Class 11: Structural Bioinformatics II

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Alphafold is a cool new bioinformatics method for structure prediction from sequence.

We can run Alphafold on our own computers by installing it or we can run on googleColab (without needing t install anything) via:

Return the full file name (i.e with the directory path) of the aligment file:

```
path <- "hiv1dimer_23119/"
aln_files <- list.files(path=path,
                        pattern="*.a3m",
                        full.names = TRUE)

aln_files
```

```
[1] "hiv1dimer_23119/hiv1dimer_23119.a3m"
```

```
library(bio3d)
aln<- read.fasta(aln_files, to.upper=TRUE)
```

```
[1] " ** Duplicated sequence id's: 101 **"
[2] " ** Duplicated sequence id's: 101 **"
```

```
attributes(aln)
```

```
$names
[1] "id"   "ali"  "call"

$class
[1] "fasta"
```

This is a big aligment - almost too big to realy look at:

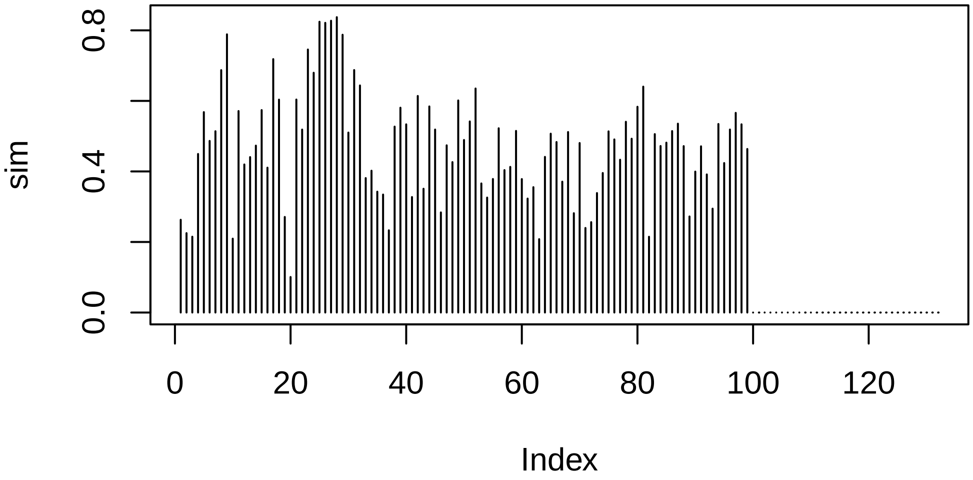
```
dim(aln$ali)
```

```
[1] 5378  132
```

Let's calculate sum summary info such as conservation scores.

```
sim <- conserv(aln)
```

```
plot(sim, typ='h')
```



We can summarize these conserved columns (the ones with high scores above) via a consensus sequence.

```
consensus(aln, cutoff=0.9)$seq
```

```
 [1] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[19] "-" "-" "-" "-" "-" "-" "D" "T" "G" "A" "-" "-" "-" "-" "-" "-" "-" "-"
[37] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[55] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
```

```
 [73] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
 [91] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[109] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[127] "-" "-" "-" "-" "-" "-"
```

Read all our structure models into R

Read the PAE (predicted aligned error files) into R to make sense of these different multichain models. There are stored as JSON format

```
library(jsonlite)
```

Find our Json files

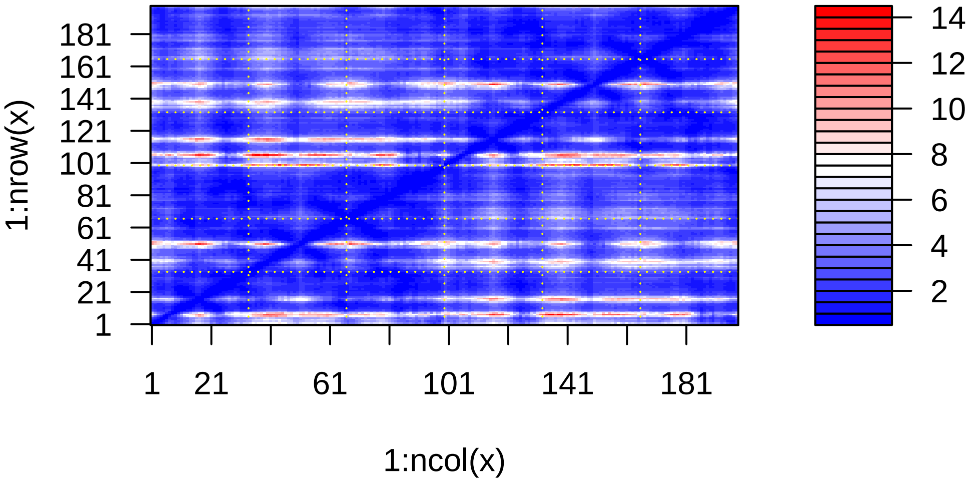
```
pae.files<-list.files(path=path,
                        pattern="*000.json",
                        full.names = TRUE)
```

```
pae5 <- read_json(pae.files[5],simplifyVector = TRUE)
pae1 <- read_json(pae.files[1],simplifyVector = TRUE)
```

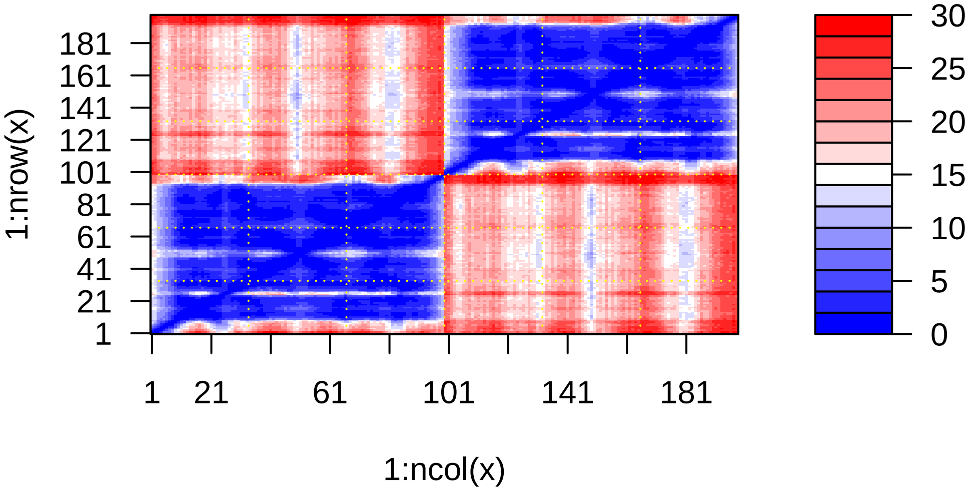
```
dim(pae1$pae)
```

```
[1] 198 198
```

```
plot.dmat(pae1$pae)
```



```
plot.dmat(pae5$pae)
```


1:nrow(x)
1:ncol(x)