Class 12_Structural Bioinformatics II

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11/4/2021

Comparative analysis of protein structures

Using the bio3d package.

```
library(bio3d)

pdb <- read.pdb("1hel")
```

```
##   Note: Accessing on-line PDB file
```

```
pdb
```

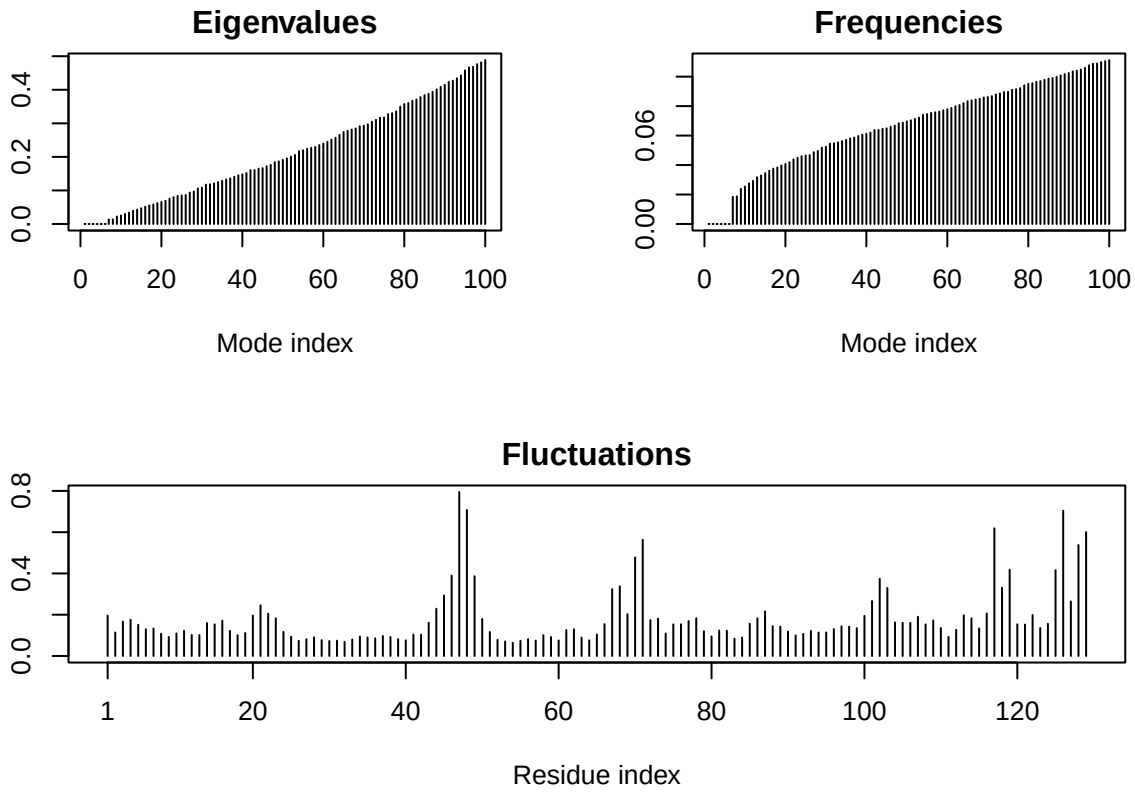
```
##
##  Call:  read.pdb(file = "1hel")
##
##    Total Models#: 1
##      Total Atoms#: 1186,  XYZs#: 3558  Chains#: 1  (values: A)
##
##      Protein Atoms#: 1001  (residues/Calpha atoms#: 129)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 185  (residues: 185)
##      Non-protein/nucleic resid values: [ HOH (185) ]
##
##    Protein sequence:
##       KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINS
##       RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDV
##       QAWIRGCRL
##
## + attr: atom, xyz, seqres, helix, sheet,
##         calpha, remark, call
```

Let's use a bioinformatics method called NMA (Normal Mode Analysis) to predict the dynamics (flexibility) of this enzyme.

```
modes <- nma(pdb)
```

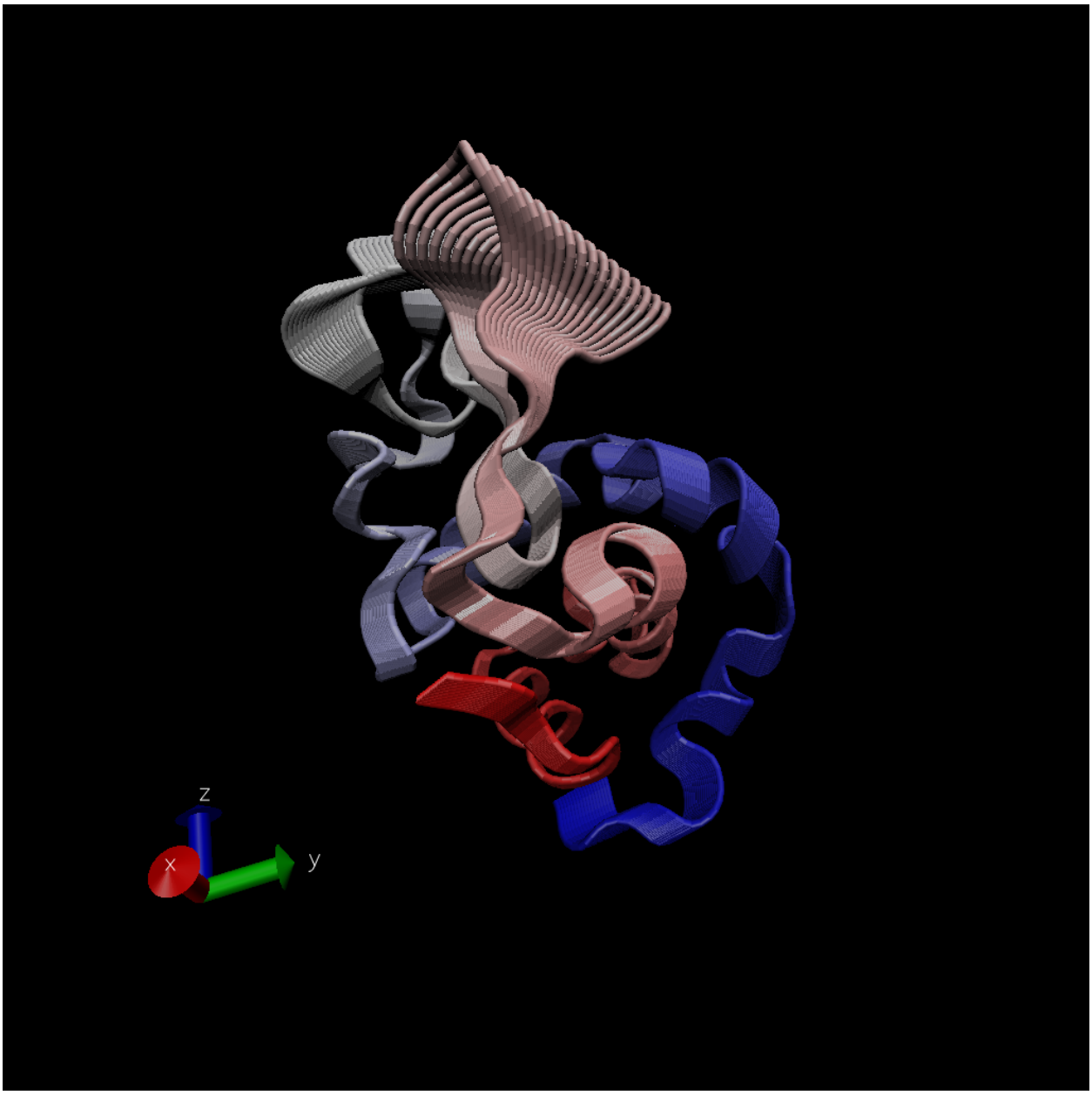
```
##  Building Hessian...     Done in 0.064 seconds.
##  Diagonalizing Hessian...    Done in 0.281 seconds.
```

```
plot.nma(modes)
```



Make a "move" of its predicted motion. We often call this a "trajectory".

```
mktrj(modes, file = "nma.pdb")
```



Analysis of ADK

```
library(bio3d)
aa <- get.seq("1ake_A")
```

```
## Warning in get.seq("1ake_A"): Removing existing file: seqs.fasta
```

```
## Fetching... Please wait. Done.
```

```
aa
```

```
##              1        .         .         .         .         .         60
## pdb|1AKE|A   MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##              1        .         .         .         .         .         60
##
##             61        .         .         .         .         .         120
## pdb|1AKE|A   DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##             61        .         .         .         .         .         120
##
##            121        .         .         .         .         .         180
## pdb|1AKE|A   VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##            121        .         .         .         .         .         180
##
##            181        .         .         .   214
## pdb|1AKE|A   YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
##            181        .         .         .   214
##
## Call:
##   read.fasta(file = outfile)
##
## Class:
##   fasta
##
## Alignment dimensions:
##   1 sequence rows; 214 position columns (214 non-gap, 0 gap)
##
## + attr: id, ali, call
```

```
# Run BLAST from BLAST
# blast <- blast.pdb(aa)
```

```
# hits <- plot(blast)
```

```
# hits$pdb.id
```

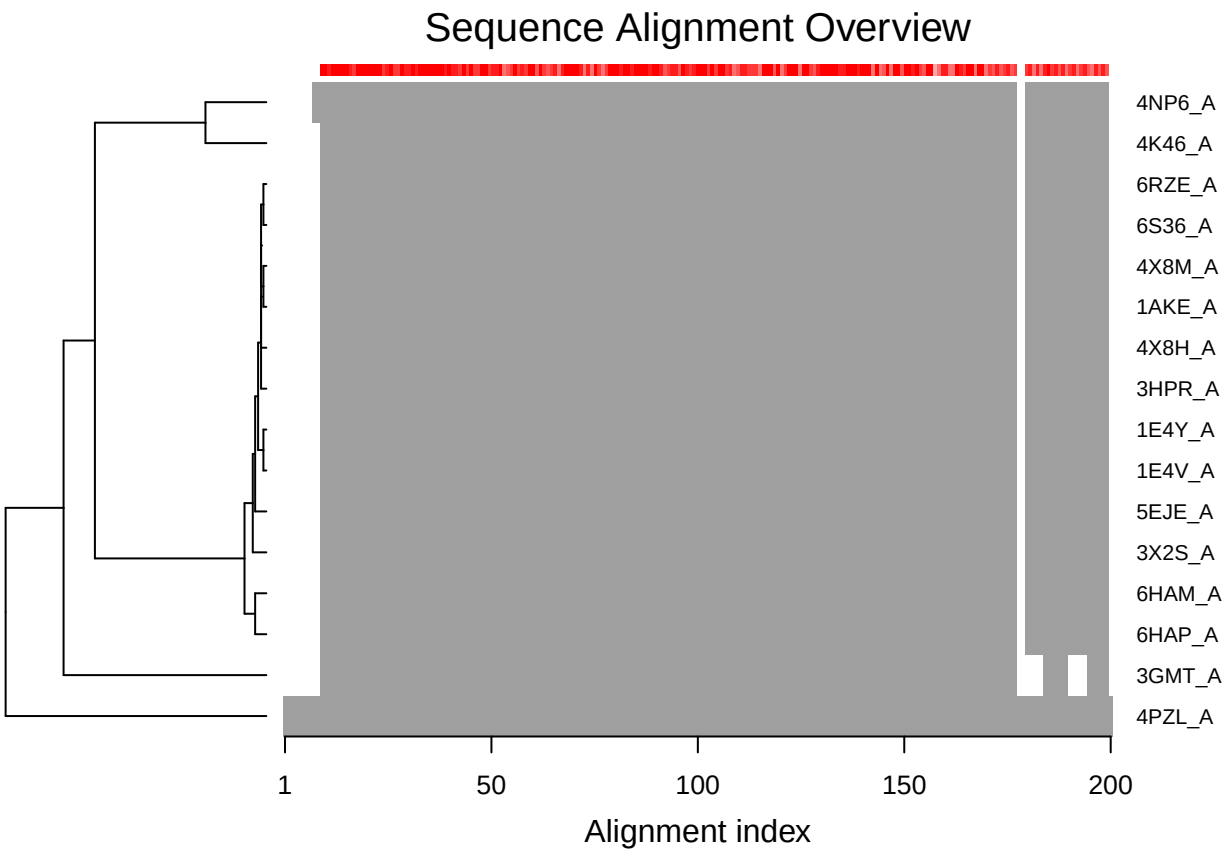
```
# Download releated PDB files
# files <- get.pdb(hits$pdb.id, path="pdbs", split=TRUE, gzip=TRUE)
```

Multiple structure alignmentcd

```
# pdbs <- pdbaln(files, fit = TRUE)
```

```
# Align releated PDBs
# pdbs <- pdbaln(files, fit = TRUE)#, exefile="msa")
#save(pdbs, blast, file="mydata.RData")
load(file="mydata.RData")
```

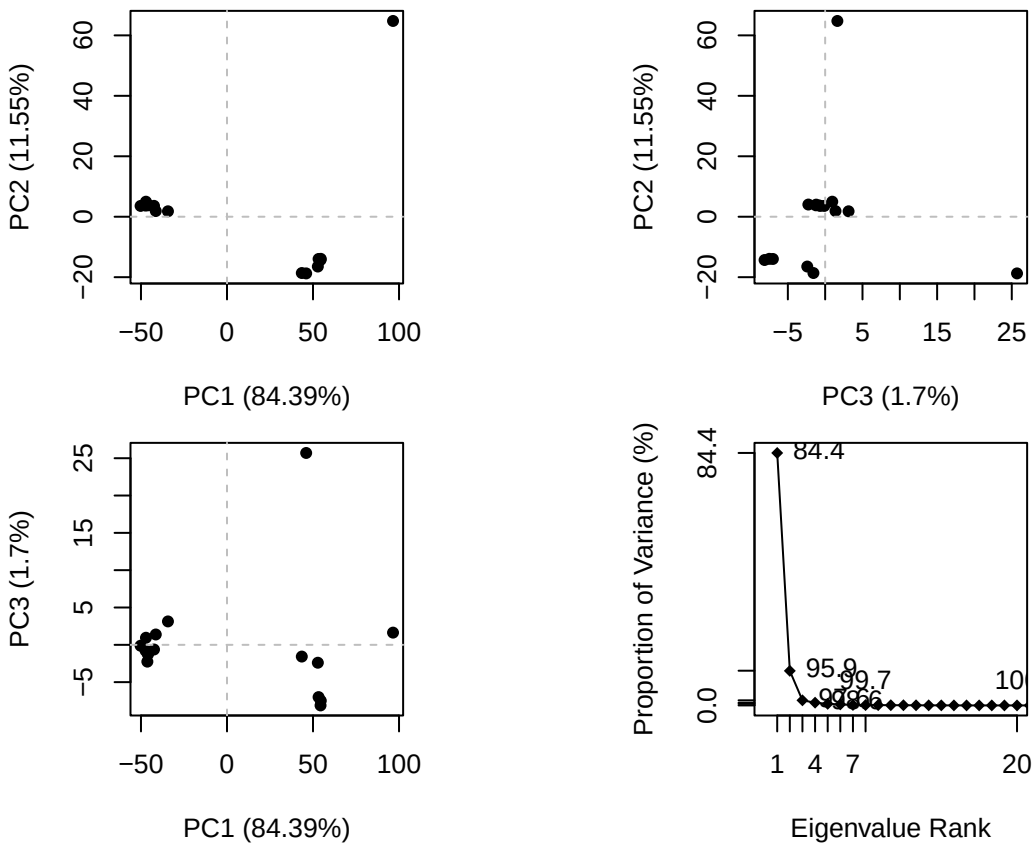
```
# Vector containing PDB codes for figure axis
ids <- basename.pdb(pdbs$id)

# Draw schematic alignment
plot(pdbs, labels=ids)
```



PCA

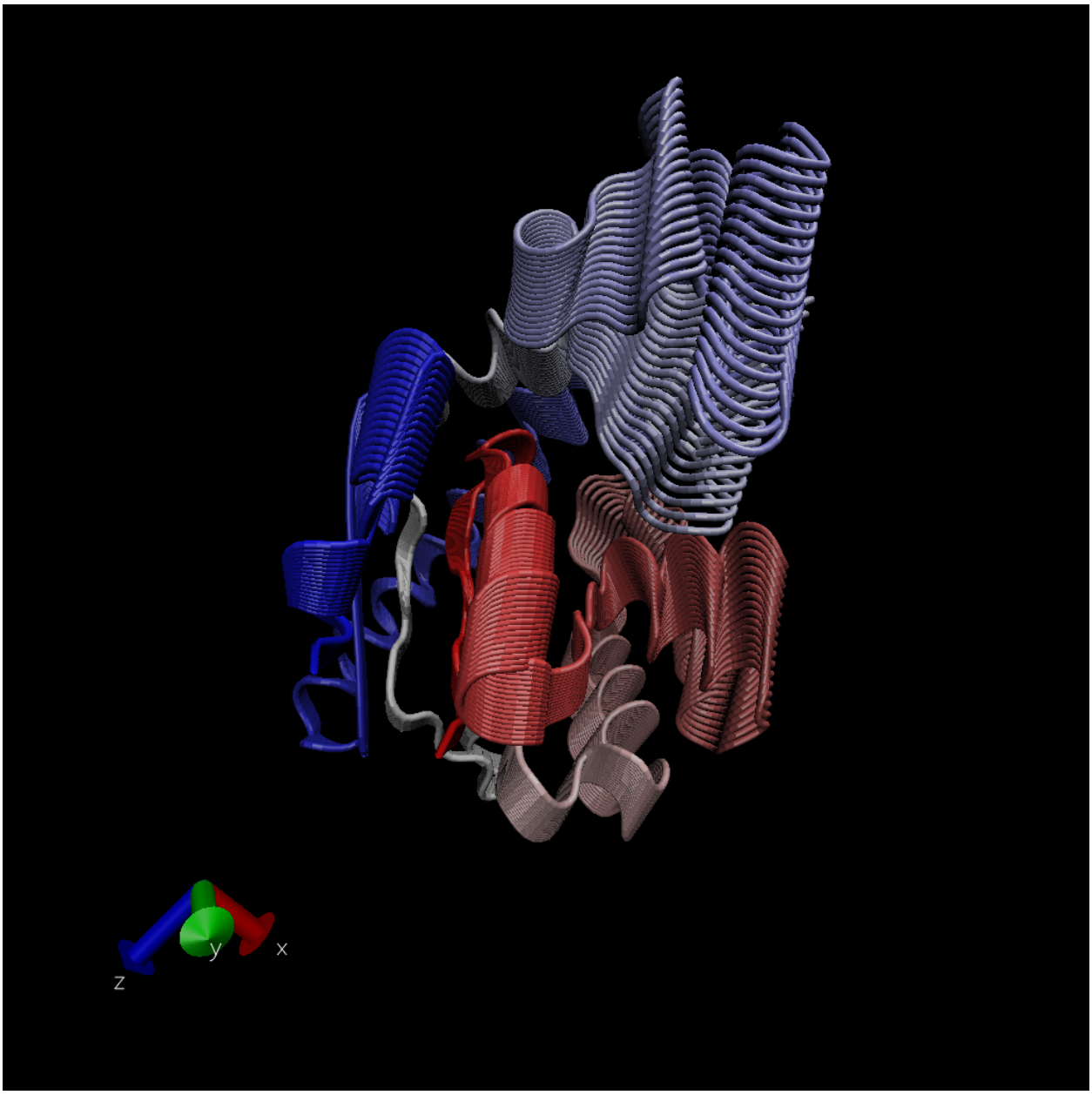
We will use the bio3d pca() function which is deigned for protein structure data.

```
# Perform PCA
pc.xray <- pca(pdbs)
plot(pc.xray)
```



Make a trajectory visualization of the motion captured by the first Principal Component.

```
# Visualize first principal component
pc1 <- mktrj(pc.xray, pc=1, file="pc_1.pdb")
```


y
x
z