Class 11: AlphaFold

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Custom analysis of resulting models

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")
```

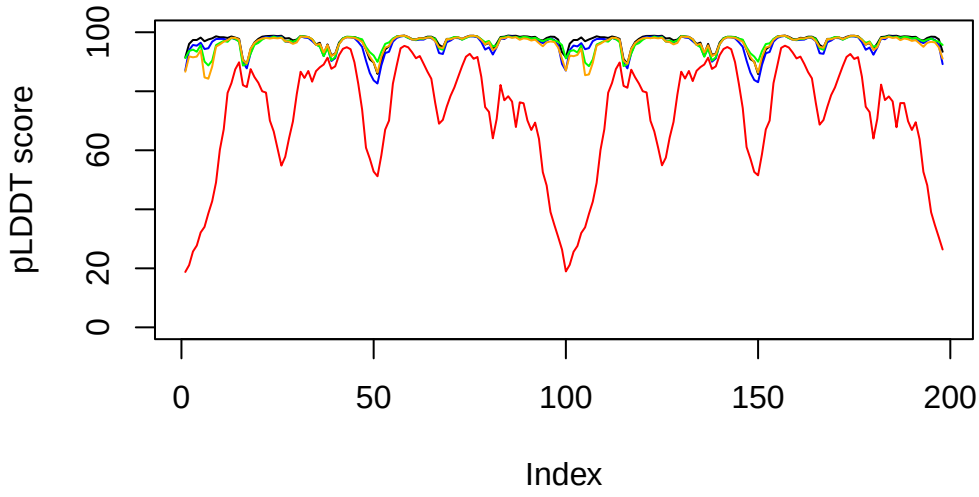
```
Reading PDB files:
dimer_23119//dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000.pdb
dimer_23119//dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb
dimer_23119//dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb
dimer_23119//dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_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_5
pdb/seq: 3   name: dimer_23119//dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4
pdb/seq: 4   name: dimer_23119//dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1
pdb/seq: 5   name: dimer_23119//dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3
```

```
library(bio3dview)

#view.pdbs(pdbs)
```

```
# Read a reference PDB structure
pdb <- read.pdb("1hsg")
```

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

```
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")
```



Predicted Alignment Error for domains

```
rd <- rmsd(pdbs)
```

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

```
rd
```

```
                                                                    dimer_23119_unrelaxed
dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000
dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000
dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
                                                                    dimer_23119_unrelaxed
dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000
dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000
```

```
dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
                                                                        dimer_23119_unrelaxed_
dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000
dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000
dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
                                                                        dimer_23119_unrelaxed_
dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000
dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000
dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
                                                                        dimer_23119_unrelaxed_
dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000
dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000
dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000
dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000
dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000
```

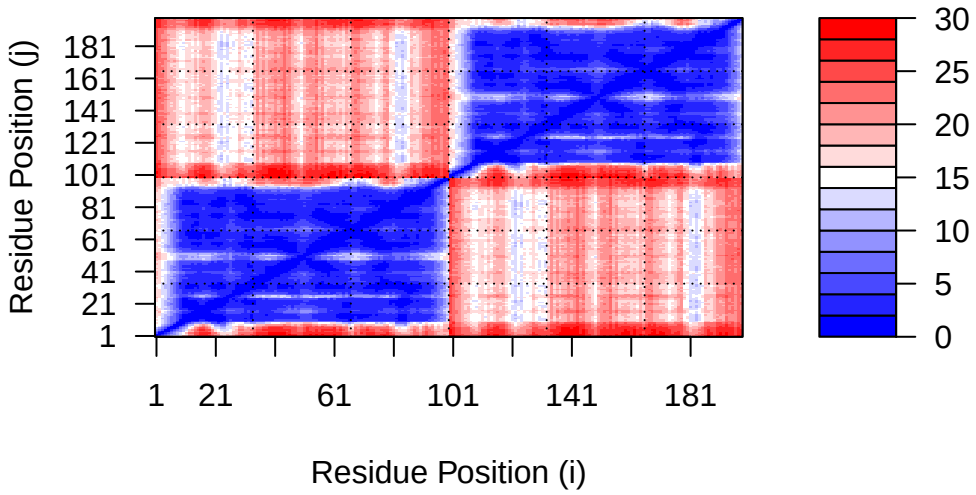
```r
library(jsonlite)

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

```
[1] "dimer_23119//dimer_23119_scores_rank_001_alphafold2_multimer_v3_model_2_seed_000.json"
[2] "dimer_23119//dimer_23119_scores_rank_002_alphafold2_multimer_v3_model_5_seed_000.json"
[3] "dimer_23119//dimer_23119_scores_rank_003_alphafold2_multimer_v3_model_4_seed_000.json"
[4] "dimer_23119//dimer_23119_scores_rank_004_alphafold2_multimer_v3_model_1_seed_000.json"
[5] "dimer_23119//dimer_23119_scores_rank_005_alphafold2_multimer_v3_model_3_seed_000.json"
```

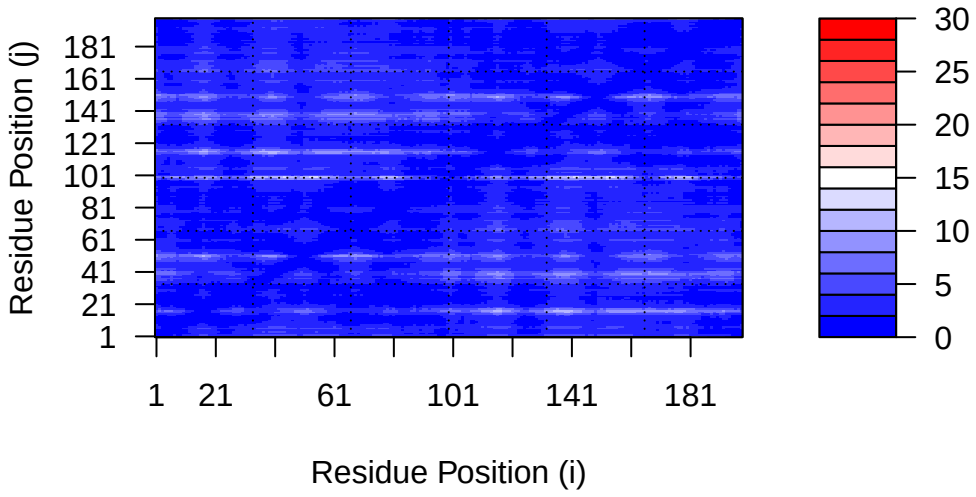
```r
pae1 <- read_json(pae_files[1],simplifyVector = TRUE)
pae5 <- read_json(pae_files[5],simplifyVector = TRUE)

attributes(pae1)
```

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

```
plot.dmat(pae5$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)",
          grid.col = "black",
          zlim=c(0,30))
```




```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)",
          grid.col = "black",
          zlim=c(0,30))
```



Score Residue Conservation from alignment file

AlphaFold returns it's large elignment 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"
```

Read the alignment file

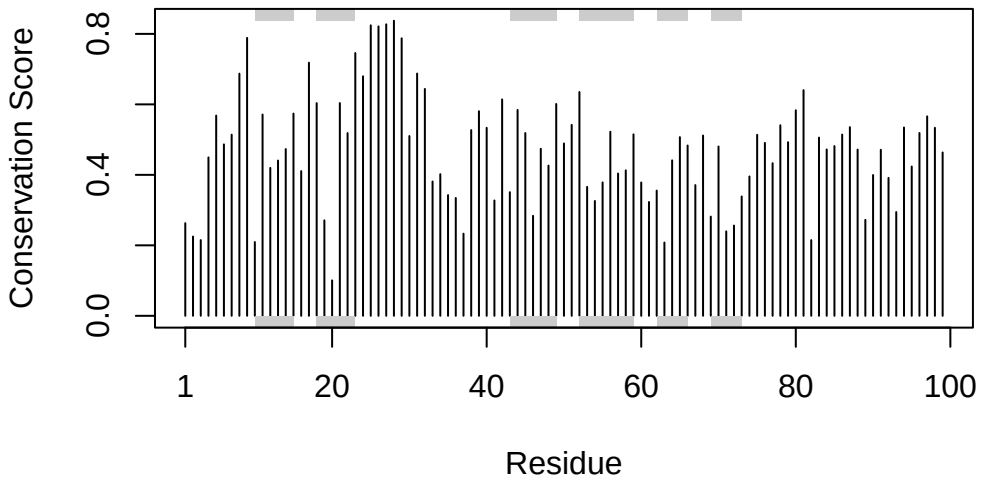
```
aln <- read.fasta(aln_file[1], to.upper = TRUE)
```

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

We can score residue conservation in the alignment with the conserv() function.

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

```
plotb3(sim[1:99], sse=trim.pdb(pdb, chain="A"),
       ylab="Conservation Score")
```



Find the consensus sequence at a very high cut-off to find invariant residues

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

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