Kernel-Based Multi-channel PolyCovNet

AI Hackathon Challenge I

Team Borides

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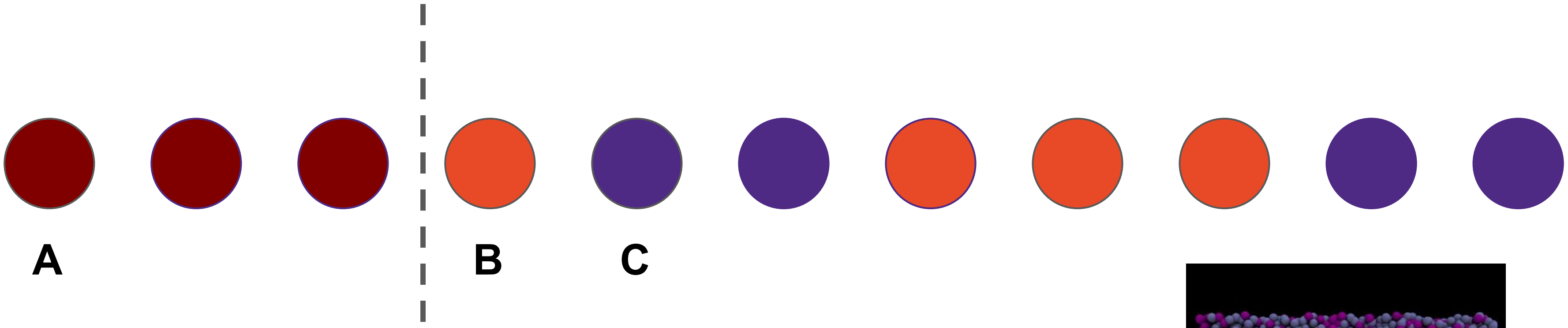
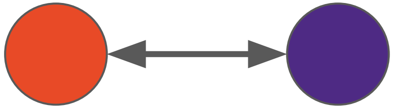
Contents

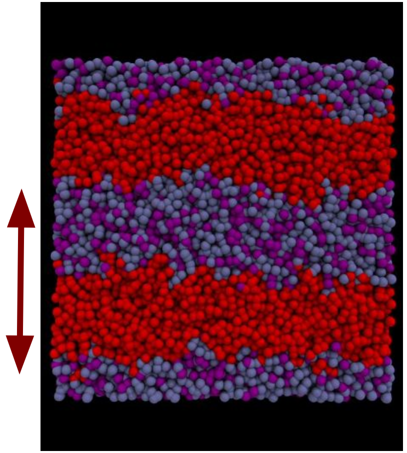
Predicting the lamellar period from monomer sequences and interaction parameters



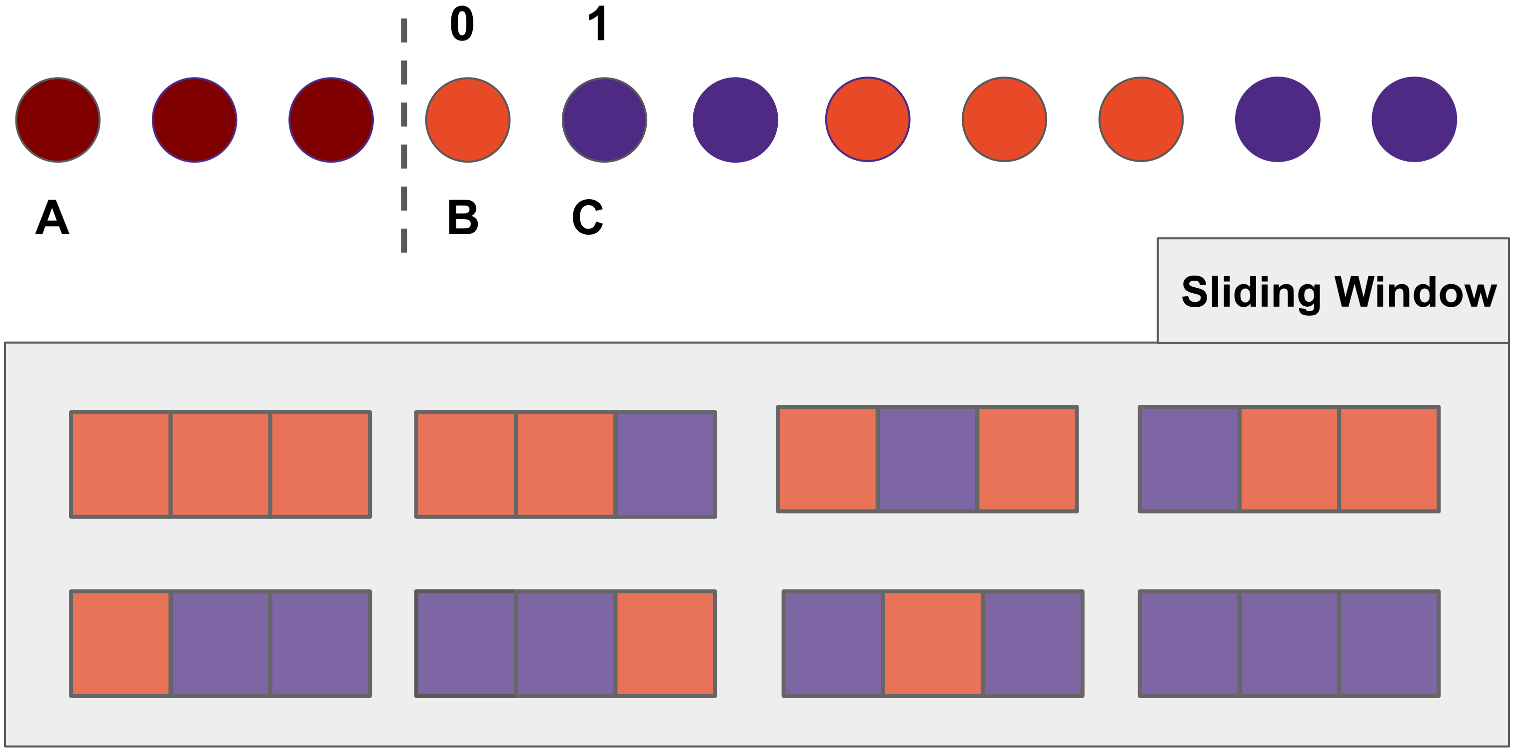


Interaction Parameter

Lamellar Period



Sliding window - extract monomer sequence features



Sliding Window Algorithm

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]

$2^4 = 16$

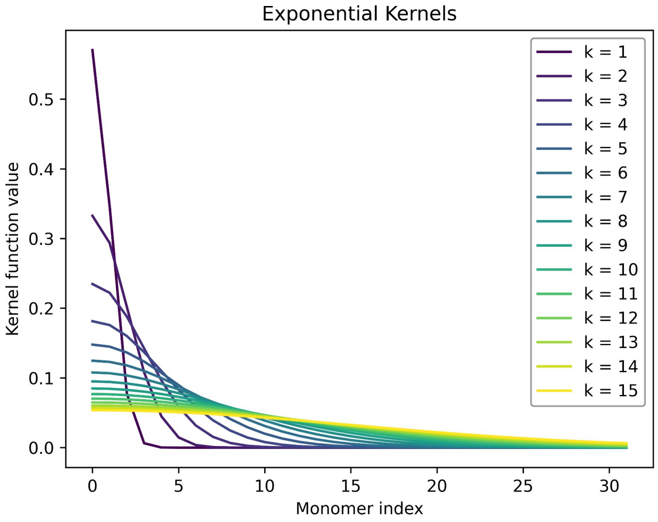
5

[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]

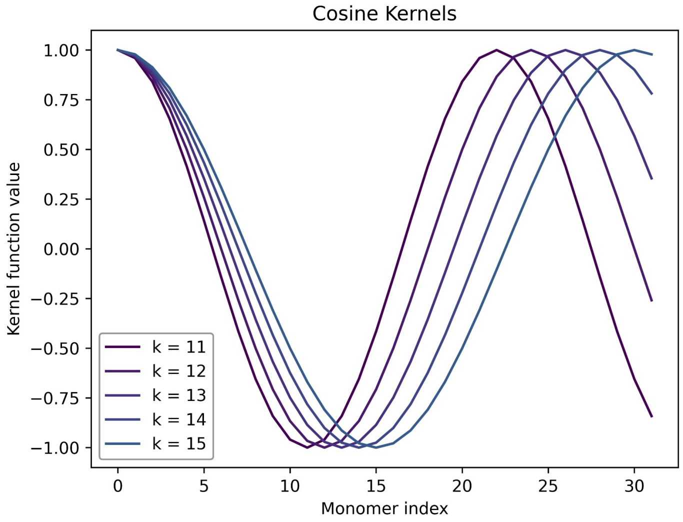
$2^5 = 32$

Non-linear kernel functions - preprocess monomer sequences

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



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

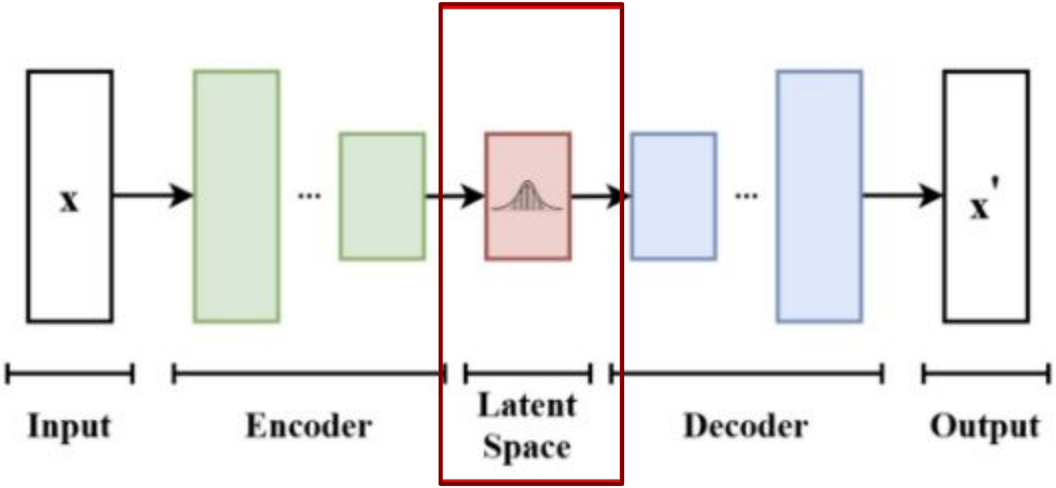


Applying the above kernels on monomer sequences ➡ Non-linearity

Variational autoencoder - extract features from monomer sequences

Monomer sequences

BBBBBCCCCC

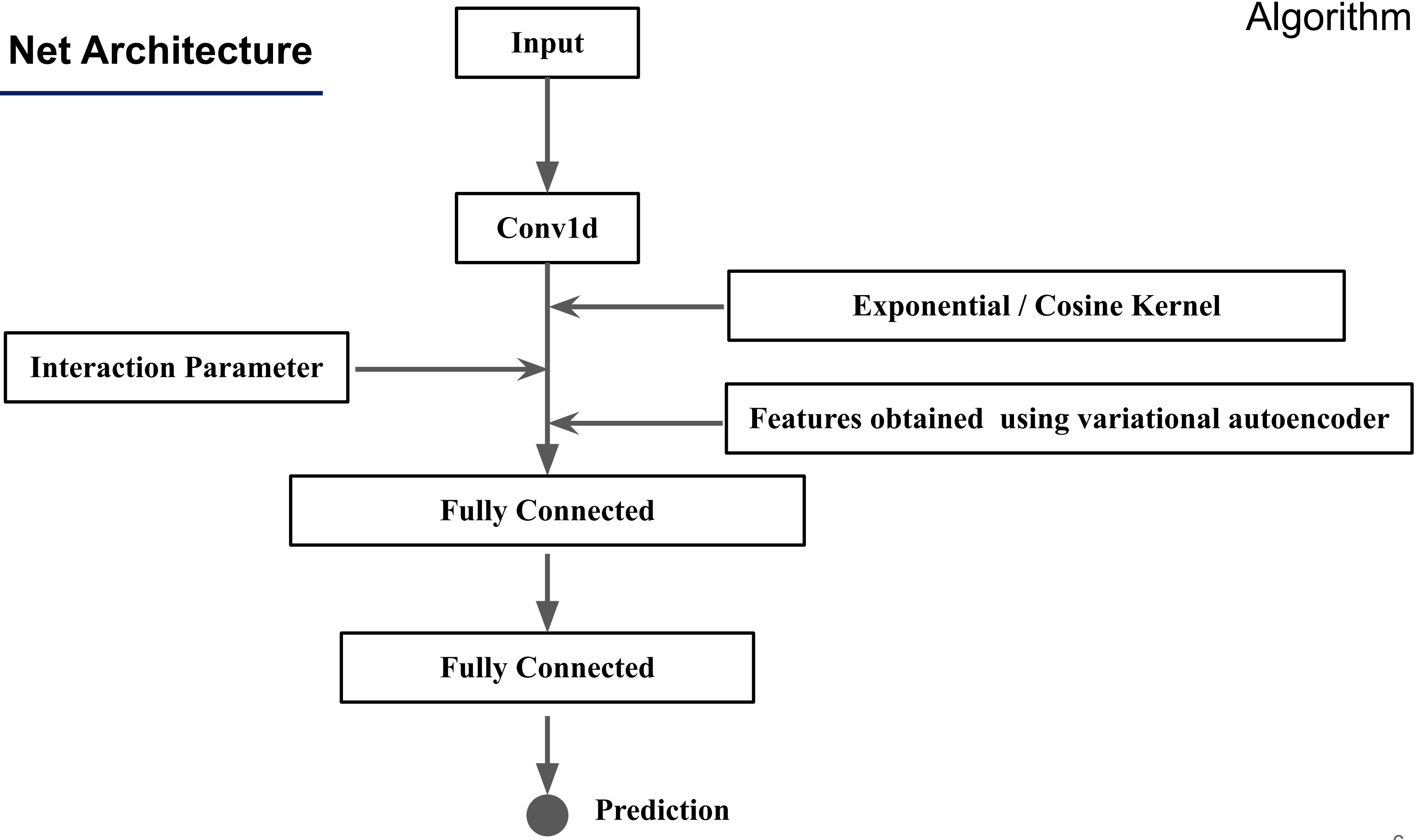


Monomer sequences

BBBBBCCCCC

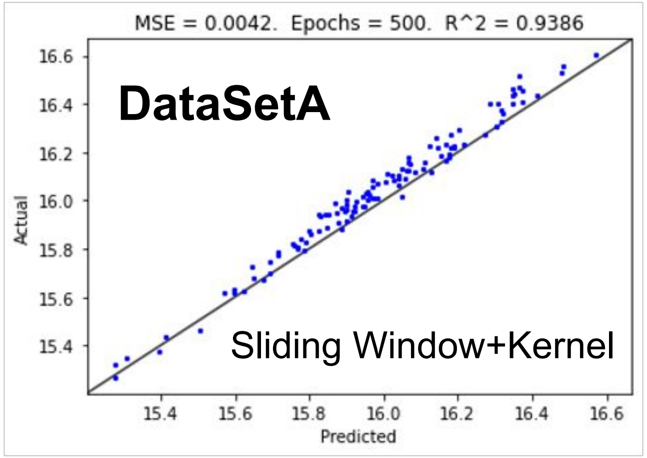
Reduced feature vectors

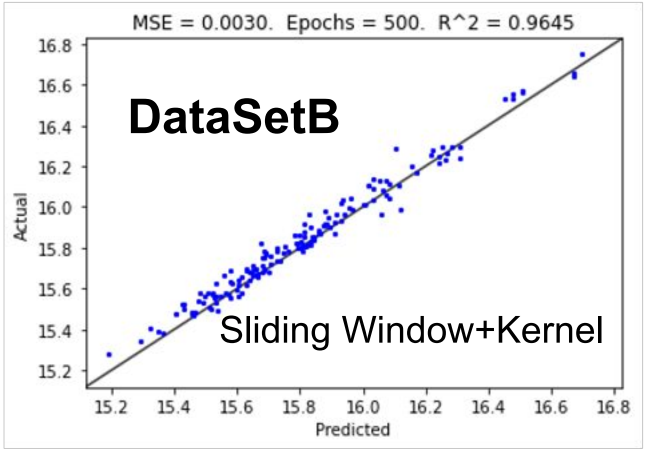
Neural Net Architecture

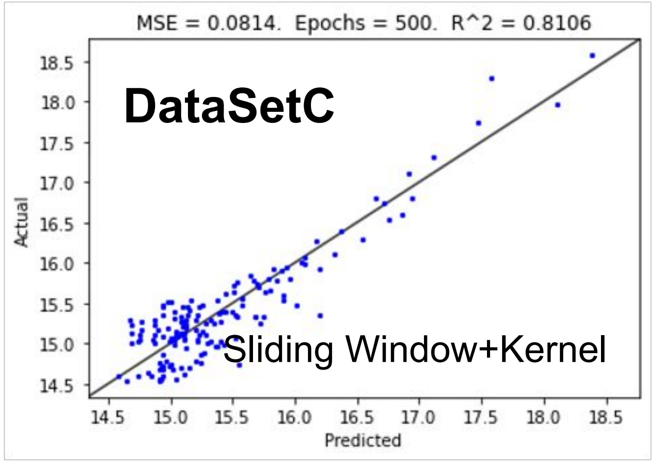


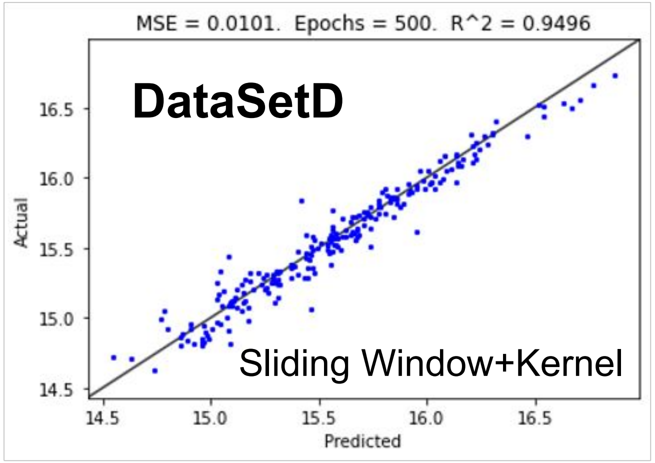
Results

w/o PC1





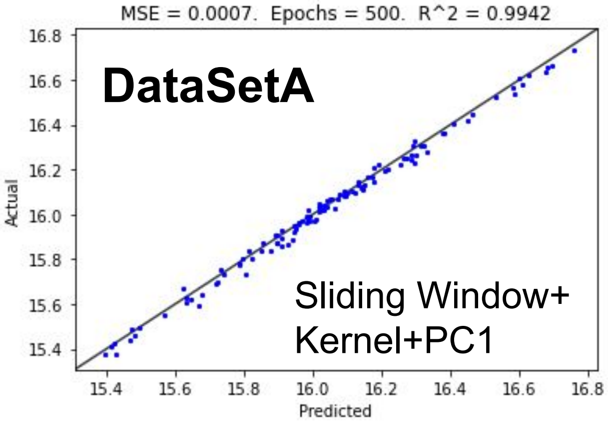


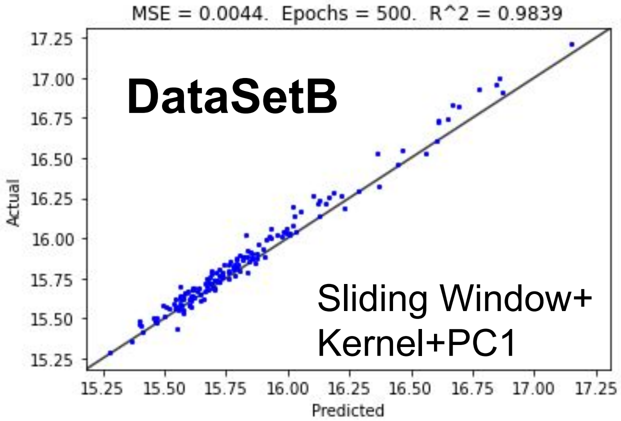


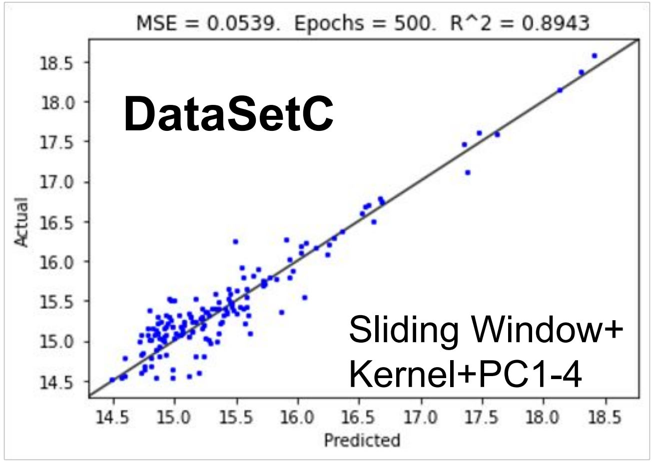
500 epoch
0.01 learning rate

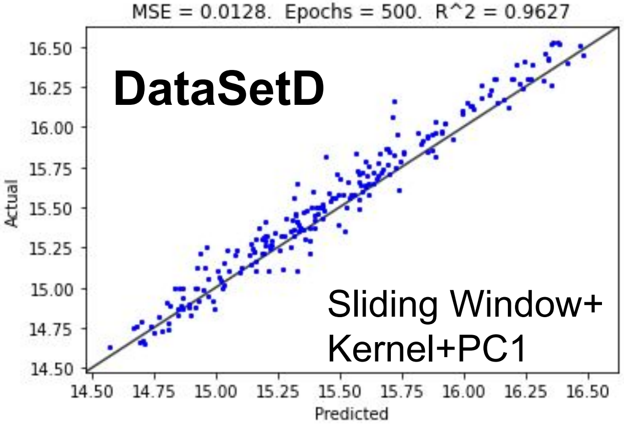
Results

w PC1



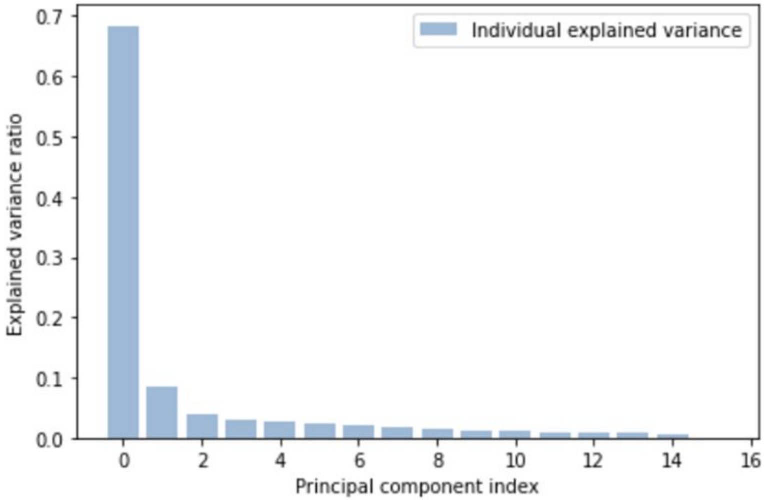




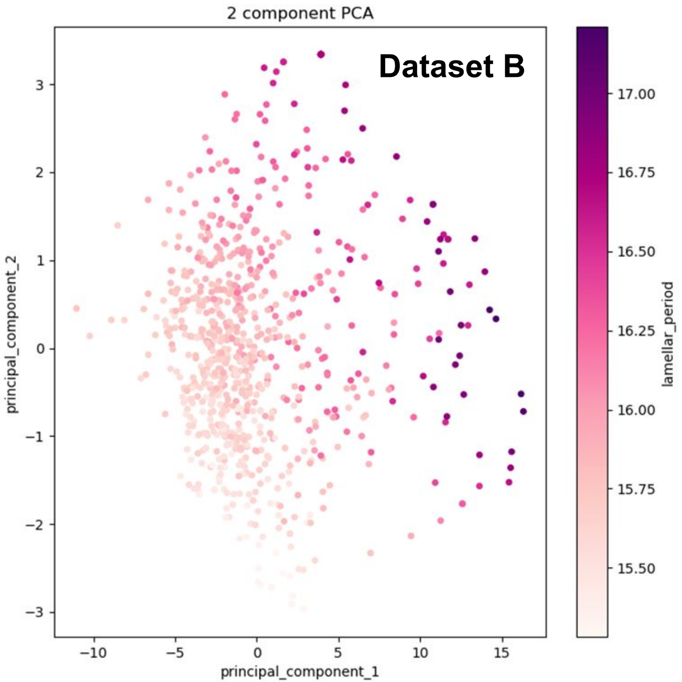


500 epoch
0.01 learning rate

Principal component analysis on the latent space



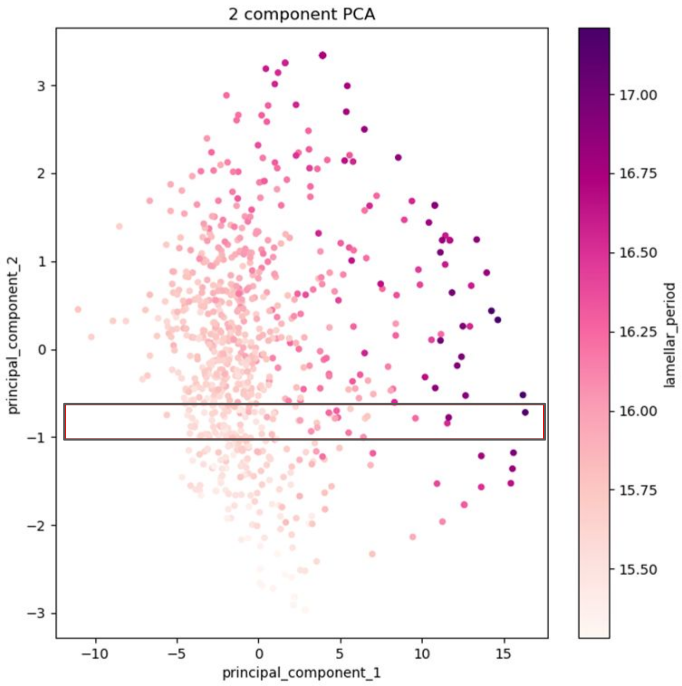
Principal component 1 dominates



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!