

Kernel-Based Multi-channel PolyCovNet

AI Hackathon Challenge I



Team Borides

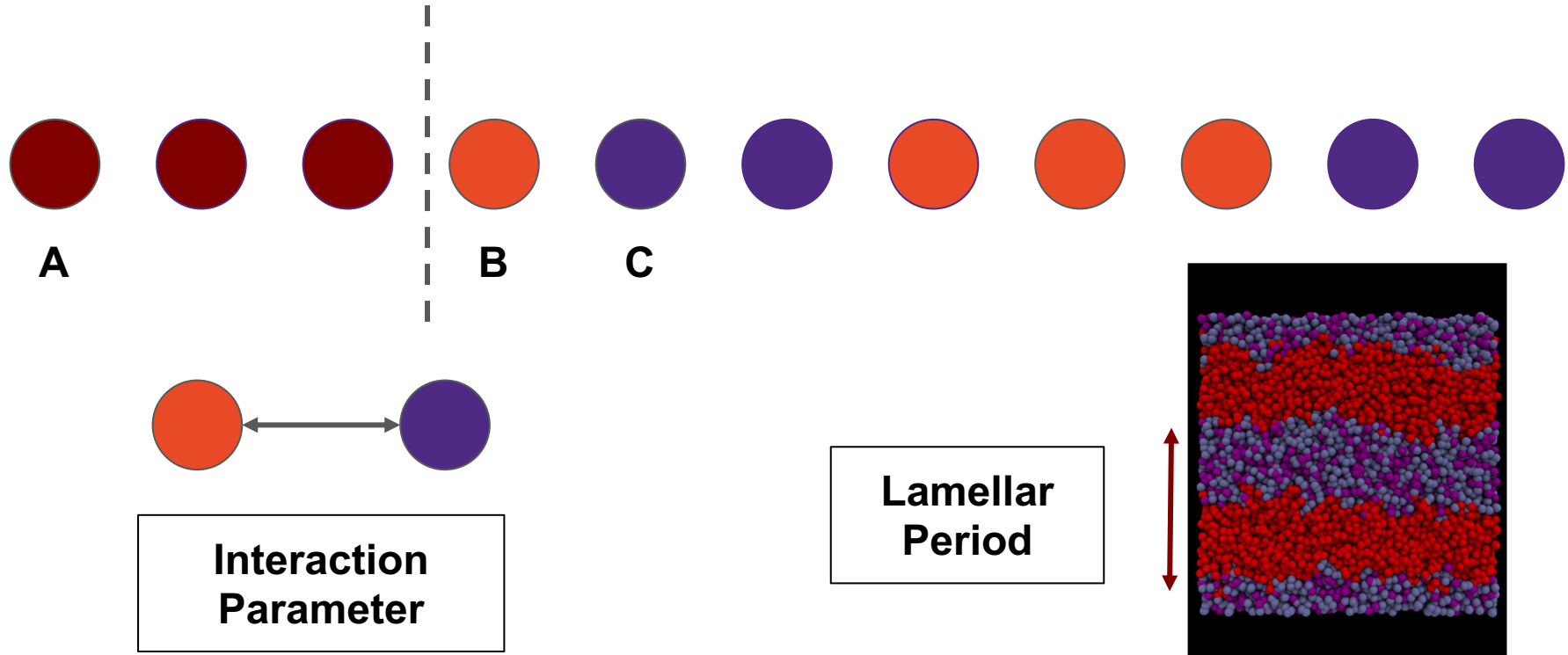
Kastan Day, Ruijie Zhu, Aria Coraor, Seonghwan Kim, Jiahui Yang

Contents

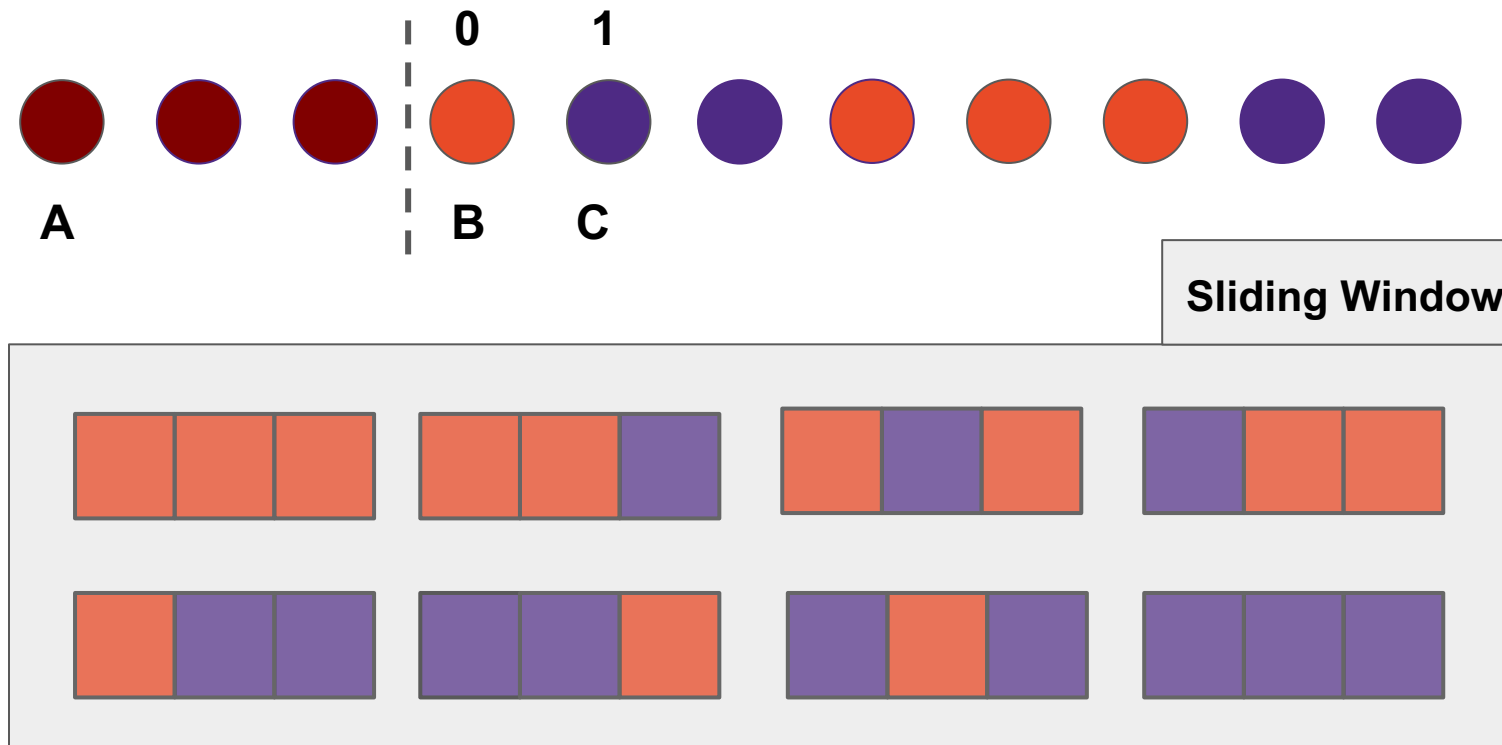
1. Problem Restatement
2. Features Engineering
3. Kernel-Based Multi-channel PolyConvNet
4. Results
5. Discussion
6. Summary

Problem Restatement

Predicting the lamellar period using monomer sequences and interaction parameters

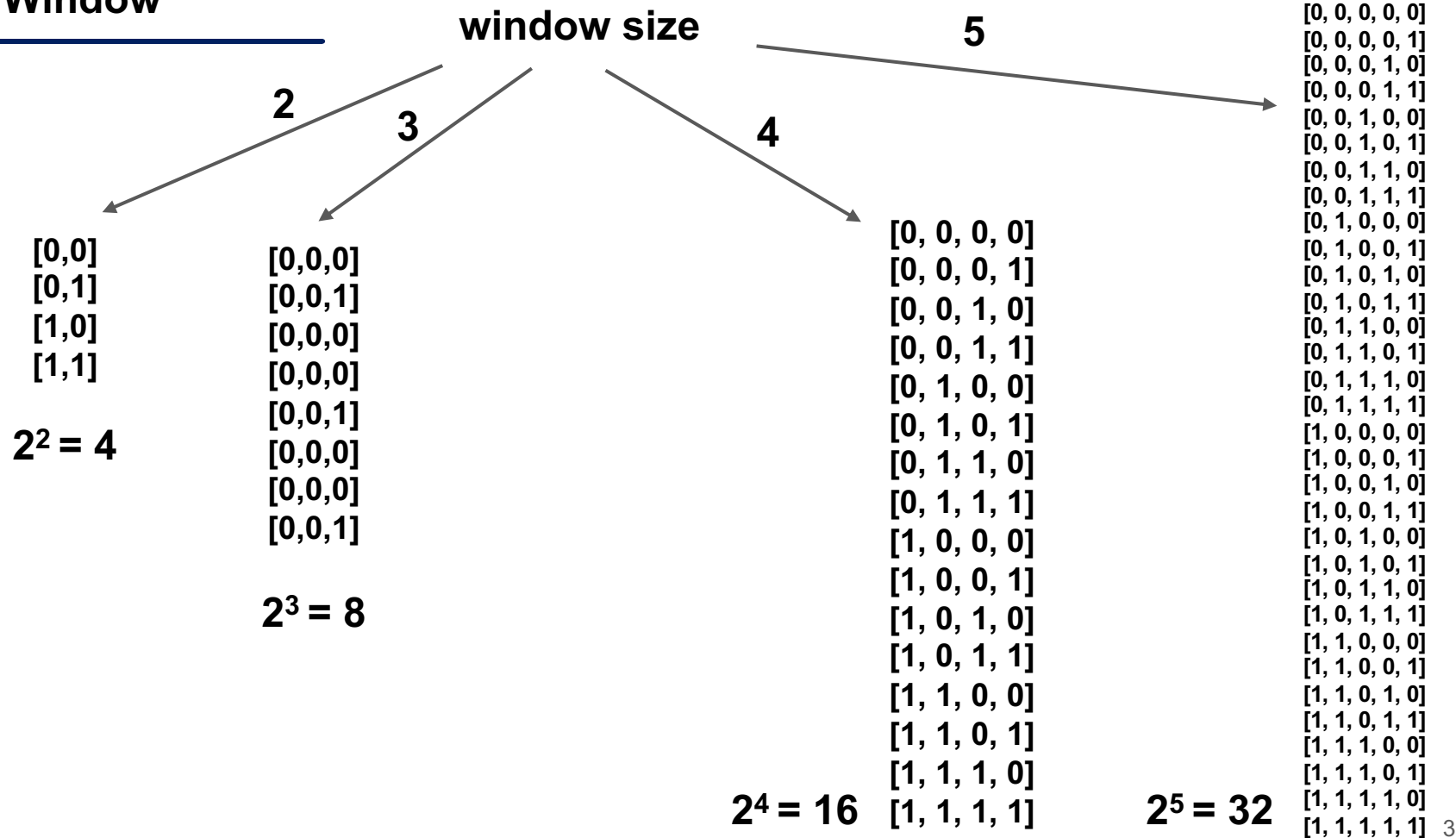


Sliding window - extract monomer sequence features



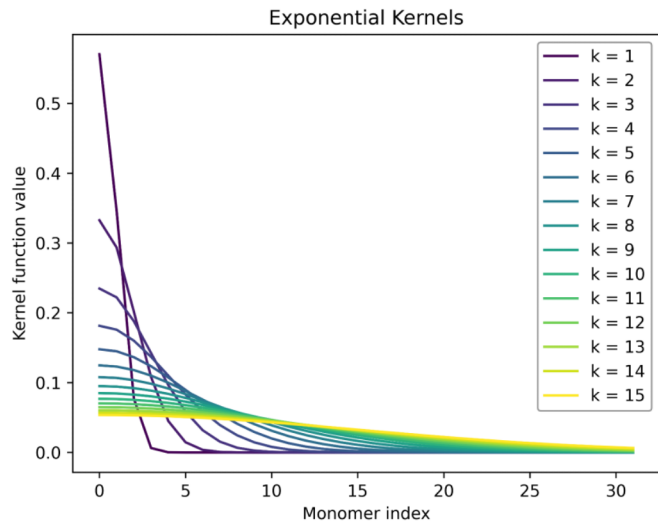
Sliding Window

Feature Engineering

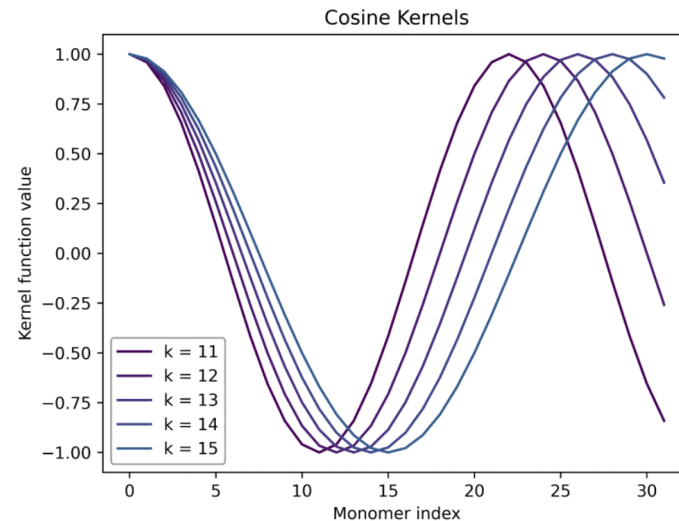


Non-linear kernel functions - preprocess monomer sequences

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

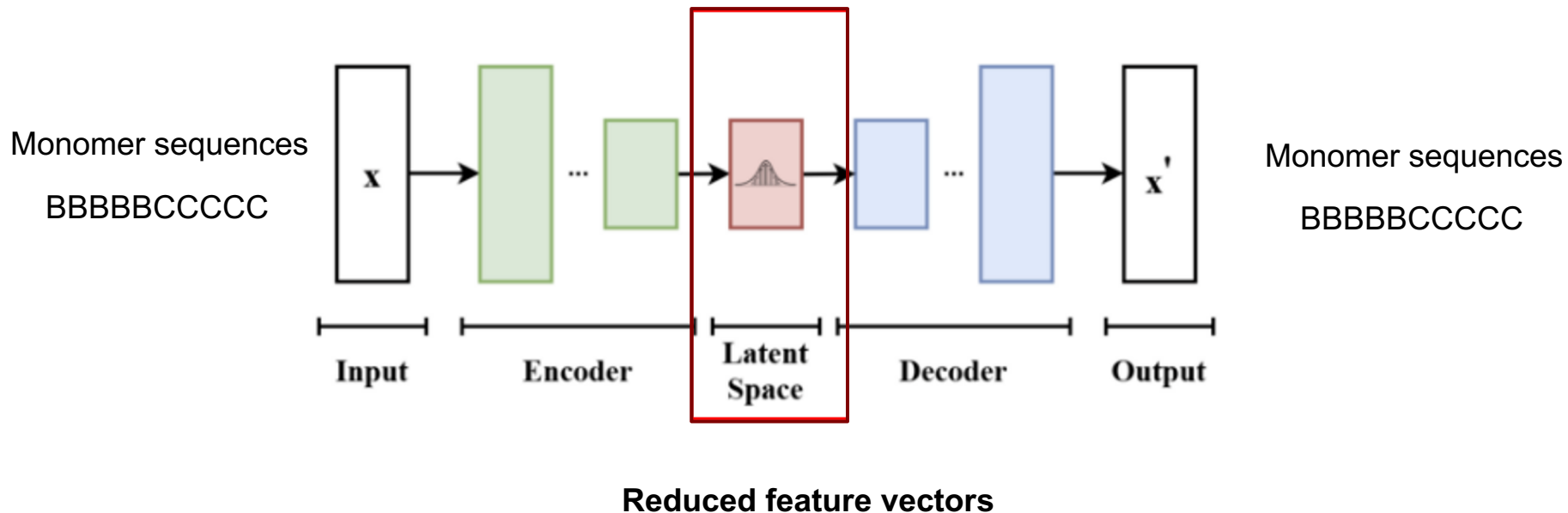


2. Cosine kernels $\cos(\frac{\pi x}{k})$

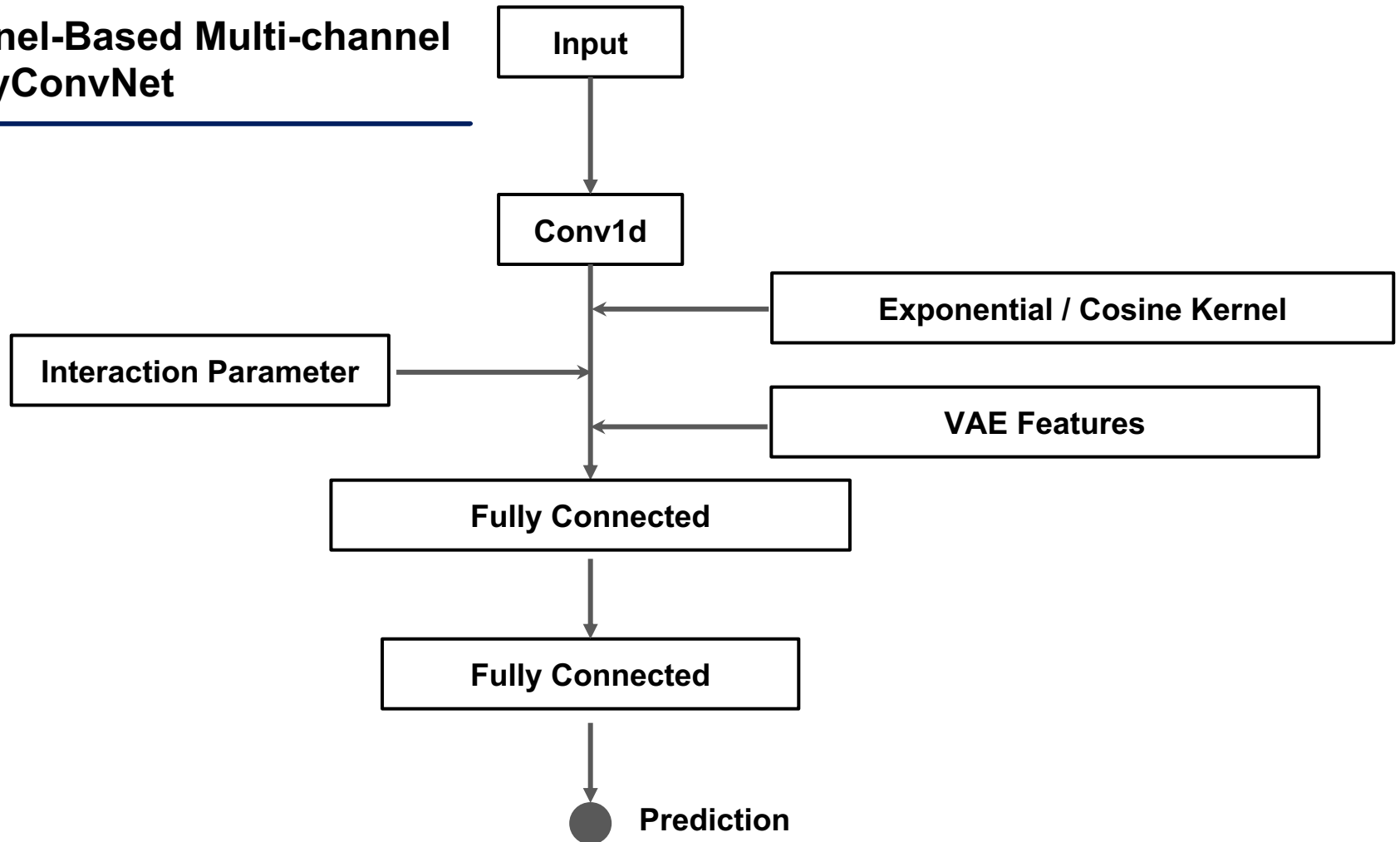


Applying the above kernels on monomer sequences ➡ Non-linearity

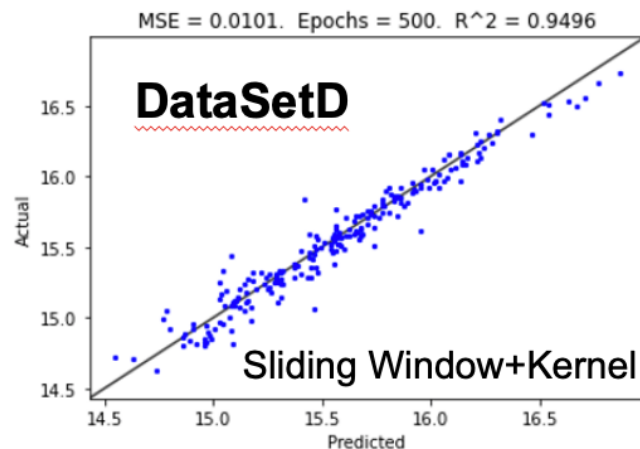
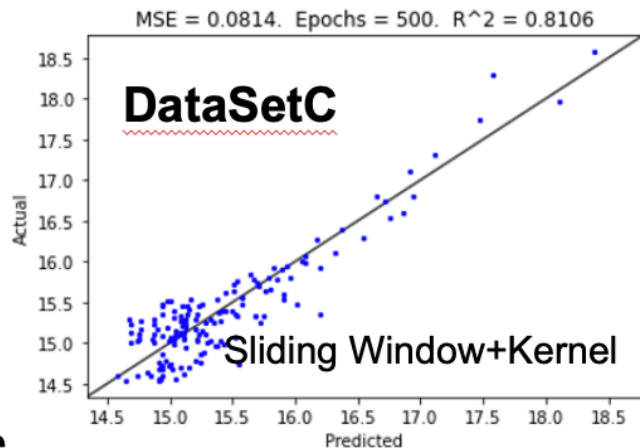
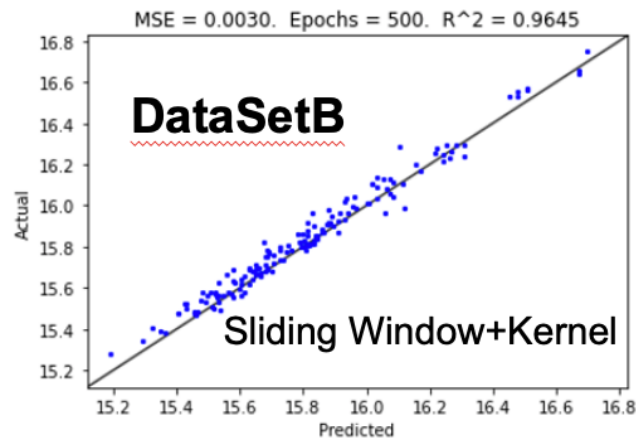
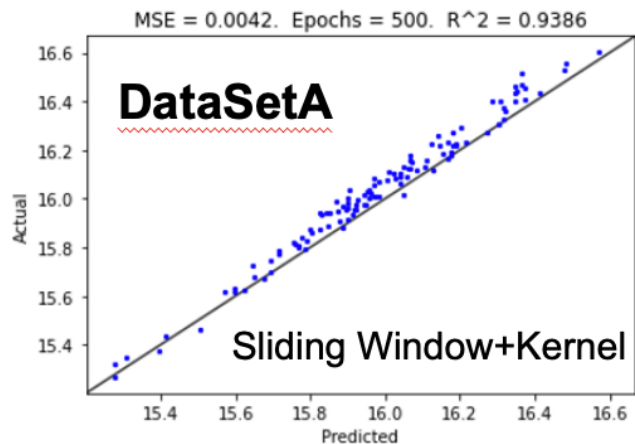
Variational autoencoder - extract features from monomer sequences



Kernel-Based Multi-channel PolyConvNet

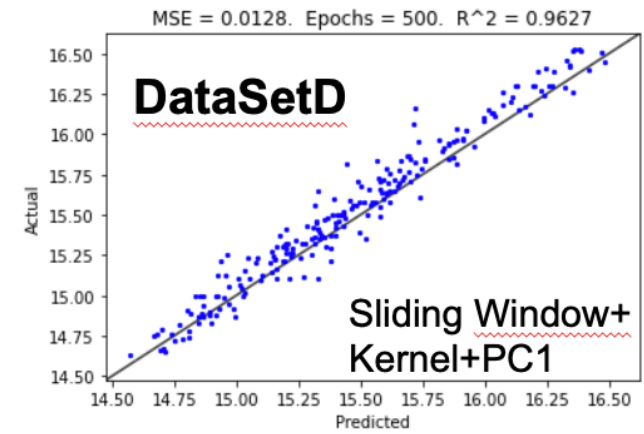
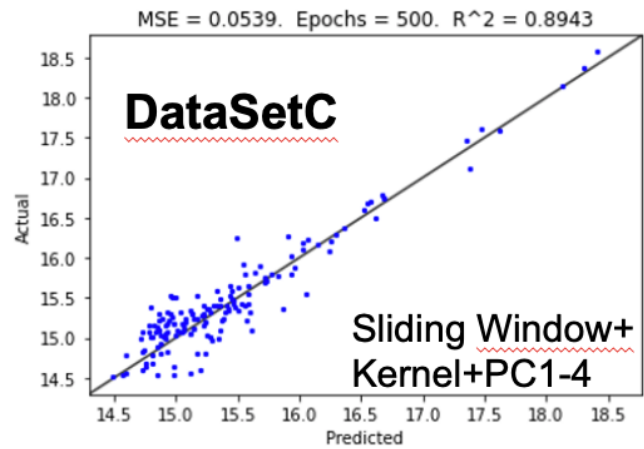
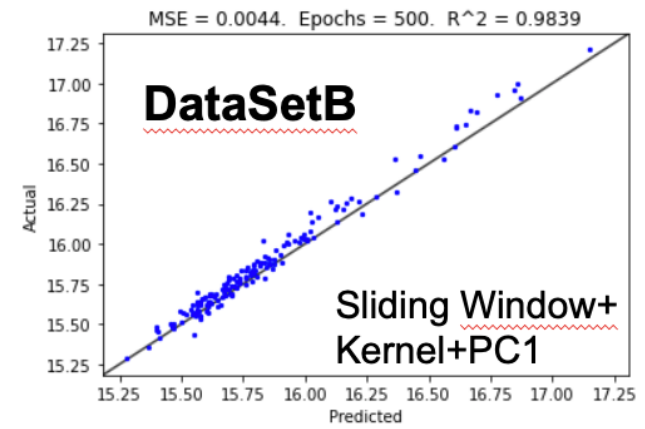
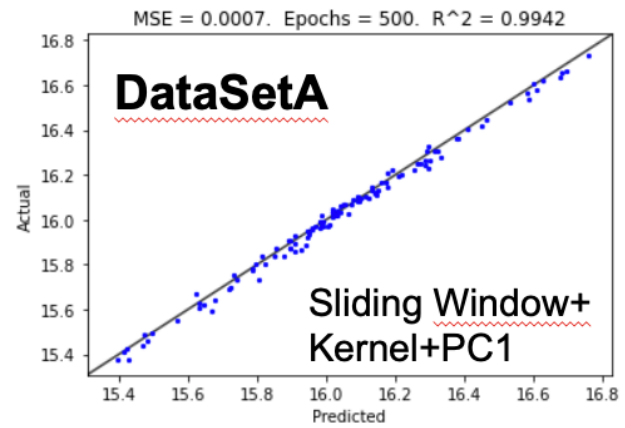


w/o PC
features



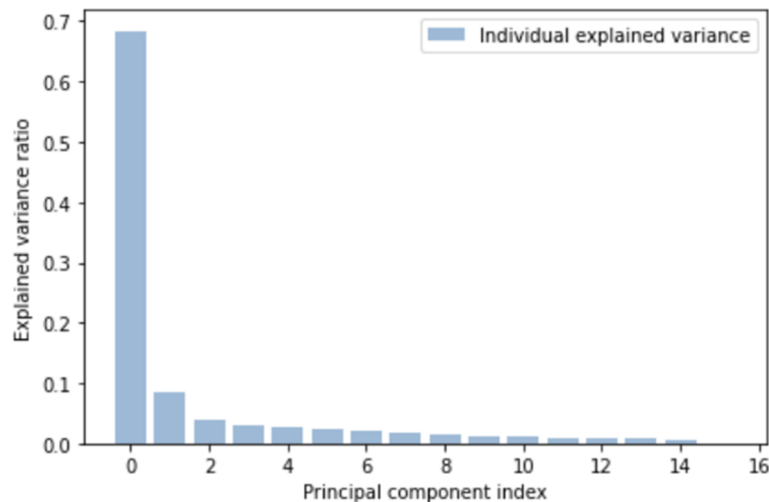
500 epoch
0.01 learning rate

w PC
features

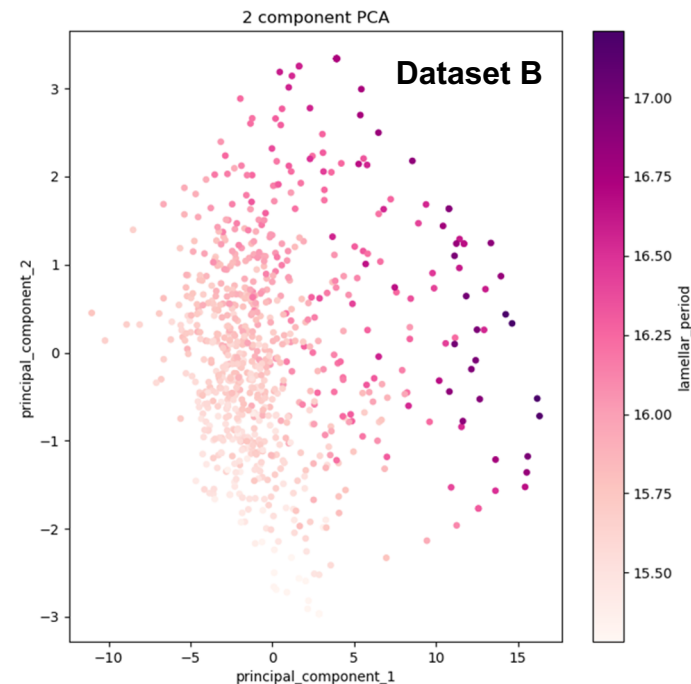


500 epoch
0.01 learning rate

Principal component analysis on the latent space



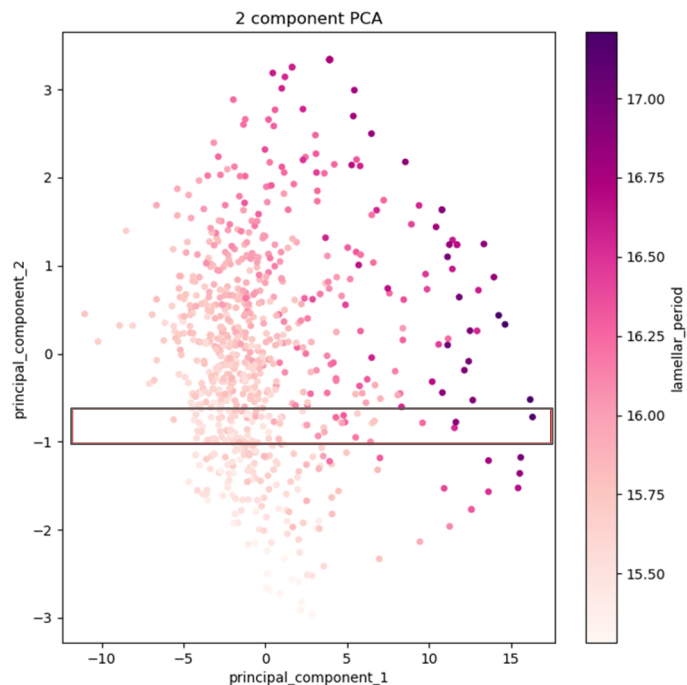
Principal component 1 dominates



Larger principal component 1

Larger lamellar period

Blockiness is important to result in a high lamellar period



Higher principal component 1

```
111111111111111111110000000000000000
111111111111111111110000000000000000
111111111111111111111000000000000000
111111111111111111111100000000000000
111111111111111111111110000000000000
```

Blockiness

```
0.875000
0.874510
0.873016
0.870445
0.866667
```

Lower principal component 1

```
1100001100111000011000000111111
0000001111111000000000000111111
1100000111011011000000000111110
01000111110110010001101000100111
10100001110001000100100100011011
```

Blockiness

```
0.498039
0.740891
0.372549
0.000000
-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!
