Class 11: Alphafold

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Here we read the results from Alphafold and try to interpret all the models and quality score metrics:

```
library(bio3d)

pth <- "dimer_23119/"
pdb.files <- list.files(path = pth, full.names = TRUE, pattern = ".pdb")
```

Align and superpose all these models

```
file.exists(pdb.files)
```

```
[1] TRUE TRUE TRUE TRUE TRUE
```

```
pdbs <- pdbaln(pdb.files, fit = TRUE, exefile = "msa")
```

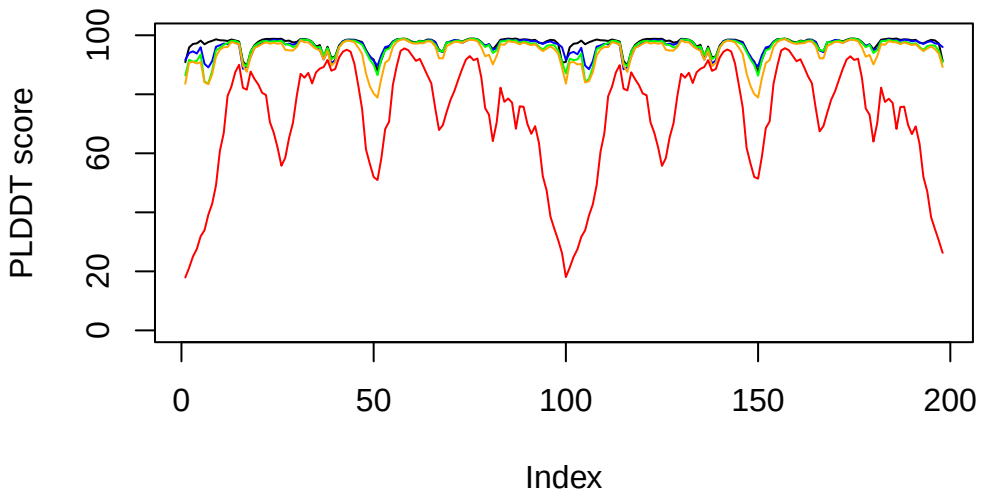
```
Reading PDB files:
dimer_23119/dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000.pdb
dimer_23119/dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_4_seed_000.pdb
dimer_23119/dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_1_seed_000.pdb
dimer_23119/dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_5_seed_000.pdb
dimer_23119/dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb
.....

Extracting sequences

pdb/seq: 1   name: dimer_23119/dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2
pdb/seq: 2   name: dimer_23119/dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_4
pdb/seq: 3   name: dimer_23119/dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_1
pdb/seq: 4   name: dimer_23119/dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_5
pdb/seq: 5   name: dimer_23119/dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3
```

```
library(bio3dview)
# view.pdbs(pdbs)
```

```
plot(pdbs$b[1,], typ="l", ylim=c(0,100), ylab="PLDDT score")
lines(pdbs$b[2,], typ="l", col="blue")
lines(pdbs$b[3,], typ="l", col="green")
lines(pdbs$b[4,], typ="l", col="orange")
lines(pdbs$b[5,], typ="l", col="red")
```




```
pdbs$sse
```

```
NULL
```

Score Residue conservation from alignment file

Alphafold returns it's large alignment file used for analysis. Here we read this file and score conservation per position

```
aln_file <- list.files(path=pth,
                       pattern=".a3m$",
                        full.names = TRUE)
aln_file
```

```
[1] "dimer_23119/dimer_23119.a3m"
```

```
aln <- read.fasta(aln_file[1], to.upper = TRUE)
```

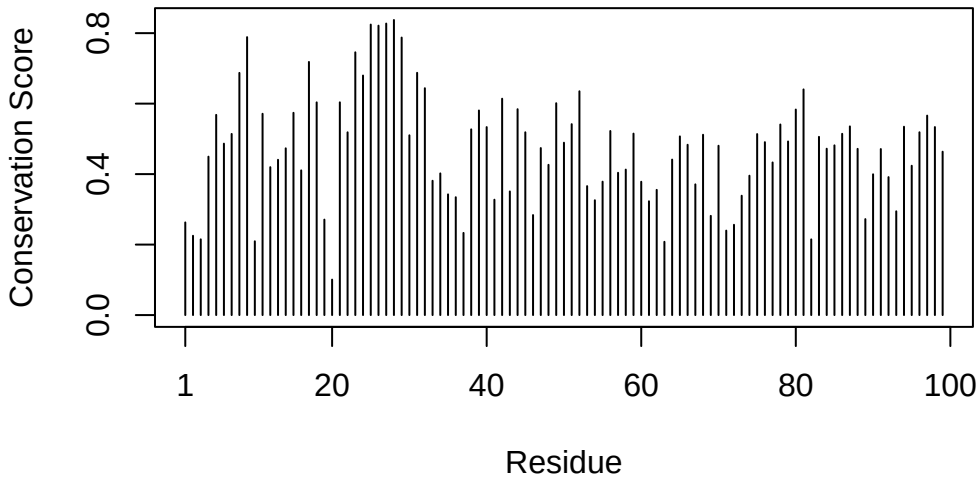
```
[1] " ** Duplicated sequence id's: 101 **"
[2] " ** Duplicated sequence id's: 101 **"
```

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

```
[1] 5378  132
```

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

```
plotb3(sim[1:99],
       ylab="Conservation Score")
```



```
con <- consensus(aln, cutoff = 0.9)
con$seq
```

```
  [1] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
 [19] "-" "-" "-" "-" "-" "-" "D" "T" "G" "A" "-" "-" "-" "-" "-" "-" "-" "-"
 [37] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
 [55] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
 [73] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
 [91] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[109] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
[127] "-" "-" "-" "-" "-" "-"
```

The sequence above shows the conserved residues which are D, T, G, and A.

Predicting Alignment Error for Domains

```
library(jsonlite)

# Listing of all PAE JSON files
pae_files <- list.files(path=pth,
                        pattern=".*model.*\\.json",
                        full.names = TRUE)
```

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

attributes(pae1)
```

```
$names
[1] "plddt"   "max_pae" "pae"     "ptm"     "iptm"
```

```
# Per-residue pLDDT scores
#  same as B-factor of PDB..
head(pae1$plddt)
```

```
[1] 90.88 95.88 97.06 97.25 98.19 96.94
```

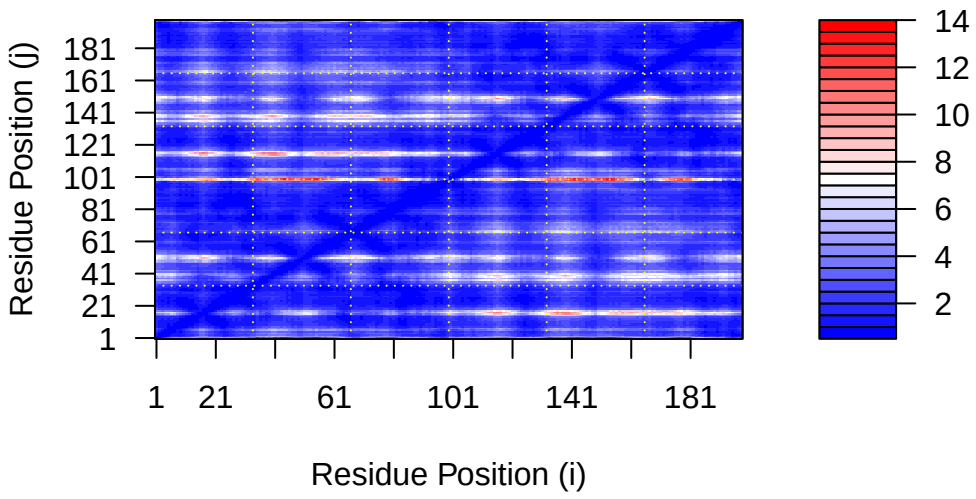
```
pae1$max_pae
```

```
[1] 13.86719
```

```
pae5$max_pae
```

```
[1] 30
```

```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)")
```



Heatmap of RMSD values

```
rd <- rmsd(pdbs, fit=T)
```

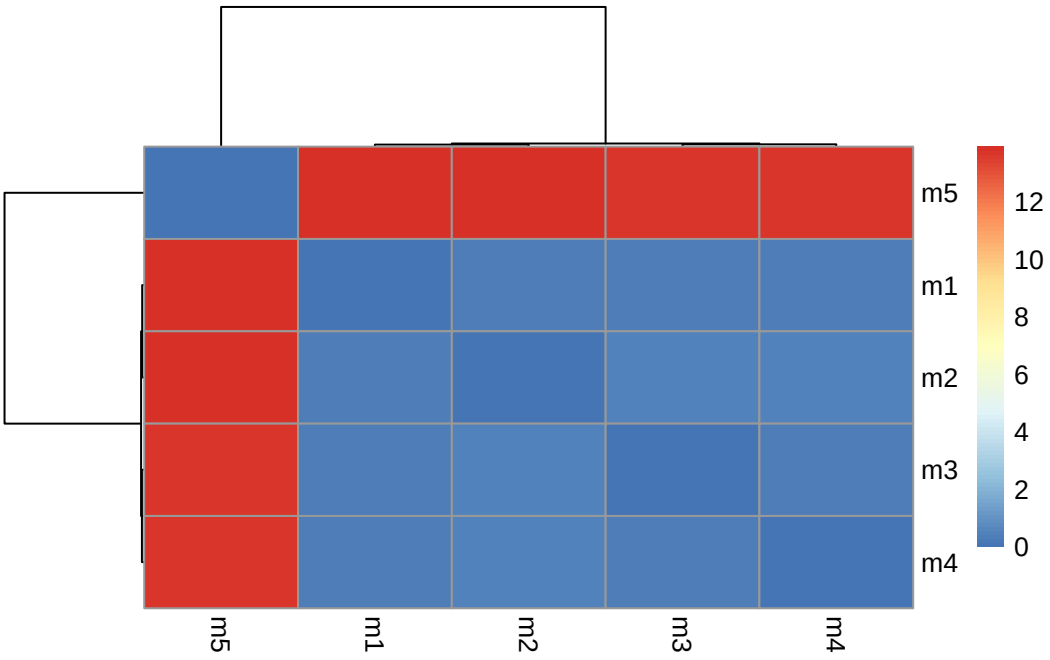
```
Warning in rmsd(pdbs, fit = T): No indices provided, using the 198 non NA positions
```

```
range(rd)
```

```
[1]  0.000 13.904
```

```
library(pheatmap)

colnames(rd) <- paste0("m", 1:5)
rownames(rd) <- paste0("m", 1:5)
pheatmap(rd)
```



The heatmap shows that models 1, 2, 3, and 4 are most similar to each other, while model 5 is the most different to all of the other models.