Extracting structural folding pattern of chromatin using chromatin condensation data

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## Introduction



#### • Hi-C experiment

- In these Heatmaps, most of the chromatin folding patterns in the nucleus can be observed.
- Topologically Associating Domains (TAD), A/B compartments, loops, and stripes are some of the most well-known structural patterns.

Cohesin

super-enhancer

stripes

From Ref [14]

one-sided cohesin extrusion

(promoter is reeled in)

promoter

Courtesy from Qiu Sun

#### Problem

- In beads-on-a-string models of chromatin, the curves which show the dependence of the Euclidean spatial inter-particle distance of chromatin chains on the genomic distance play an important role to reveal the information of condensation of chromatin across whole genome.
- We have a computational modeling for chromatin in drosophila genome based on MD simulation[2] which we can extract these curves from the distance matrices of position of beads on ensemble of chromatin chain.
- What I am interested in is whether we can obtain Hi-C folding patterns following training the data with CNN?



Each curve represents one specific trajectory in the MD simulation.

- Provide data set as the symmetric square matrices
- We have 18 trajectories that show different chromosome configurations in Drosophila. In molecular dynamic simulation of chromatin chains in the Drosophila genome, we have 400K different configurations that correspond to 400K different timesteps for each trajectory. [2]

### Milestone 1

dataset

# Milestone 2

- Training the 2D matrices using Convolutional Neural Networks (ImageNet[3], LeNet [4] or AlexNet[5]).
- Training the 2D matrices using one of VGG[6], InceptionNet[7, 8, 9] ResNet[10] and DenseNet[11].





Increasing the resolution using HiCNN[12] or HiCNN2[13] approaches





#### Milestone 4

• Metrics for evaluation:

Comparing the result's mean squared error and Pearson's correlation coefficients with experimental high-resolution Hi-C data

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