Final Project

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```r
setwd("~/phylometh_exercises-")
```

#loading Library

```r
library(ape)
library(phangorn)
library(seqinr)
```

```
##
## Attaching package: 'seqinr'

## The following objects are masked from 'package:ape':
##
##     as.alignment, consensus
```

#Alignment and Conversion of data #Interleaved:the function starts to read the sequences after it finds one or more spaces (or tabulations). All #characters before the sequences are taken as the taxa names after removing the leading and trailing spaces (so #spaces in taxa names are not allowed). It is assumed that the taxa names are not repeated in the subsequent #blocks of nucleotides.

```r
mammals <- read.dna("~/phylometh_exercises-/primates.dna", format="interleaved")
mammals_phyDat <- phyDat(mammals, type = "DNA", levels = NULL)

# Subset (first ten)
mammals10 <- subset(mammals_phyDat, 1:10)
mammals10_phyDat <- phyDat(mammals10, type = "DNA", levels = NULL)
```

#Comparing different nucleotide or amino acid substitution models

```r
mt <- modelTest(mammals10)
```

```
## [1] "JC+I"
## [1] "JC+G"
## [1] "JC+G+I"
## [1] "F81+I"
## [1] "F81+G"
## [1] "F81+G+I"
## [1] "K80+I"
## [1] "K80+G"
## [1] "K80+G+I"
## [1] "HKY+I"
## [1] "HKY+G"
## [1] "HKY+G+I"
## [1] "SYM+I"
## [1] "SYM+G"
## [1] "SYM+G+I"
## [1] "GTR+I"
## [1] "GTR+G"
## [1] "GTR+G+I"
```

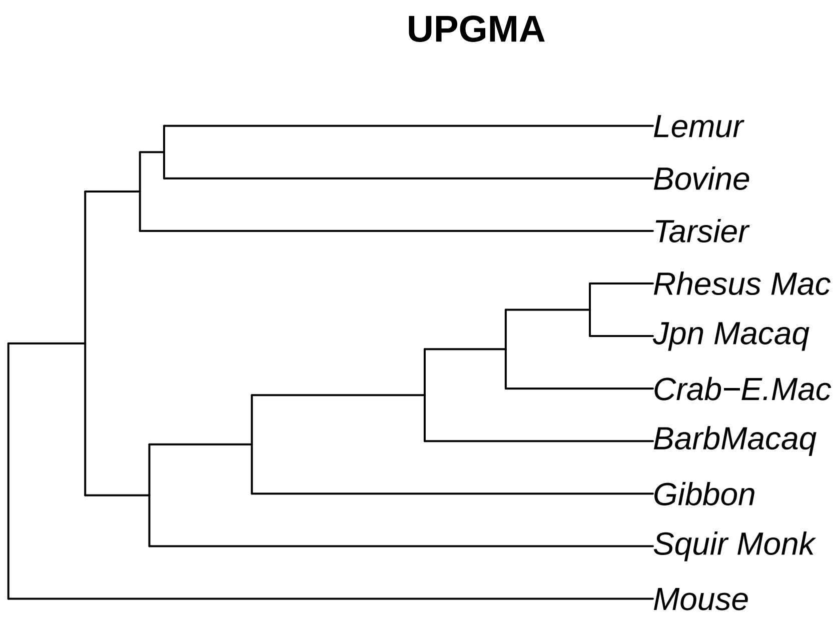
```
print (mt)
```

```
##      Model df    logLik      AIC          AICw     AICc         AICcw      BIC
## 1       JC 17 -2348.727 4731.453 1.015172e-131 4734.313 6.760843e-131 4790.048
## 2     JC+I 18 -2346.692 4729.385 2.856095e-131 4732.596 1.595573e-130 4791.426
## 3     JC+G 18 -2348.426 4732.852 5.045428e-132 4736.063 2.818656e-131 4794.893
## 4   JC+G+I 19 -2346.712 4731.425 1.029722e-131 4735.010 4.772319e-131 4796.913
## 5      F81 20 -2206.835 4453.671  2.119608e-71 4457.652  8.058328e-71 4522.606
## 6    F81+I 21 -2203.862 4449.724  1.525358e-70 4454.124  4.703117e-70 4522.105
## 7    F81+G 21 -2205.054 4452.108  4.629541e-71 4456.508  1.427421e-70 4524.490
## 8  F81+G+I 22 -2203.861 4451.721  5.617673e-71 4456.564  1.388572e-70 4527.550
## 9      K80 18 -2301.019 4638.039 1.955405e-111 4641.250 1.092397e-110 4700.080
## 10   K80+I 19 -2297.749 4633.498 1.893960e-110 4637.082 8.777693e-110 4698.986
## 11   K80+G 19 -2298.851 4635.701 6.293413e-111 4639.286 2.916727e-110 4701.189
## 12 K80+G+I 20 -2297.747 4635.494 6.980091e-111 4639.475 2.653692e-110 4704.429
## 13     HKY 21 -2056.374 4154.748  1.724267e-06 4159.148  5.316410e-06 4227.129
## 14   HKY+I 22 -2048.676 4141.352  1.397503e-03 4146.194  3.454337e-03 4217.181
## 15   HKY+G 22 -2045.236 4134.473  4.357813e-02 4139.315  1.077161e-01 4210.301
## 16 HKY+G+I 23 -2042.963 4131.926  1.556797e-01 4137.234  3.048900e-01 4211.201
## 17     SYM 22 -2195.356 4434.712  2.773590e-67 4439.554  6.855740e-67 4510.541
## 18   SYM+I 23 -2194.096 4434.192  3.598326e-67 4439.499  7.047120e-67 4513.467
## 19   SYM+G 23 -2190.897 4427.794  8.818587e-66 4433.101  1.727071e-65 4507.069
## 20 SYM+G+I 24 -2190.899 4429.797  3.238684e-66 4435.594  4.965990e-66 4512.519
## 21     GTR 25 -2052.104 4154.209  2.257535e-06 4160.519  2.677625e-06 4240.377
## 22   GTR+I 26 -2043.425 4138.850  4.883551e-03 4145.699  4.425923e-03 4228.465
## 23   GTR+G 26 -2039.920 4131.840  1.625575e-01 4138.688  1.473246e-01 4221.455
## 24 GTR+G+I 27 -2037.562 4129.124  6.318996e-01 4136.536  4.321810e-01 4222.186
```

```
dna_dist <- dist.ml(mammals10, model="JC69")
```

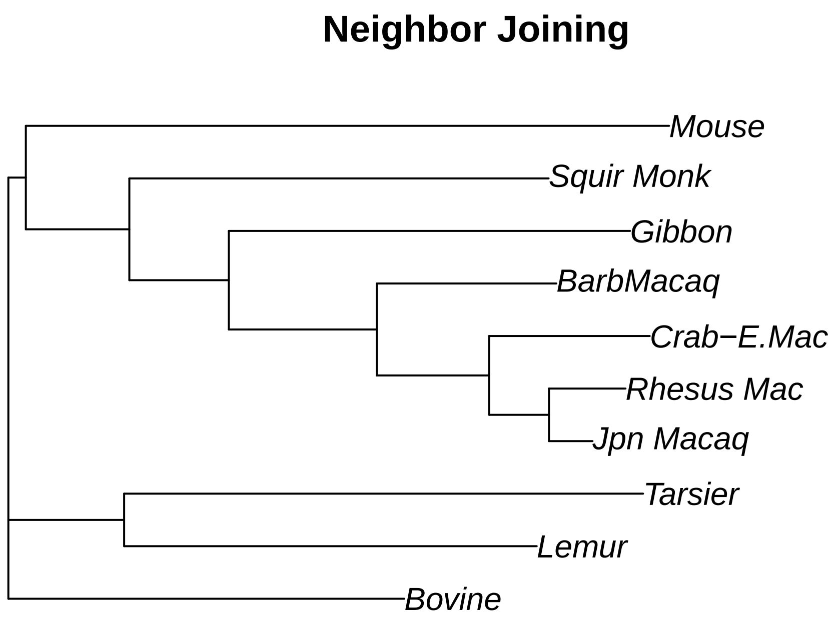
#Estimating tress from distance matrices using neighbor-joining and UPGMA(Unweighted Pair Group Method with #Arithmetic mean) algorithms. #UPGMA is a simple agglomerative hierarchical clustering method

```
mammals_UPGMA <- upgma(dna_dist)
mammals_NJ  <- NJ(dna_dist)
plot(mammals_UPGMA, main="UPGMA")
```



#ploting Neighnor joining #Neighnor joining is a bottom-up (agglomerative) clustering method for the creation of phylogenetic trees #Bottom-up (agglomerative) is a type of hierachical clustering where each observation starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy

```
plot(mammals_NJ, main = "Neighbor Joining")
```



#Parsimony can be used to fit the data of the trees and compare their respective parisimony scores #optim.parismony() gives you a detailed search through the nearest-neighbor interchange (NNI) and subtree pruning #and regrafting (SPR). #pratchet() will perform the search with the parsimony ratchet algorithm.

```
parsimony(mammals_UPGMA, mammals10_phyDat)
```

```
## [1] 586
```

```
parsimony(mammals_NJ, mammals10_phyDat)
```

```
## [1] 580
```

```
mammals_optim <- optim.parsimony(mammals_NJ, mammals10_phyDat)
```

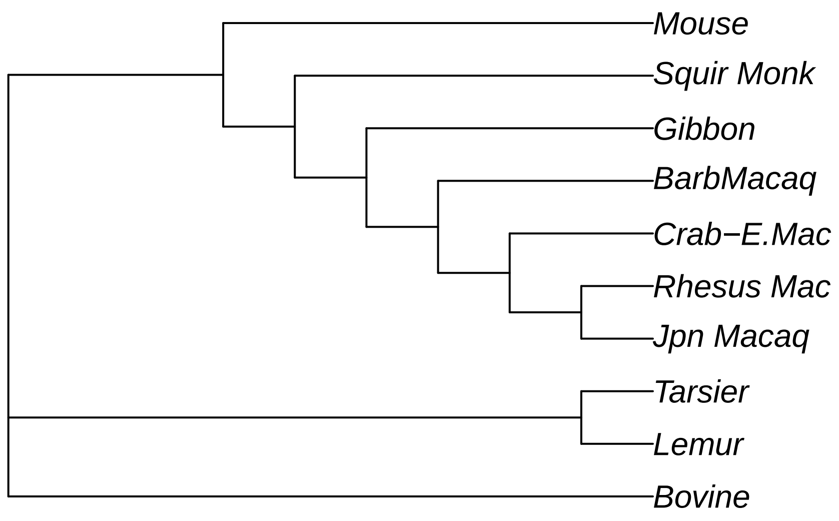
```
## Final p-score 580 after  0 nni operations
```

```
mammals_pratchet <- pratchet(mammals10)
```

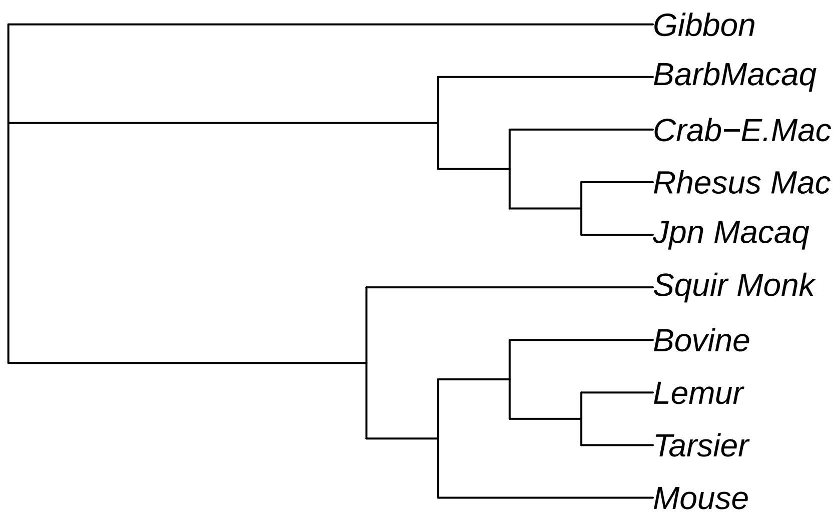
```
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
## [1] "Best pscore so far: 580"
```

#plot mammals_optim and mammals_pratchet

```
plot(mammals_optim)
```



```
plot(mammals_pratchet)
```



#Maximum Likelihood and Bootstrapping #These are more computationally intensive methods than the distance matrix method #Maximum Likelihood helps you to estimate model parameters by align all your sequenced data in a statistical frame work. #pml() can beb used to compute likelihood of a given tree. #To optimize the tree topology and branch length for a selected model of nucleotide evolution, the function optim.pml() can be used

```
fit <- pml(mammals_NJ, mammals10)
print(fit)
```

```
##
##  loglikelihood: -2352.64
##
## unconstrained loglikelihood: -1230.335
##
## Rate matrix:
##   a c g t
## a 0 1 1 1
## c 1 0 1 1
## g 1 1 0 1
## t 1 1 1 0
##
## Base frequencies:
## 0.25 0.25 0.25 0.25
```

```r
fitJC <- optim.pml(fit, model = "JC", rearrangement = "stochastic")
```

```
## optimize edge weights:  -2352.64 --> -2348.727
## optimize edge weights:  -2348.727 --> -2348.727
## optimize topology:  -2348.727 --> -2348.727
## 0
## [1] "Ratchet iteration  1 , best pscore so far: -2348.72667645298"
## [1] "Ratchet iteration  2 , best pscore so far: -2348.72667643957"
## [1] "Ratchet iteration  3 , best pscore so far: -2348.71352776233"
## [1] "Ratchet iteration  4 , best pscore so far: -2348.71352776233"
## [1] "Ratchet iteration  5 , best pscore so far: -2348.71352776233"
## [1] "Ratchet iteration  6 , best pscore so far: -2348.71352776233"
## [1] "Ratchet iteration  7 , best pscore so far: -2348.71352762916"
## [1] "Ratchet iteration  8 , best pscore so far: -2348.71352762916"
## [1] "Ratchet iteration  9 , best pscore so far: -2348.71352762916"
## [1] "Ratchet iteration  10 , best pscore so far: -2348.71352762916"
## [1] "Ratchet iteration  11 , best pscore so far: -2348.71352762916"
## [1] "Ratchet iteration  12 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  13 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  14 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  15 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  16 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  17 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  18 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  19 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  20 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  21 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  22 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  23 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  24 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  25 , best pscore so far: -2348.71352754831"
## [1] "Ratchet iteration  26 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  27 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  28 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  29 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  30 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  31 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  32 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  33 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  34 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  35 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  36 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  37 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  38 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  39 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  40 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  41 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  42 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  43 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  44 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  45 , best pscore so far: -2348.71352752024"
## [1] "Ratchet iteration  46 , best pscore so far: -2348.71352752024"
## optimize edge weights:  -2348.714 --> -2348.714
## optimize topology:  -2348.714 --> -2348.714
## 0
## optimize edge weights:  -2348.714 --> -2348.714
```

```
logLik(fitJC)
```

```
## 'log Lik.' -2348.714 (df=17)
```

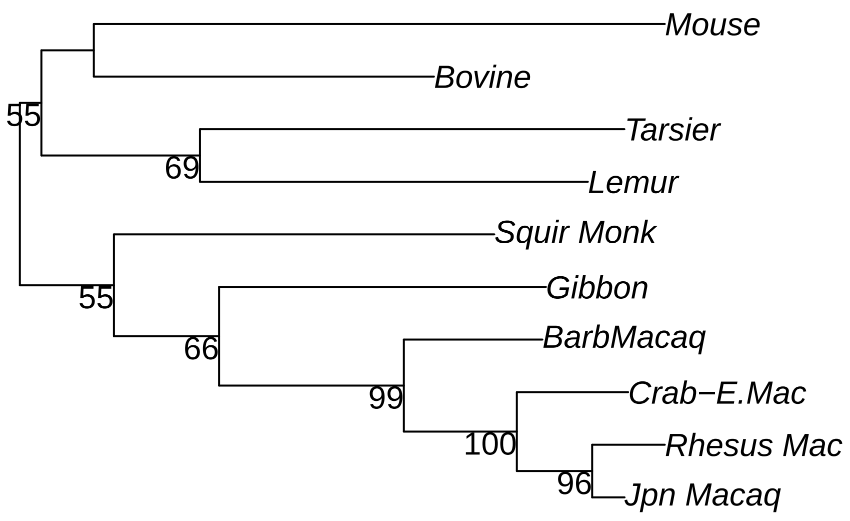
```
bs <- bootstrap.pml(fitJC, bs=100, optNni=TRUE, multicore=TRUE, control = pml.control(trace=0))
```

```
## Warning in if (!is.na(tmp)) {: the condition has length > 1 and only the first
## element will be used
```

```
## Warning in if (tmp == 1) {: the condition has length > 1 and only the first
## element will be used
```

```
## Warning in if (tmp == 2) do_rearr <- extras$rearrangement %in% c("NNI", : the
## condition has length > 1 and only the first element will be used
```

```
plotBS(midpoint(fitJC$tree), bs, p = 50, type="p")
```



#Exporting Trees #write.tree () allows you to export the output in Newick format

```r
write.tree(bs, file="bootstrap_example.tre")
```