Class10: Structural Bioinformatics pt1

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What is in the PDB database

The main repository of biomolecular structure info is the PDB < www.rcsb.org >.

Let's see what this database contains:

```
stats <- read.csv("pdb_stats.csv", row.names=1)
stats
```

	X.ray	EM	NMR	Multiple.methods	Neutron	Other
Protein (only)	161,663	12,592	12,337	200	74	32
Protein/Oligosaccharide	9,348	2,167	34	8	2	0
Protein/NA	8,404	3,924	286	7	0	0
Nucleic acid (only)	2,758	125	1,477	14	3	1
Other	164	9	33	0	0	0
Oligosaccharide (only)	11	0	6	1	0	4

	Total
Protein (only)	186,898
Protein/Oligosaccharide	11,559
Protein/NA	12,621
Nucleic acid (only)	4,378
Other	206
Oligosaccharide (only)	22

> Q1: What percentage of structures in the PDB are solved by X-Ray and Electron Microscopy.

```
as.numeric(stats$X.ray)
```

Warning: NAs introduced by coercion

```
[1]   NA  NA  NA  NA 164   11
```

We got to get rid of the commas. Can you find a function to get rid of the commas?

```
x <- stats$X.ray
sum(as.numeric(gsub(",","", x)))
```

```
[1] 182348
```

I am going to turn this into a function and then use `apply()` to work on the entire table of data

```
sumcomma <- function(x) {
  sum(as.numeric(gsub(",","", x)))
}

sumcomma(stats$X.ray)
```

```
[1] 182348
```

```
n.total <- sumcomma(stats$Total)
n.total
```

```
[1] 215684
```

```
sumcomma(stats$EM)
```

```
[1] 18817
```

```
apply(stats, 2, sumcomma)
```

```
        X.ray                EM              NMR Multiple.methods
       182348             18817            14173              230
       Neutron            Other            Total
           79               37           215684
```

```r
apply(stats, 2, sumcomma)/ sumcomma(stats$Total)
```

```
        X.ray             EM            NMR Multiple.methods
   0.8454405519    0.0872433746   0.0657118748    0.0010663749
      Neutron          Other          Total
   0.0003662766    0.0001715473   1.0000000000
```

Q2: What proportion of structures in the PDB are protein?

Q3: Type HIV in the PDB website search box on the home page and determine how many HIV-1 protease structures are in the current PDB?

In UniProt there are 248,805,733 entries which compared to PDB protein entries (186, 898) means there are only ~7% of known sequences 248,805,733 - 186,898

```r
186898/248805733 * 100
```

```
[1] 0.07511804
```

Visualizing the HIV-1 protein strucutre

Mol* ("mol-star") viewer is now everywhere. The homepage is here: https://molstar.org/viewer

I want to insert my image from Mol* here

Working with bio3d package

```r
library(bio3d)
```

```r
pdb <- read.pdb("1hsg")
```
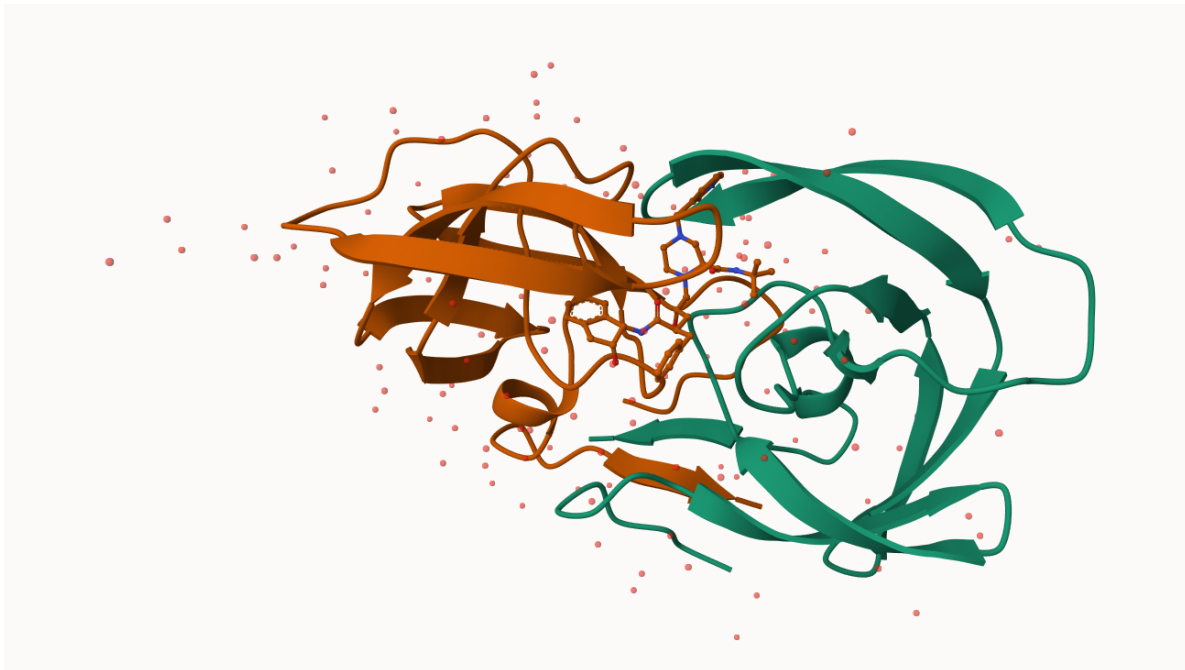
```
 Note: Accessing on-line PDB file
```

```r
pdb
```

Figure 1: My first molecular image

```
 Call:  read.pdb(file = "1hsg")

   Total Models#: 1
     Total Atoms#: 1686,  XYZs#: 5058  Chains#: 2  (values: A B)

     Protein Atoms#: 1514  (residues/Calpha atoms#: 198)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 172  (residues: 128)
     Non-protein/nucleic resid values: [ HOH (127), MK1 (1) ]

   Protein sequence:
     PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYD
     QILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFPQITLWQRPLVTIKIGGQLKE
     ALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTP
     VNIIGRNLLTQIGCTLNF

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```

```r
head(pdb$atom)
```

```
  type eleno elety  alt resid chain resno insert      x      y     z o     b
1 ATOM     1     N <NA>   PRO     A     1   <NA> 29.361 39.686 5.862 1 38.10
2 ATOM     2    CA <NA>   PRO     A     1   <NA> 30.307 38.663 5.319 1 40.62
3 ATOM     3     C <NA>   PRO     A     1   <NA> 29.760 38.071 4.022 1 42.64
4 ATOM     4     O <NA>   PRO     A     1   <NA> 28.600 38.302 3.676 1 43.40
5 ATOM     5    CB <NA>   PRO     A     1   <NA> 30.508 37.541 6.342 1 37.87
6 ATOM     6    CG <NA>   PRO     A     1   <NA> 29.296 37.591 7.162 1 38.40
  segid elesy charge
1  <NA>     N   <NA>
2  <NA>     C   <NA>
3  <NA>     C   <NA>
4  <NA>     O   <NA>
5  <NA>     C   <NA>
6  <NA>     C   <NA>
```

```r
pdbseq(pdb)[25]
```

```
 25
"D"
```

Predicting functional motions of a single structure

We can do a bioinformatics prediction of functional motions (i.e. flexibility/dynamics):

```r
pdb <- read.pdb("6s36")
```

```
 Note: Accessing on-line PDB file
  PDB has ALT records, taking A only, rm.alt=TRUE
```

```r
pdb
```

```
 Call:  read.pdb(file = "6s36")

   Total Models#: 1
```

```
Total Atoms#: 1898,  XYZs#: 5694  Chains#: 1  (values: A)

Protein Atoms#: 1654  (residues/Calpha atoms#: 214)
Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

Non-protein/nucleic Atoms#: 244  (residues: 244)
Non-protein/nucleic resid values: [ CL (3), HOH (238), MG (2), NA (1) ]

Protein sequence:
   MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
   DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDKI
   VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
   YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

+ attr: atom, xyz, seqres, helix, sheet,
       calpha, remark, call
```
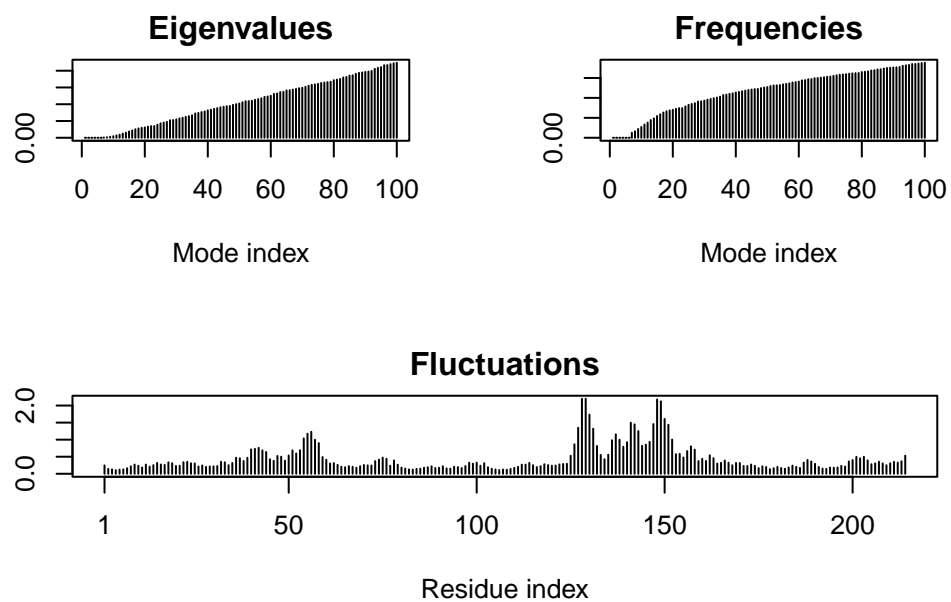
```
m <- nma(pdb)
```

```
Building Hessian...      Done in 0.022 seconds.
Diagonalizing Hessian...  Done in 0.464 seconds.
```

```
plot(m)
```

Eigenvalues

Frequencies

Fluctuations

```
mktrj(m, file="adk_m7.pdb")
```