Machine Learning Seminar 3.
Layout learning.

March 12, 2020

1 R skills

1. Run scripts which are available online.

```
source("http://ashipunov.info/shipunov/school/biol_240/ncov.r", echo=TRUE)
plot(log(confirmed) ~ dt, data=cc, type="b", xlab="Date",
 ylab="Confirmed cases (log)")
```

2. Homework: how to make the `scriptb.r` (`http://ashipunov.info/shipunov/school/biol_240/scriptb.r`) work?

```
## will produce error:
## source("http://ashipunov.info/shipunov/school/biol_240/scriptb.r", echo=TRUE
## t1 <- read.table("trees_m.txt") # this the place of error
## file.show("trees_m.txt") # look on data
## str(t1) # look on result (1)
## head(t1) # look on result (2)
## look on script:
## url.show("http://ashipunov.info/shipunov/school/biol_240/scriptb.r")
## this is how to do it properly:
trees.m <- data.frame(trees[1]*2.54, trees[2]*30.48, trees[3]*(30.38^3))
write.table(trees.m, file="trees_m.txt", row.names=FALSE, quote=FALSE)
t2 <- read.table("trees_m.txt", h=TRUE)
t2.scaled <- scale(t2)
boxplot(t2.scaled)
## do not forget to remove the file (but be careful with this command!)
## unlink("trees_m.txt")
```

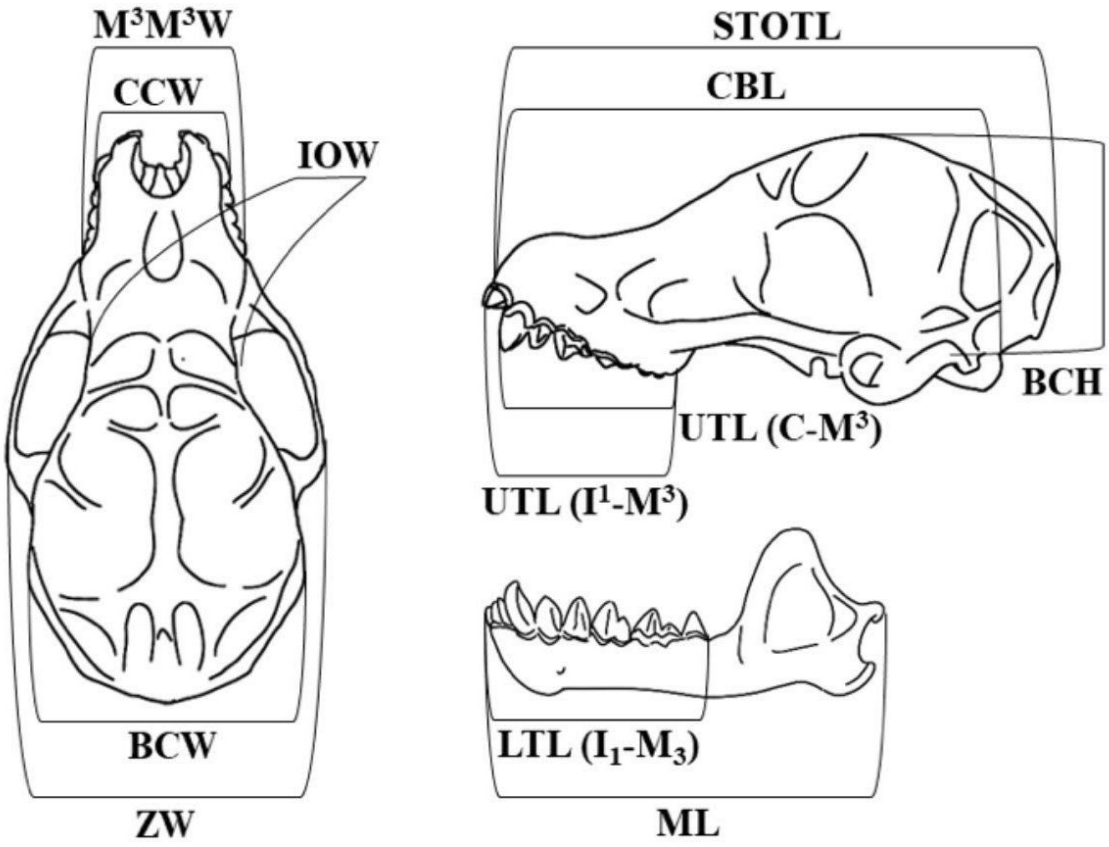
3. More about PCA: biplot, convex hulls and overlap

```
iris.p <- prcomp(iris[, -5], scale=TRUE)
iris.p # loadings (importances of variables)
summary(iris.p) # total variance explained (importances of components)
biplot(iris.p, xpd=TRUE) # shows both original and PCA variables
iris[16, ] # row number 16

library(shipunov) # install also 'PBSmapping' package
```

```
plot(iris.p$x, col=iris$Species)
iris.h <- Hulls(iris.p$x[, 1:2], groups=iris$Species)
summary(Overlap(iris.h))
iris.h <- Hulls(iris.p$x[, 1:2], groups=iris$Species)
summary(Overlap(iris.h))
```

4. How to use *Murina hilgendorfi* data.



Craniodental and mandibular measurements by caliper (linear measurement)

```
## 'sample_murina_hilgendorfi.xls' converted into tab-delimited text file
mh <- read.table(
 "http://ashipunov.info/shipunov/school/biol_240/sample_murina_hilgendorfi.txt",
 h=TRUE, sep="\t")
str(mh)
Str(mh) # useful command: shows number of variable and presence of missing data
sapply(mh[, -(1:4)], Normality) # some variab;es are not normal
mh.cor <- cor(mh[, -(1:4)], method="spearman") # correlation matrix, non-parametric
Pleiad(mh.cor, corr=TRUE, breaks=3) # correlogramm

mh.p <- prcomp(mh[, -(1:4)], scale=TRUE)
palette(rainbow(nlevels(mh$locality)))
plot(mh.p$x, col=mh$locality, pch=as.character(mh$locality))
mh.ph <- Hulls(mh.p$x, groups=mh$locality)
mh.ov <- Overlap(mh.ph)
summary(mh.ov) # calculates overlap of each with all others
palette("default")
Biarrows(mh.p$x, scale(mh[, -(1:4)]), ar.col=1, tx.col=1) # biplot-like
```

```
library(Rdimtools)
mh.i <- do.isomap(scale(mh[, -(1:4)]), type=c("enn", 6))
palette(rainbow(nlevels(mh$locality)))
plot(mh.i$Y, col=mh$locality, pch=as.character(mh$locality))
mh.ih <- Hulls(mh.i$Y, groups=mh$locality)
palette("default")
Biarrows(mh.i$Y, scale(mh[, -(1:4)]), ar.col=1, tx.col=1)
summary(Overlap(mh.ih))

library(uwot)
mh.u <- umap(scale(mh[, -(1:4)]))
oldpal <- palette(rainbow(nlevels(mh$locality)))
plot(mh.u, col=mh$locality, pch=as.character(mh$locality))
mh.uh <- Hulls(mh.u, groups=mh$locality)
palette(oldpal)
Biarrows(mh.u, scale(mh[, -(1:4)]), ar.col=1, tx.col=1)
summary(Overlap(mh.uh))
```

2 Layout Learning

1. Distances: Euclidean, Gower, Jaccard

```
iris.d <- dist(iris[, -5], method="euclidean")
library(shipunov)
iris.g <- Gower.dist(iris) # note that I did not remove 5th column
bin <- +t(moldino > 0) # make binary (occurrence) dataset
library(vegan)
bin.j <- vegdist(bin, dist="jaccard")
```

2. Multidimensional scaling (MDS = PCoA), biplot, surrogate variance and loadings

```
iris.c1 <- cmdscale(iris.d)
plot(iris.c1, col=iris$Species)
Hulls(iris.c1, groups=iris$Species)
MDSv(iris.c1) # importances of dimensions (surrogate explained variance)
Biarrows(iris.c1, scale(iris[, -5])) # biplot-like but for MDS

iris.c2 <- cmdscale(iris.g)
plot(iris.c2, col=iris$Species)
Hulls(iris.c2, groups=iris$Species) # much better -- because we told species

library(MASS)
iris.mds <- isoMDS(dist(iris[, -5]) + 1e-9) # non-metric MDS
cor(iris[, 1:4], iris.mds$points) # variable importances ("loadings")
library(shipunov)
(vv <- MDSv(iris.mds$points)) # dimension importance ("explained variance")
xxlab <- paste0("Dim 1 (", round(vv[1], 2), "%)")
yylab <- paste0("Dim 1 (", round(vv[2], 2), "%)")
abb <- abbreviate(iris$Species, 1, method="both.sides")
plot(iris.mds$points, pch=abb, xlab=xxlab, ylab=yylab)
```

```
Biarrows(iris.mds$points, iris[, -5]) # biplot for MDS
iris.mds.h <- Hulls(iris.mds$points, groups=iris[, 5], usecolors=rep(1, 3), lty=2)
summary(Overlap(iris.mds.h))

library(vegan)
mh.d <- dist(mh[, -(1:4)])
# # run several times, not always converged:
mh.mds <- metaMDS(mh.d, distance="euclidean")
palette(rainbow(nlevels(mh$locality)))
plot(mh.mds$points, col=mh$locality, pch=as.character(mh$locality))
mh.h2 <- Hulls(mh.mds$points, groups=mh$locality)
summary(Overlap(mh.h2))
palette("default")
Biarrows(mh.mds$points, mh[, -c(1:4)], ar.col=1, tx.col=1, lty=2)
```

3. Inferential PCA and MDS

```
library(vegan)
anosim(iris.c1, iris$Species, dist="euclidean")
anosim(iris.c2, iris$Species, dist="euclidean")
anosim(iris.p$x[, 1:2], iris$Species, dist="euclidean")
```

4. Hierarchical clustering and linkage; bootstrap

```
iris.10 <- iris[c(rep(0, 9), 1) > 0, ] # select every 10th row
iris.10d <- dist(iris.10[, -5])
iris.10dh <- hclust(iris.10d, method="ward.D")
plot(iris.10dh, labels=iris.10$Species)

library(shipunov)
iris.10b <- Bclust(iris.10[, -5])
plot(iris.10b$hclust, labels=iris.10$Species)
Bclabels(iris.10b$hclust, iris.10b$values, col="red", pos=3, offset=0.1)

## clustering overlaps
mh.ov # all overlaps
mh.ov[is.na(mh.ov)] <- 0
mh.od <- as.dist(1-mh.ov) # use overlap as distance
plot(hclust(mh.od)) # which groups are closer by overlap
```

5. How to “reverse” trees (and make super-trees)

```
library(shipunov)
iris.h1 <- hclust(dist(iris[, -5]), method="ward.D")
iris.h2 <- hclust(dist(iris[, -5]), method="single")
iris.b1 <- MRH(iris.h1) # raw data from trees
iris.b2 <- MRH(iris.h2)
iris.12 <- cbind(iris.b1, iris.b2) # merge trees data
plot(cmdscale(dist(iris.12)), col=iris$Species) # result
```

6. Partitioning with desired number of clusters; fuzzy methods

```
iris.k <- kmeans(iris[, -5], centers=3)
plot(iris.p$x, col=iris$Species, pch=iris.k$cluster)
library(shipunov)
Misclass(iris$Species, iris.k$cluster, best=TRUE)

mh.k <- kmeans(mh[, -(1:4)], centers=5)
palette(rainbow(nlevels(mh$locality)))
plot(mh.p$x, col=mh$locality, pch=mh.k$cluster)
palette("default")
## Misclass(mh$locality, mh.k$cluster, best=TRUE) # does not work with 9 classes...
new <- as.character(mh$locality) # colnvert locality to character
new2 <- ifelse(!new %in% c("W", "I", "L", "U"), "C", new) # 5 classes only
Misclass(new2, mh.k$cluster, best=TRUE) # insteresting!

library(cluster)
iris.f <- fanny(iris[, -5], k=3)
iris.fzz <- apply(iris.f$membership, 1, var) # fuzziness
tt <- quantile(iris.fzz, 0.25) # threshold
iris.p <- prcomp(iris[, -5], scale=TRUE) # we need it for plotting
plot(iris.p$x, col=iris[, 5], pch=ifelse(iris.fzz < tt, 1, 19))
```

7. *Ad hoc* partitioning: mean-shift and others

```
library(meanShiftR)
iris.m <- meanShift(as.matrix(iris[, -5]))
plot(iris.p$x, col=iris$Species, pch=iris.m$assignment)
library(shipunov)
Misclass(iris.m$assignment, iris$Species, best=TRUE)

mh.m <- meanShift(as.matrix(mh[, -(1:4)]))
palette(rainbow(nlevels(mh$locality)))
plot(mh.p$x, col=mh$locality, pch=mh.m$assignment) # not useful...
palette("default")
```

3 Future

Machine learning in the strict sense: supervised methods. LDA, MANOVA (including nonparametric), recursive partitioning, bagging and boosting, rules methods, k-NN, SVM, neural networks, semi-supervised methods. Geometric morphometry in R.