# Kernel-Based Multi-channel PolyCovNet

AI Hackathon Challenge I

**Team Borides**

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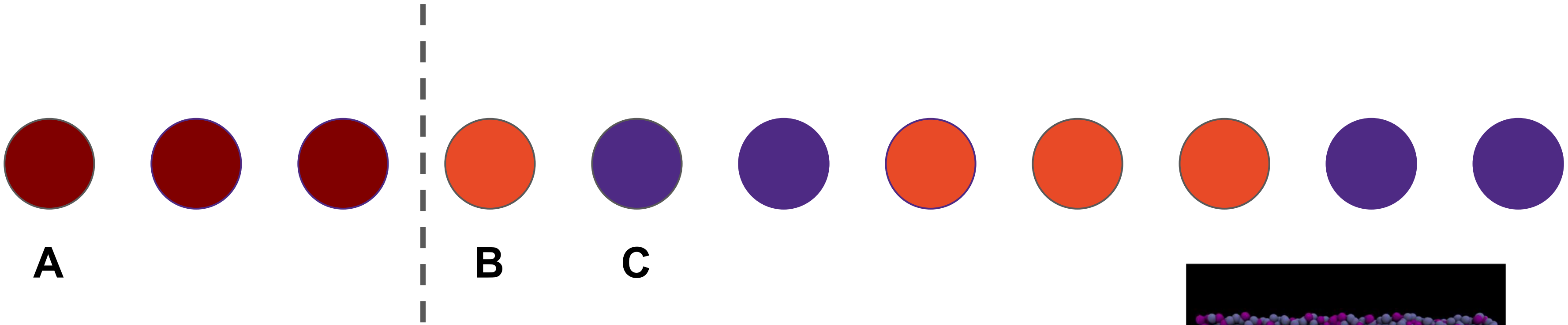
# Contents

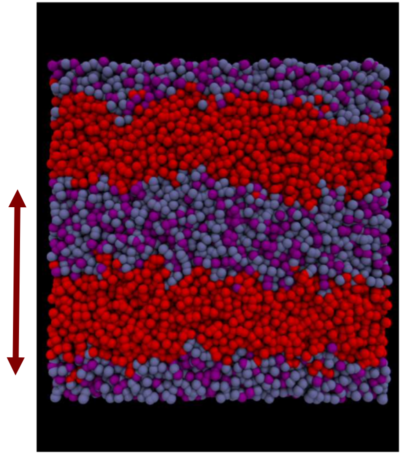
# Problem Restatement

Predicting the lamellar period using monomer sequences and interaction parameters

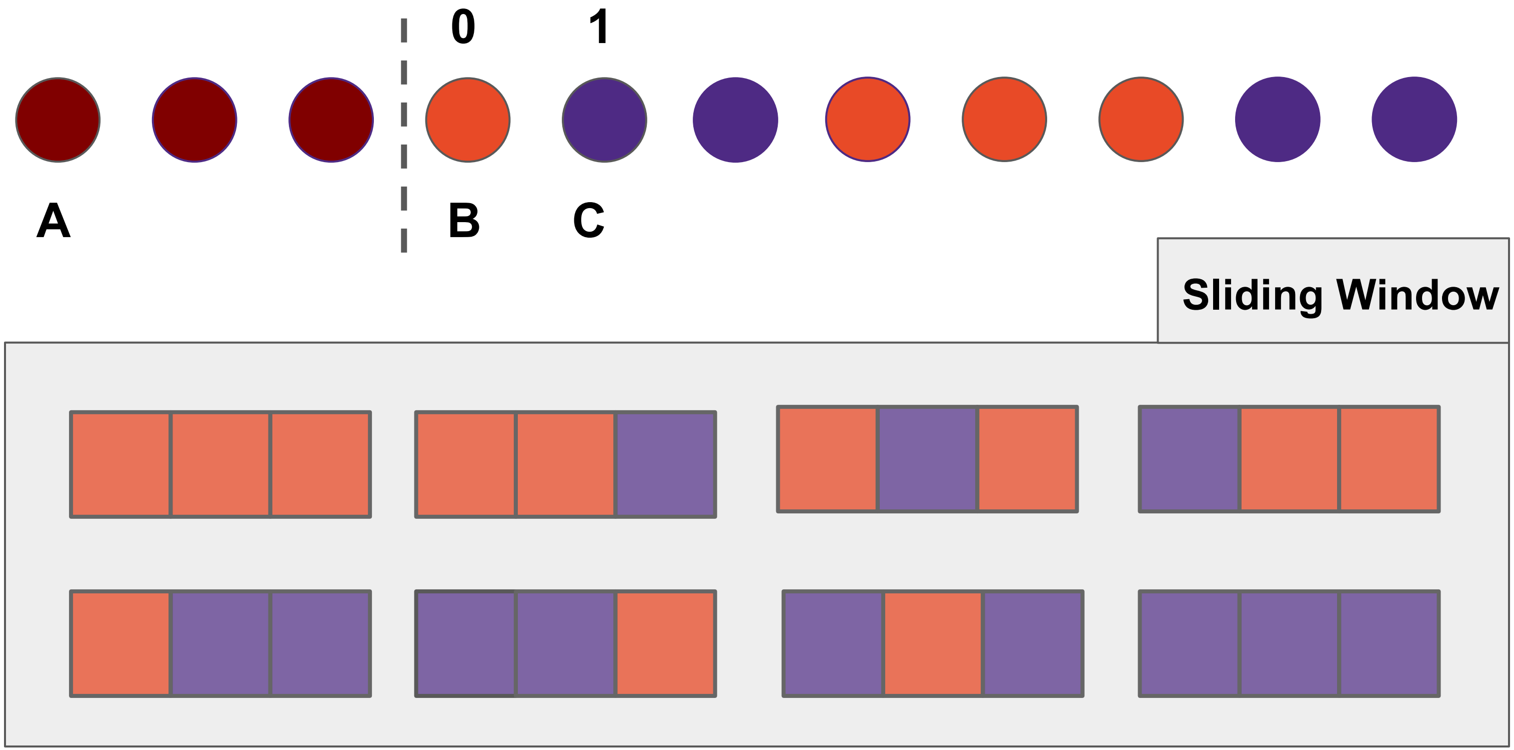



**Interaction Parameter**

**Lamellar Period**



# Sliding window - extract monomer sequence features



# Sliding Window

## Feature Engineering

**window size**

**2**

[0,0]
[0,1]
[1,0]
[1,1]

$2^2 = 4$

**3**

[0,0,0]
[0,0,1]
[0,0,0]
[0,0,0]
[0,0,1]
[0,0,0]
[0,0,0]
[0,0,1]

$2^3 = 8$

**4**

[0, 0, 0, 0]
[0, 0, 0, 1]
[0, 0, 1, 0]
[0, 0, 1, 1]
[0, 1, 0, 0]
[0, 1, 0, 1]
[0, 1, 1, 0]
[0, 1, 1, 1]
[1, 0, 0, 0]
[1, 0, 0, 1]
[1, 0, 1, 0]
[1, 0, 1, 1]
[1, 1, 0, 0]
[1, 1, 0, 1]
[1, 1, 1, 0]
[1, 1, 1, 1]

$2^4 = 16$

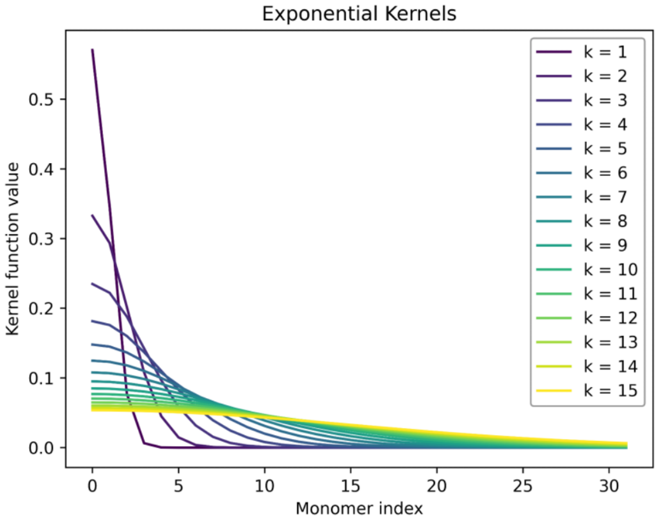
**5**

[0, 0, 0, 0, 0]
[0, 0, 0, 0, 1]
[0, 0, 0, 1, 0]
[0, 0, 0, 1, 1]
[0, 0, 1, 0, 0]
[0, 0, 1, 0, 1]
[0, 0, 1, 1, 0]
[0, 0, 1, 1, 1]
[0, 1, 0, 0, 0]
[0, 1, 0, 0, 1]
[0, 1, 0, 1, 0]
[0, 1, 0, 1, 1]
[0, 1, 1, 0, 0]
[0, 1, 1, 0, 1]
[0, 1, 1, 1, 0]
[0, 1, 1, 1, 1]
[1, 0, 0, 0, 0]
[1, 0, 0, 0, 1]
[1, 0, 0, 1, 0]
[1, 0, 0, 1, 1]
[1, 0, 1, 0, 0]
[1, 0, 1, 0, 1]
[1, 0, 1, 1, 0]
[1, 0, 1, 1, 1]
[1, 1, 0, 0, 0]
[1, 1, 0, 0, 1]
[1, 1, 0, 1, 0]
[1, 1, 0, 1, 1]
[1, 1, 1, 0, 0]
[1, 1, 1, 0, 1]
[1, 1, 1, 1, 0]
[1, 1, 1, 1, 1]

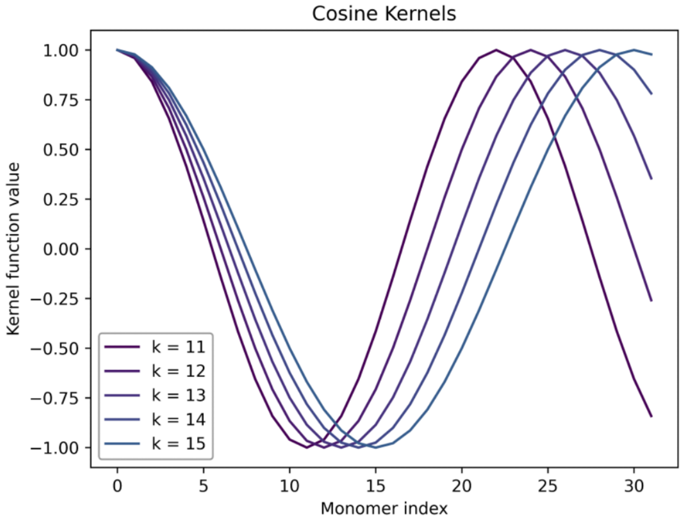
$2^5 = 32$

# Non-linear kernel functions - preprocess monomer sequences

1. Exponential kernels $\exp(\frac{x^2}{2k^2})$




2. Cosine kernels $\cos(\frac{\pi x}{k})$

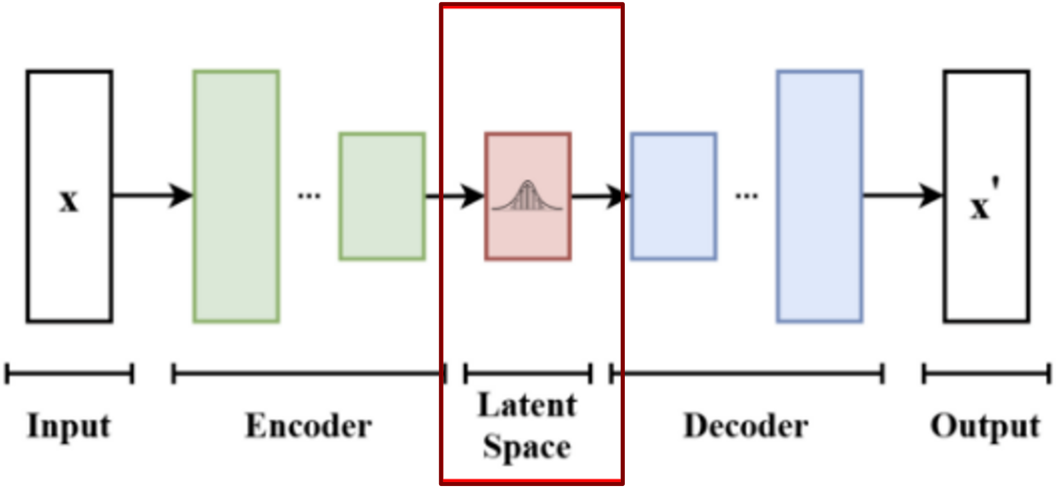



Applying the above kernels on monomer sequences ➡ Non-linearity

# Variational autoencoder - extract features from monomer sequences

Monomer sequences

BBBBBCCCCC

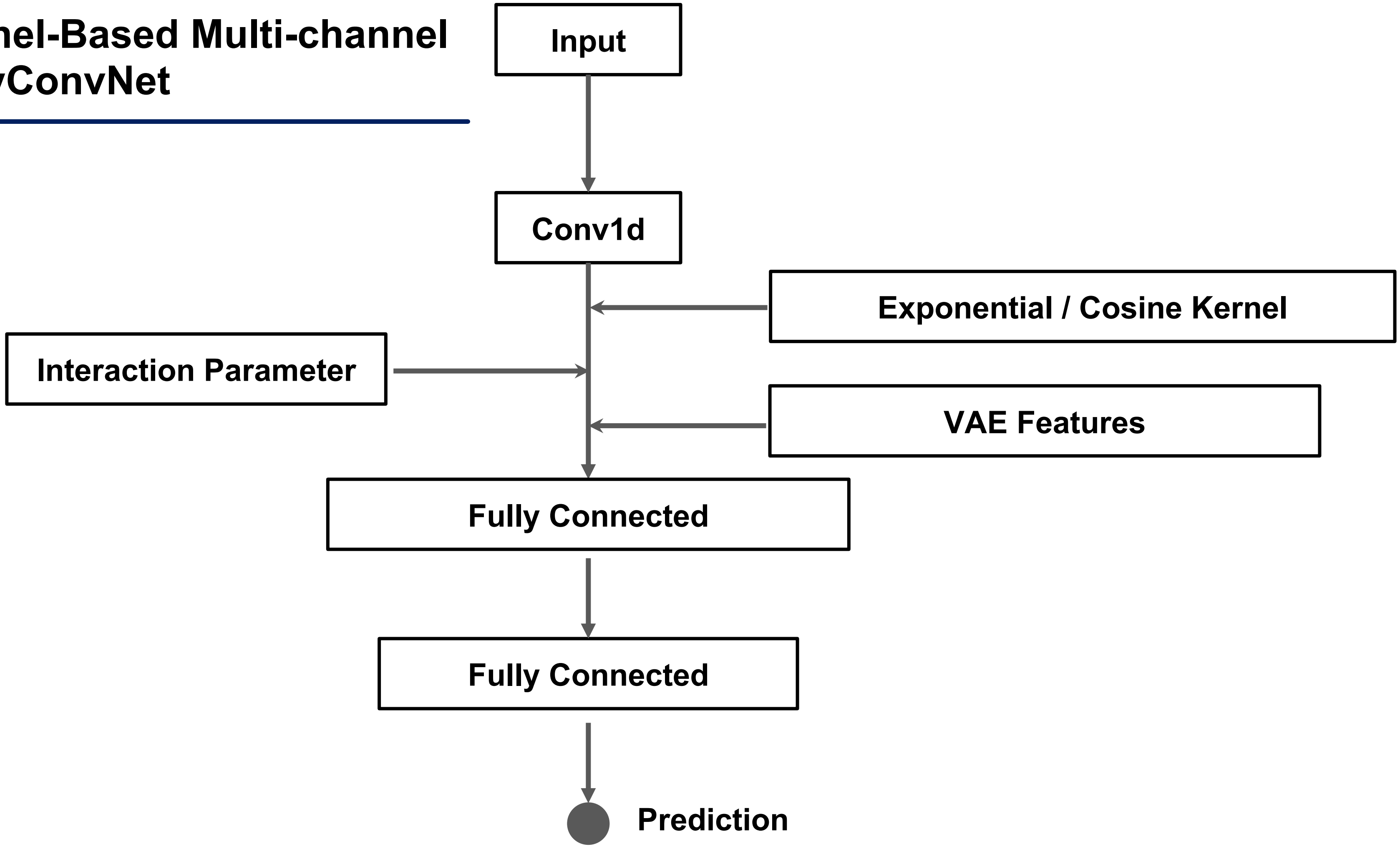



Monomer sequences

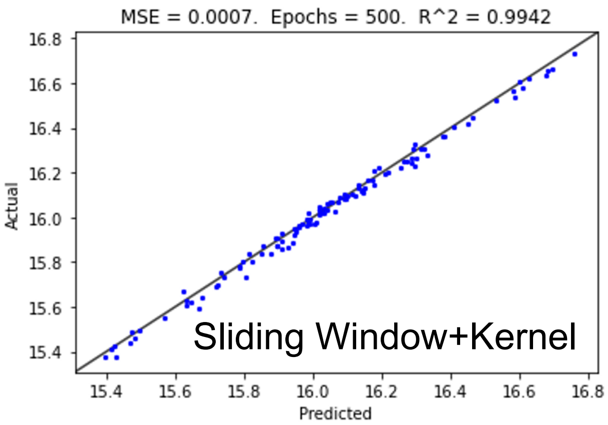
BBBBBCCCCC

**Reduced feature vectors**

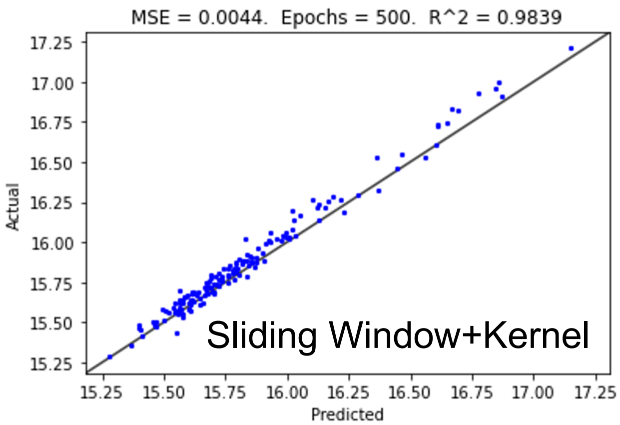
# Kernel-Based Multi-channel PolyConvNet



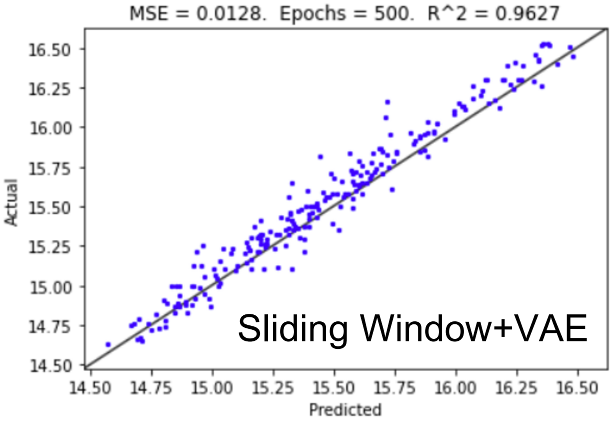
# Results



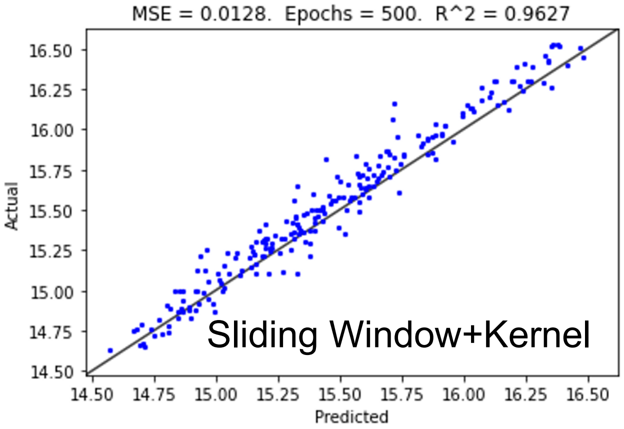

**DataSetA**




**DataSetB**



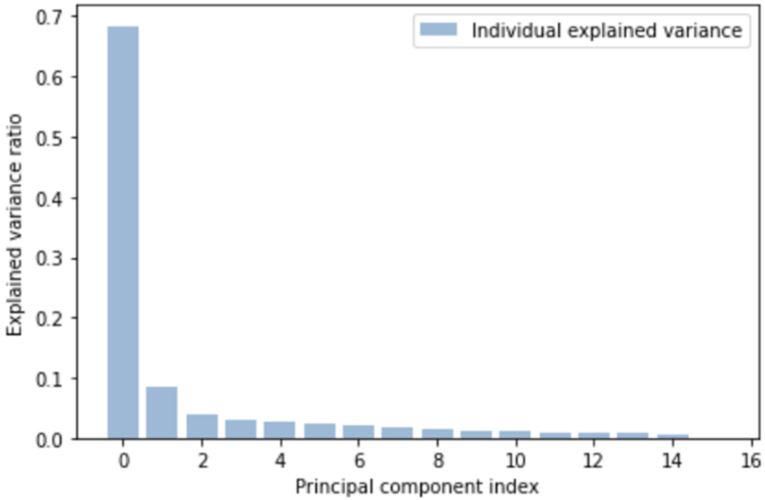

**DataSetC**



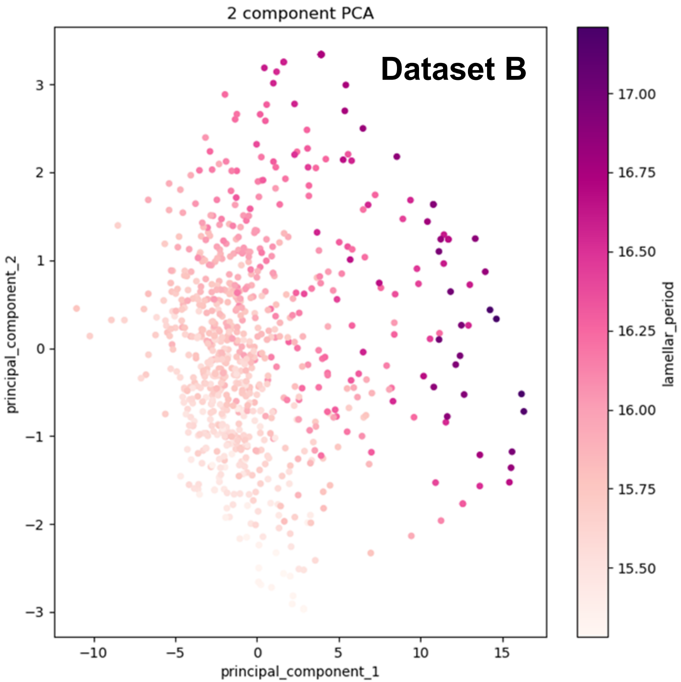

**DataSetD**

**500 epoch**
**0.01 learning rate**

# Principal component analysis on the latent space



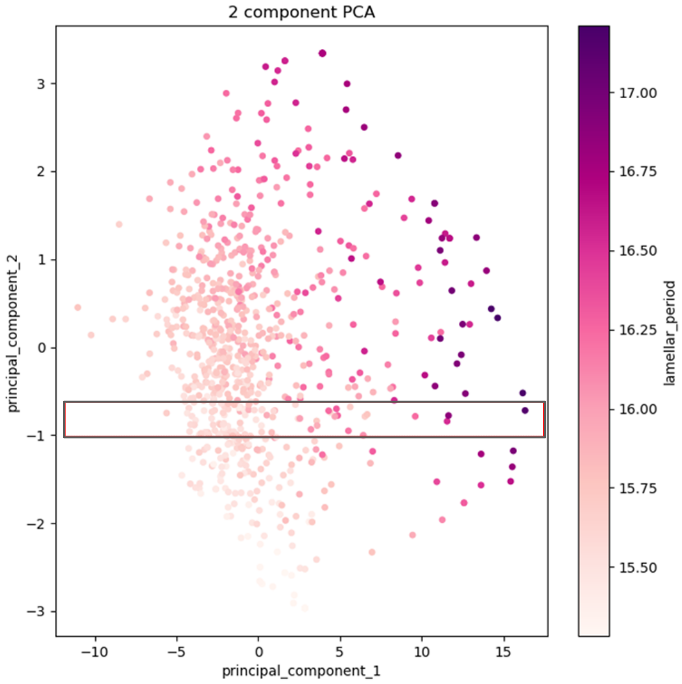

**Principal component 1 dominates**




**Larger** principal component 1

**Larger** lamellar period

# Blockiness is important to result in a high lamellar period




| Higher principal component 1 | Blockiness |
|---|---|
| 11111111111111110000000000000000 | 0.875000 |
| 11111111111111100000000000000000 | 0.874510 |
| 11111111111111111100000000000000 | 0.873016 |
| 11111111111111111110000000000000 | 0.870445 |
| 11111111111111111111000000000000 | 0.866667 |

| Lower principal component 1 | Blockiness |
|---|---|
| 11000011001110000110000000111111 | 0.498039 |
| 00000011111110000000000000111111 | 0.740891 |
| 11000001110110110000000001111110 | 0.372549 |
| 01000111110110010001101000100111 | 0.000000 |
| 10100001110001000100100100011011 | -0.036437 |

# Computational Efficiency (500 epochs)

| Feature Generation | Time (min) |
|---|---|
| 2-channel Sliding Window Features | 0.5 |
| Exponential / Cosine Kernel Features | 0.08 |
| VAE Features | 30 |

| Model Training / Validation | Time (min) |
|---|---|
| Training | 1 |
| Validation | 0.02 |

* All runtimes are reported using ThetaGPU

# Thank you!