory plotting
trajLines <- function(t, x, ...) {
    x[x == 0] <- NA
    alive <- range(which(!is.na(x)))

    x[min(alive) - 1] <- 0
    x[max(alive) + 1] <- 0

    t <- t[!is.na(x)]
    x <- x[!is.na(x)]

    lines(t, x, ...)
}
```

```r
# the actual plotting

pdf('ms/fig_pkx-fbeta.pdf', width = 4.25 * 1.25, height = 4 * 1.25)

layout(matrix(c(1, 2, 1, 3), nrow = 2))

par(oma = c(0, 3, 0, 0) + 0.25, mar = c(4, 0, 0, 0) + 0.25,
    mgp = c(2, 0.5, 0), cex.lab = 1.4)

plot(1, xlim = c(540, 0), xaxt = 'n', xaxs = 'i', xlab = '',
     ylim = c(0, max(lo, mi, hi, na.rm = TRUE)), type = 'n')

trajLines(tbinMid, lo, col = cols['lo'], lwd = 2)
trajLines(tbinMid, mi, col = cols['mi'], lwd = 2)
trajLines(tbinMid, hi, col = cols['hi'], lwd = 2)

text(c(450, 230, 10), c(4, 5.25, 2), labels = c(miFam, loFam, hiFam),
     col = cols[c('mi', 'lo', 'hi')], pos = c(3, 4, 2))

paleoAxis(1)
mtext('Millions of years ago', side = 1, line = 3.5)
mtext('Standardized richness', side = 2, line = 2)

legend('topright', legend = 'A', pch = NA, bty = 'n', cex = 1.4)

# scale fluctuations
par(mar = c(3, 0, 1, 0) + 0.25)
plot(pAll, xlim = c(-4, 4), col = 'gray', ylim = c(0, 1.025),
     xlab = 'Scaled fluctuations')
mtext('Cumultive density', side = 2, line = 2)

for(i in 1:length(pHighlight)) lines(pHighlight[[i]], col = cols[i], lwd = 2)

curve(pnorm(x, lower.tail = FALSE), lwd = 2, add = TRUE)

legend('topright', legend = 'B', pch = NA, bty = 'n', cex = 1.4)

# CDF of beta
betaCDF <- simpECDF(sstatPBDBfam3TP$beta, complement = TRUE)
plot(betaCDF, ylim = c(0, 1.025),
     log = 'x', xaxt = 'n', yaxt = 'n',
     xlab = expression(beta), col = 'gray')

theseBeta <- sstatPBDBfam3TP$beta[c(loFam, miFam, hiFam)]
points(theseBeta, approxfun(betaCDF)(theseBeta), bg = cols, pch = 21, cex = 1.2)

logAxis(1, expLab = TRUE)

curve(pgamma(x, sstatPBDBfam3TP$gam.par[1], sstatPBDBfam3TP$gam.par[2],
             lower.tail = FALSE),
      col = 'black', lwd = 2, add = TRUE)

legend('topright', legend = 'C', pch = NA, bty = 'n', cex = 1.4)
```

```
dev.off()
```

To-do

- remove all deprecated files and folders. . . do it in one fell swoop so we can roll back if needed ever
- make the 3TPub script seapparate and have it save (made script, haven't tried running):
    1. the plot of diversity through time (maybe not?)
- make a sepparate script for the plotting of the sstat analysis including:
    1. first it needs to make the corrected diversity fluctuations
    2. the main sstat style CDF
        - need to remove the raw data from the plot
        - need to make sure 95% CI still works
    3. the f(beta) plot
    4. the p_k(x) plot
    5. example trajectories
- do KS analysis with Families
- run clean functions on sepkoski
- manuscript text
    - add more recent citations
    - add more thurough explaination and justification of correction approach
    - respond to other reviewer comments