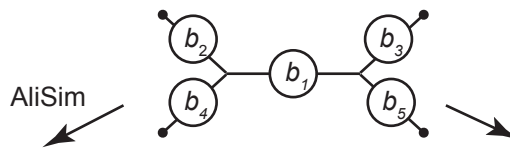


Tree with branch lengths \mathbf{b}



AliSim

Multiple sequence alignment (MSA)

```

A G T T G T T A G T
A G T T G A T A T G
A G T T G A A A T G
A G T T G A T A T G
    
```

Site pattern frequency feature vector

```

0.01 0.04 0.02 0.09 0.05
    
```

Table of true branch lengths

```

b1 b2 b3 b4 b5
0.9 0.3 0.2 0.2 1.1
... ..
... ..
    
```

Convolutional Neural Network (CNN)

Multilayer Perceptron (MLP)

\mathbf{X}

\mathbf{Y}

```

A G T T G T T A G T
A G T T G A T A T G
A G T T G A A A T G
A G T T G A T A T G
    
```

```

b1 b2 b3 b4 b5
0.9 0.3 0.2 0.2 1.1
... ..
... ..
    
```

2D convolution

Pooling

Flattening

MLP

```

A G T T G T T A G T
A G T T G A T A T G
A G T T G A A A T G
A G T T G A T A T G
    
```

\mathbf{X}

\mathbf{Y}

```

0.01 0.04 0.02 0.09 0.05
    
```

```

b1 b2 b3 b4 b5
0.9 0.3 0.2 0.2 1.1
... ..
... ..
    
```

```

0.01
0.04
0.02
0.09
0.05
    
```

Input

Output

Regression of observed on estimated values (ROE)

\mathbf{X} (= estimated $\hat{\mathbf{Y}}$)

\mathbf{Y}

```

b1 b2 b3 b4 b5
0.7 0.2 0.1 0.4 0.9
... ..
... ..
    
```

```

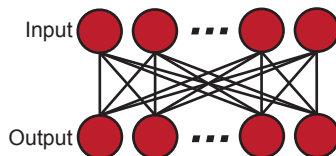
b1 b2 b3 b4 b5
0.9 0.3 0.2 0.2 1.1
... ..
... ..
    
```

Predicted branch lengths

```

0.7 0.2 0.1 0.4 0.9
    
```

Simple input-output layer perceptron



Multi-output multiple linear regression

$$\mathbf{Y} = \mathbf{X}^T \mathbf{W}$$

Equivalent to