# Bioinformatics Lab 2

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```
# Dependencies and data
library(ape)
## Warning: package 'ape' was built under R version 4.4.2
library(dplyr)
##
## Attaching package: 'dplyr'
## The following object is masked from 'package:ape':
##
##
       where
## The following objects are masked from 'package:stats':
##
##
       filter, lag
## The following objects are masked from 'package:base':
##
##
       intersect, setdiff, setequal, union
lizards_accession_numbers <- c("JF806202", "HM161150", "FJ356743", "JF806205",
                                "JQ073190", "GU457971", "FJ356741", "JF806207",
                                "JF806210", "AY662592", "AY662591", "FJ356748",
                                "JN112660", "AY662594", "JN112661", "HQ876437",
                                "HQ876434", "AY662590", "FJ356740", "JF806214",
                                "JQ073188", "FJ356749", "JQ073189", "JF806216",
                                "AY662598", "JN112653", "JF806204", "FJ356747",
                                "FJ356744", "HQ876440", "JN112651", "JF806215",
                                "JF806209")
lizards_sequences<-ape::read.GenBank(lizards_accession_numbers)</pre>
print(lizards_sequences)
## 33 DNA sequences in binary format stored in a list.
##
## Mean sequence length: 1982.879
      Shortest sequence: 931
##
```

```
##
       Longest sequence: 2920
##
## Labels:
## JF806202
## HM161150
## FJ356743
## JF806205
## JQ073190
## GU457971
## ...
##
## Base composition:
       a
             С
## 0.312 0.205 0.231 0.252
## (Total: 65.44 kb)
ape::write.dna(lizards_sequences,
               file = "lizard_seqs.fasta",
               format = "fasta",
               append = FALSE,
               nbcol = 6,
               colsep = " ",
               colw = 10)
```

## Question 1

### Q 1.1

Simulate an artificial DNA sequence dataset. It should contain 33 sequences. The lengths of the sequences should be the same as in the lizard dataset, i.e. for each real sequence simulate an artificial one. The simulation rule is as follows, each nucleotide is to be independently and randomly drawn from the distribution given by the base composition (frequencies) in the true lizard sequences. Save your dataset in a fasta format le. Remember to give unique names to your sequences. Report on the base composition in your simulated data.

The base composition of the respective simulated sequences will be roughly the same as the true base compositions, due to the law of large numbers. Example:

```
# Base frequences of the first real sequence
base.freq(lizards_sequences[1])

## a c g t
## 0.2898696 0.2026078 0.2437312 0.2637914

# Base frequences of the first simulated sequence
base.freq(sim_sequences[1])

## a c g t
## 0.2855711 0.2084168 0.2294589 0.2765531
```

### Question 2

### Q 2.1

Report some basic statistics on each sequence dataset: individual base composition, GC content, CpG, ApT content. Also translate your sequences into protein sequences (see Lab 1) and report on the amino acid composition. In your simulated sequences, how many times did you observe a stop codon inside your sequence? Does this occur in your true sequences? Comment.

```
# Create empty dataframe
df base stats <- data.frame(Accession=character(),</pre>
                             GC cont=numeric(),
                             CpG_cont=numeric(),
                             ApT_cont=numeric())
for(i in 1:33){
  # GC content
  gc_cont <- base.freq(lizards_sequences[1])[c(2,3)] %>% sum()
  \# CpG and ApT contents
  dna_string <- as.character(lizards_sequences)[[i]] %>% paste(collapse = "")
  CpG_cont <- gregexpr(pattern="cg", text=dna_string)[[1]] %>% length() %>% {2*./nchar(dna_string)}
  ApT_cont <- gregexpr(pattern="at", text=dna_string)[[1]] %>% length() %>% {2*./nchar(dna_string)}
  # Store values
  new_row <- data.frame(Accession=lizards_accession_numbers[i],</pre>
                        GC cont=gc cont,
                        CpG_cont=CpG_cont,
```

```
ApT_cont=ApT_cont)

df_base_stats <- rbind(df_base_stats, new_row)
}

df_base_stats

## Accession GC_cont CpG_cont ApT_cont
## 1 JF806202 0.446339 0.02605210 0.1543086</pre>
```

```
JF806202 0.446339 0.02605210 0.1543086
## 2
      HM161150 0.446339 0.02288667 0.1247693
## 3
      FJ356743 0.446339 0.02421308 0.1189900
## 4
      JF806205 0.446339 0.02973241 0.1427156
## 5
      JQ073190 0.446339 0.02713704 0.1492537
## 6
      GU457971 0.446339 0.02199817 0.1429881
      FJ356741 0.446339 0.02144587 0.1224490
## 7
## 8
       JF806207 0.446339 0.02191235 0.1593625
## 9
       JF806210 0.446339 0.02107280 0.1551724
## 10 AY662592 0.446339 0.02054795 0.1273973
## 11 AY662591 0.446339 0.02201705 0.1264205
## 12 FJ356748 0.446339 0.02210708 0.1291883
## 13 JN112660 0.446339 0.01819505 0.1375546
## 14 AY662594 0.446339 0.02044413 0.1290095
## 15 JN112661 0.446339 0.02037846 0.1317322
## 16 HQ876437 0.446339 0.02191235 0.1314741
## 17 HQ876434 0.446339 0.03000000 0.1440000
## 18 AY662590 0.446339 0.01345133 0.1267257
## 19 FJ356740 0.446339 0.01684802 0.1375921
## 20
      JF806214 0.446339 0.02182540 0.1468254
## 21 JQ073188 0.446339 0.01630435 0.1521739
## 22 FJ356749 0.446339 0.01935707 0.1251296
## 23 JQ073189 0.446339 0.01520387 0.1478922
## 24
      JF806216 0.446339 0.03200000 0.1360000
## 25 AY662598 0.446339 0.02044413 0.1254847
## 26 JN112653 0.446339 0.01516361 0.1332801
      JF806204 0.446339 0.01393035 0.1512438
## 28 FJ356747 0.446339 0.02075406 0.1272916
## 29 FJ356744 0.446339 0.02006226 0.1286752
## 30 HQ876440 0.446339 0.02641509 0.1415094
      JN112651 0.446339 0.01533966 0.1322133
## 32
      JF806215 0.446339 0.02193420 0.1395813
      JF806209 0.446339 0.02363050 0.1460795
```

We will now translate the sequences to proteins.

```
# Translate to proteins
# Get codon table and Open Reading Frame (ORF)
cod_orf_info <- read.delim("codon_and_orf.txt", header = TRUE, sep = ",")

lizard_proteins <- list()
sim_proteins <- list()
for(i in 1:33){
    # Translate true lizard sequences
    true_protein <- ape::trans(lizards_sequences[[i]],</pre>
```

Now we can determine the composition of amino acids in the proteins.

```
## Composition of Amino Acids in JF806202
## A C D E F G H I K L M N P
                                    QRSTVWY
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JF806202 (simulated)
## * A C D E F G H I K L M N P
                                       QRSTV
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in HM161150
## A C D E F G H I K L M N P
                                    O R S T
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in HM161150 (simulated)
## * A C D E F G H I K L M N P Q R S T V
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
##
## Composition of Amino Acids in FJ356743
## A C D E F G H I K L M N P
                                    QRST
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in FJ356743 (simulated)
## * A C D E F G H I K L M N P Q R S
                                                      Y
                                              Τ
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21
##
## Composition of Amino Acids in JF806205
## A C D E F G H I K L M N P
                                     QRSTVWY
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JF806205 (simulated)
```

```
## * A C D E F G H I K L M N P Q R S T V W Y
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in JQ073190
## A C D E F G H I K L M N P
                                    QRSTV
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JQ073190 (simulated)
## * A C D E F G H I K L M N P
                                       Q R S
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in GU457971
## A C D E F G H I K L M N P
                                    QRSTV
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in GU457971 (simulated)
## * A C D E F G H I K L M N P Q R S T V
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in FJ356741
## A C D E F G H I K L M N P
                                    QRSTVWY
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in FJ356741 (simulated)
## * A C D E F G H I K L M N P
                                      QRST
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in JF806207
## A C D E F G H I K L M N P Q R S T V
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JF806207 (simulated)
## * A C D E F G H I K L M N P Q R S
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in JF806210
## A C D E F G H I K L M N P Q R S T V
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JF806210 (simulated)
## * A C D E F G H I K L M N P Q R S T
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21
## Composition of Amino Acids in AY662592
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in AY662592 (simulated)
## * A C D E F G H I K L M N P Q R S
                                              Т
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in AY662591
                                    Q R S T V W
## A C D E F G H I K L M N P
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in AY662591 (simulated)
## * A C D E F G H I K L M N P
                                       Q R S
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21
## Composition of Amino Acids in FJ356748
## A C D E F G H I K L M N P Q R S T V W Y
```

```
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in FJ356748 (simulated)
## * A C D E F G H I K L M N P Q R S T
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in JN112660
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JN112660 (simulated)
## * A C D E F G H I K L M N P Q R S
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in AY662594
## A C D E F G H I K L M N P Q R S T V
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in AY662594 (simulated)
## * A C D E F G H I K L M N P Q R S T
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in JN112661
## A C D E F G H I K L M N P Q R S T V W
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in JN112661 (simulated)
## * A C D E F G H I K L M N P Q R S T
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in HQ876437
## A C D E F G H I K L M N P Q R S T V
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in HQ876437 (simulated)
## * A C D E F G H I K L M N P Q R S T V
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in HQ876434
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in HQ876434 (simulated)
## * A C D E F G H I K L M N P Q R S T V
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
##
## Composition of Amino Acids in AY662590
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in AY662590 (simulated)
## * A C D E F G H I K L M N P Q R S T V
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in FJ356740
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in FJ356740 (simulated)
## * A C D E F G H I K L M N P Q R S T V
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
##
```

```
## Composition of Amino Acids in JF806214
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JF806214 (simulated)
## * A C D E F G H I K L M N P Q R S
                                               Τ
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in JQ073188
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JQ073188 (simulated)
## * A C D E F G H I K L M N P Q R S
                                              T
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in FJ356749
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in FJ356749 (simulated)
## * A C D E F G H I K L M N P Q R S T V W Y
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
##
## Composition of Amino Acids in JQ073189
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JQ073189 (simulated)
## * A C D E F G H I K L M N P Q R S T V W Y
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in JF806216
## A C D E F G H I K L M N P Q R S T V W Y
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in JF806216 (simulated)
## * A C D E F G H I K L M N P Q R S
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in AY662598
## A C D E F G H I K L M N P Q R S T V W
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22 3 10
## Composition of Amino Acids in AY662598 (simulated)
## * A C D E F G H I K L M N P Q R S T
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in JN112653
## A C D E F G H I K L M N P Q R S T V W
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in JN112653 (simulated)
## * A C D E F G H I K L M N P Q R S T
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
## Composition of Amino Acids in JF806204
## A C D E F G H I K L M N P Q R S T V
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in JF806204 (simulated)
## * A C D E F G H I K L M N P Q R S T V W Y
```

```
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21 3 21
##
## Composition of Amino Acids in FJ356747
## A C D E F G H I K L
                             M
                               N P
                                     QRST
## 23 8 23 32 13 19 9 21 20 30
                             9 11 15
                                     5 19 25 15 22
## Composition of Amino Acids in FJ356747 (simulated)
## * A C D E F G H I K L M N P
                                        Q R S
                                  9 19 7 26 36 25 21
## 17 13 11 14 12 11 16 4 20 13 28 6
##
## Composition of Amino Acids in FJ356744
## A C D E F G H I K L M N
                                     QRST
                                  Ρ
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in FJ356744 (simulated)
## * A C D E F G H I K L M N
                                    Ρ
                                        QRS
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21
##
## Composition of Amino Acids in HQ876440
## A C D E F G H I K L M N P
                                     QRST
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in HQ876440 (simulated)
## * A C D E F G H I K L M N P
                                        QRS
                                               Т
                                                       Υ
## 17 13 11 14 12 11 16 4 20 13 28 6
                                  9 19 7 26 36 25 21
##
## Composition of Amino Acids in JN112651
## A C D E F G H I K L M N P
                                     QRST
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in JN112651 (simulated)
## * A C D E F G H I K L M
                                  N P
                                        QRS
                                                       Y
                                                Τ
                                  9 19 7 26 36 25 21
## 17 13 11 14 12 11 16 4 20 13 28 6
##
## Composition of Amino Acids in JF806215
## A C D E F G H I K L M N P
                                     QRST
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in JF806215 (simulated)
## * A C D E F G H I K L
                               Μ
                                  N
                                     Ρ
                                        Q R S
                                                Τ
## 17 13 11 14 12 11 16 4 20 13 28 6
                                  9 19 7 26 36 25 21
## Composition of Amino Acids in JF806209
## A C D E F G H I K L M N P
                                     QRSTV
## 23 8 23 32 13 19 9 21 20 30 9 11 15 5 19 25 15 22
## Composition of Amino Acids in JF806209 (simulated)
## * A C D E F G H I K L M N P
                                        QR
                                               Τ
## 17 13 11 14 12 11 16 4 20 13 28 6 9 19 7 26 36 25 21
                                                    3 21
```

Now we will count how many times the stop codons (taa, tag, tga) occur in the respective sequences. Because the simulated sequences are random, the stop codons will occur frequently.

```
# Positions of stop codons in simulated sequence (example)

sim_seq_n_stopcodons <- c()
liz_seq_n_stopcodons <- c()
for(i in 1:33){
    ### Get number of stop codons in *simulated* sequences
    n_taa <- as.character(sim_sequences[[i]] %>%
```

```
paste(collapse="")) %>%
    gregexpr(pattern="taa", text=.) %>%
   unlist() %>% length()
  n_tag <- as.character(sim_sequences[[i]] %>%
                          paste(collapse="")) %>%
    gregexpr(pattern="tag", text=.) %>%
   unlist() %>% length()
  n tga <- as.character(sim sequences[[i]] %>%
                          paste(collapse="")) %>%
    gregexpr(pattern="tga", text=.) %>%
   unlist() %>% length()
  sim_seq_n_stopcodons <- c(sim_seq_n_stopcodons, n_taa+n_tag+n_tga)</pre>
  ### Get number of stop codons in *true* sequences
  n_taa <- as.character(lizards_sequences)[[i]] %>%
                          paste(collapse="") %>%
    gregexpr(pattern="taa", text=.) %>%
   unlist() %>% length()
  n tag <- as.character(lizards sequences)[[i]] %>%
                          paste(collapse="") %>%
    gregexpr(pattern="tag", text=.) %>%
   unlist() %>% length()
 n_tga <- as.character(lizards_sequences)[[i]] %>%
                          paste(collapse="") %>%
    gregexpr(pattern="tga", text=.) %>%
   unlist() %>% length()
  liz_seq_n_stopcodons <- c(liz_seq_n_stopcodons, n_taa+n_tag+n_tga)</pre>
print(sim_seq_n_stopcodons)
## [1] 59 149 174 57 87 65 165 62 78 189 177 184 185 173 160 62 66 179 188
## [20] 65 88 184 88 57 188 145 60 178 180 60 156 61 57
print(liz_seq_n_stopcodons)
        52 131 140 50 78 61 145 57 60 143 138 144 143 144 132 54 55 151 144
## [1]
        56 76 141 78 50 136 124 56 145 139 57 141 57 54
## [20]
\#cat("Number\ of\ stop\ codons\ in\ simulated\ sequences:\n",\ sim\_seq\_n\_stopcodons,\ "\n")
\#cat("Number\ of\ stop\ codons\ in\ true\ sequences:\n",\ liz\_seq\_n\_stopcodons,\ "\n")
# Positions of stop codons in true sequenes
#as.character(lizards_sequences)[[1]] %>% paste(collapse = "") %>%
# gregexpr(pattern="taa", text=.) %>% unlist()
```