Artificial Neural networks for the prediction of phage protein function

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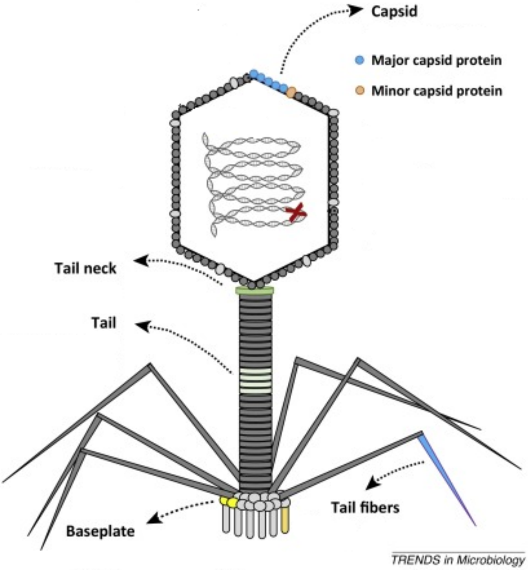
BacterioPhage



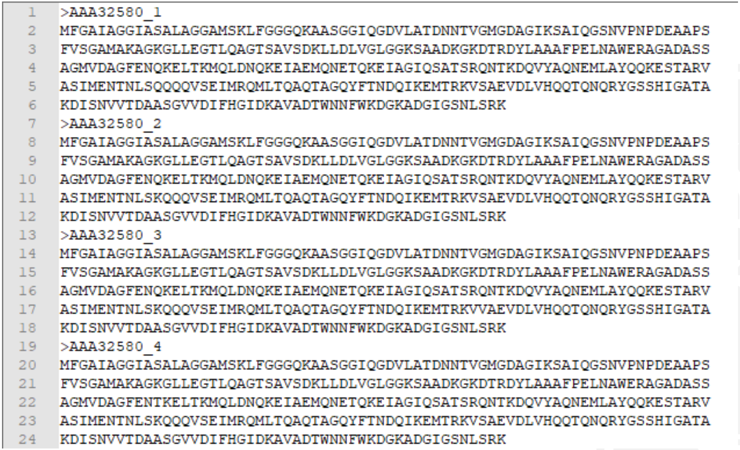
TRENDS in Microbiology

Databases

Class	Raw sequences	After manual curation	After 90% dereplication
Major capsid	112,987	105,653	13,172
Minor capsid	2,901	1,903	656
Baseplate	75,599	19,293	2,090
Major tail	66,513	35,030	3,249
Minor tail	94,628	80,467	3,886
Portal	210,064	189,143	18,622
Tail fiber	29,132	18,514	3,191
Tail shaft	37,885	35,570	4,933
Collar	4,224	3,709	1,262
Head-Tail joining	60,270	58,658	6,713
Other	733,006	-	162,709

Table: The classes database by the numbers

Protein Sequences



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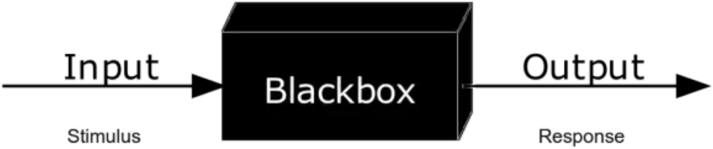
KDISNVVTDAASGVVDIFHGIDKAVADTWNNFWKDGKADGIGSNLSRK
```

F:Sequence –> Function



Input

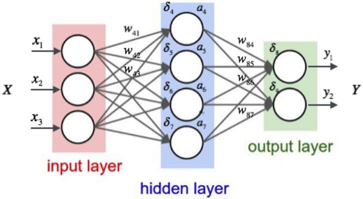
Blackbox

Output

Stimulus

Response

Artificial Neural Networks



ANN have been shown to be universal approximators of continuous functions in $\mathbb{R}^n$

$$d = \left(\int_0^{2\pi} |f_1(t) - f_2(t)|^p \, dt \right)^{\frac{1}{p}}$$

where $1 < p < \infty$

Artificial Neural Networks

$$\begin{pmatrix} Z_1 \\ Z_2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ Z_{408} \end{pmatrix} = X$$

$$\begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \\ Y_6 \\ Y_7 \\ Y_8 \\ Y_9 \\ Y_{10} \\ Y_{11} \end{pmatrix} = Y$$

where $\sum_{n=1}^{11} Y_n = 1$

The 'black box' function

$$Y = F(X) = \underbrace{[10 \ast 200]}_{W_3} \left(\underbrace{[200 \ast 200]}_{W_2} \left(\underbrace{[200 \ast 408]}_{W_1} \underbrace{[408 \ast 1]}_{X} + \underbrace{[200 \ast 1]}_{\delta_1} \right) + \underbrace{[200 \ast 10]}_{\delta_2} \right) + \underbrace{[10 \ast 1]}_{\delta_1}$$

289,866 Trainable parameters

Precision and Recall

$$precision = \frac{TP}{TP + FP}$$

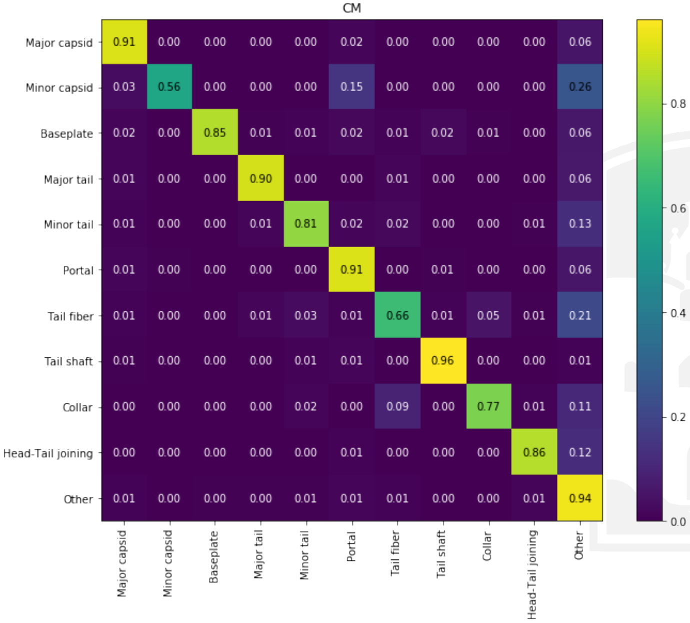
$$recall = \frac{TP}{FN + TP}$$

$$F1 = \frac{2 \cdot precision \cdot recall}{precision + recall}$$

Accuracy

	$Precision$	$Recall$	$f1 - score$	$Support$
$Major\ capsid$	0.88	0.92	0.90	1232
$Minor\ capsid$	0.27	0.57	0.36	51
$Baseplate$	0.54	0.87	0.67	180
$Major\ tail$	0.82	0.88	0.85	289
$Minor\ Tail$	0.65	0.77	0.70	345
$Portal$	0.87	0.90	0.88	1640
$Tail\ Fiber$	0.54	0.67	0.60	272
$Tail\ shaft$	0.91	0.94	0.93	444
$Collar$	0.75	0.80	0.77	129
$Head - Tail\ Joining$	0.74	0.84	0.79	647
$Other$	0.97	0.93	0.95	15254
$weighted\ avg$	0.82	0.79	0.79	675

Results Confusion matrix



CM

	Major capsid	Minor capsid	Baseplate	Major tail	Minor tail	Portal	Tail fiber	Tail shaft	Collar	Head-Tail joining	Other
Major capsid	0.91	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.06
Minor capsid	0.03	0.56	0.00	0.00	0.00	0.15	0.00	0.00	0.00	0.00	0.26
Baseplate	0.02	0.00	0.85	0.01	0.01	0.02	0.01	0.02	0.01	0.00	0.06
Major tail	0.01	0.00	0.00	0.90	0.00	0.00	0.01	0.00	0.00	0.00	0.06
Minor tail	0.01	0.00	0.00	0.01	0.81	0.02	0.02	0.00	0.00	0.01	0.13
Portal	0.01	0.00	0.00	0.00	0.00	0.91	0.00	0.01	0.00	0.00	0.06
Tail fiber	0.01	0.00	0.00	0.01	0.03	0.01	0.66	0.01	0.05	0.01	0.21
Tail shaft	0.01	0.00	0.00	0.00	0.01	0.01	0.00	0.96	0.00	0.00	0.01
Collar	0.00	0.00	0.00	0.00	0.02	0.00	0.09	0.00	0.77	0.01	0.11
Head-Tail joining	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.86	0.12
Other	0.01	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.01	0.94

Weighted average

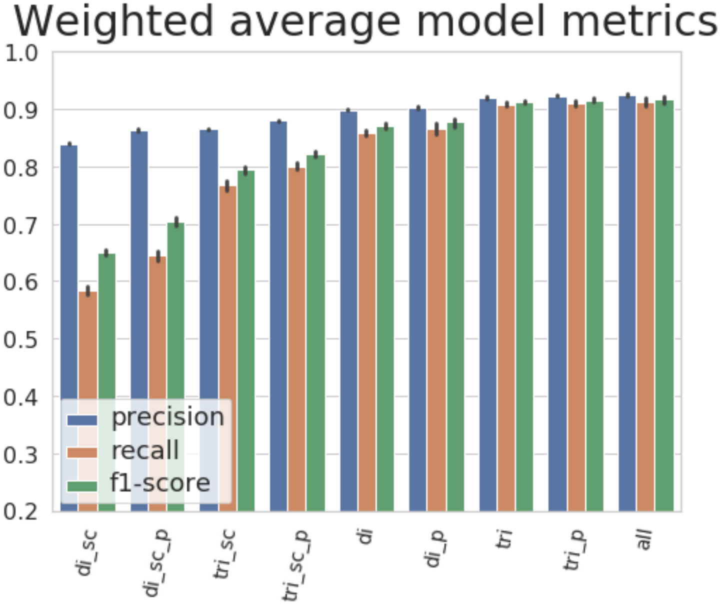
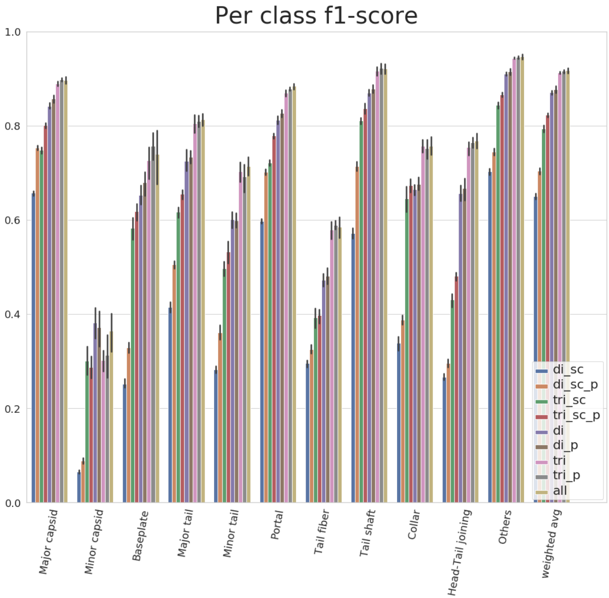


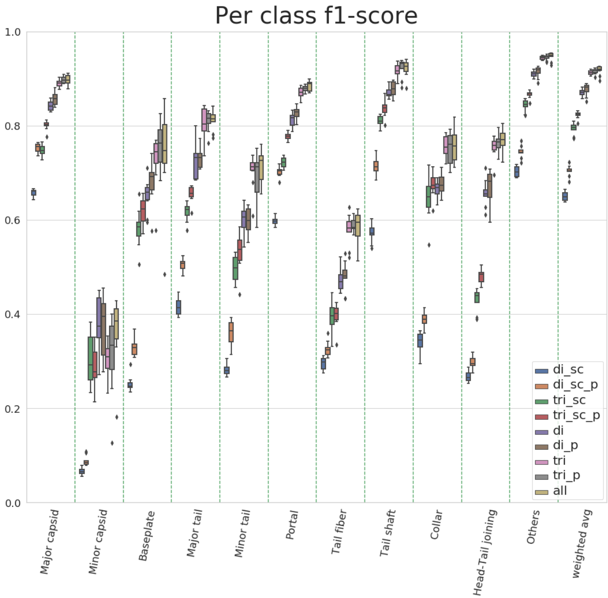
Table: Side chain grouping

Hydrophobic	A,I,L,M,V
Hydrophylic	N,Q,S,T
Small turn	G,P
disulfide	C
Positive charge	H,K,R
Negative charge	D,E
Aromatic	F,W,Y

Per class f1-score



Per class f1-score



website

http://edwards.sdsu.edu/PhANNies/