Unsupervised machine learning algorithms can detect dynamical heterogeneities in 2D glass former liquids from the structural heterogeneities

Unsupervised Machine Learning in 2D Glasses

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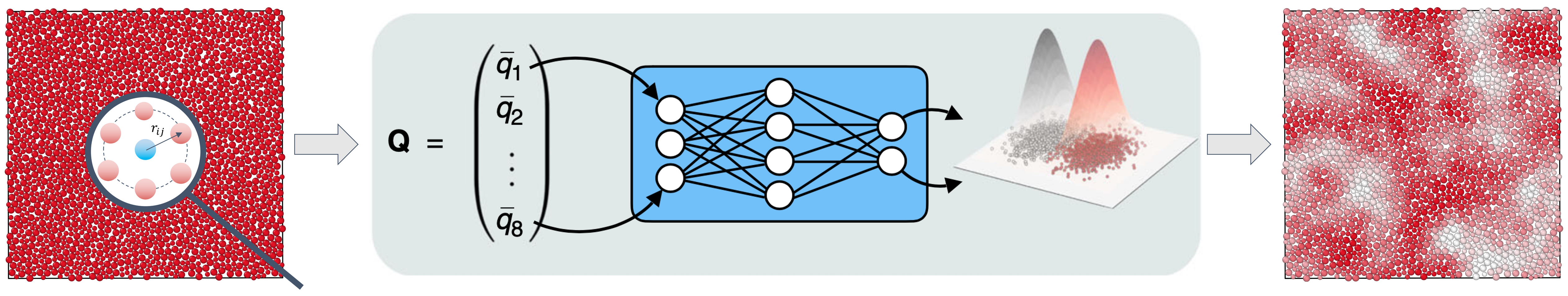


INTRODUCTION

- We use an unsupervised machine learning (UML) technique to autonomously find structural variations in a 2D glassy system [1].
- We then show that these structural variations strongly correlate with the future dynamics of the particles. This demonstrates the strong link between structure and glassy dynamics [2].

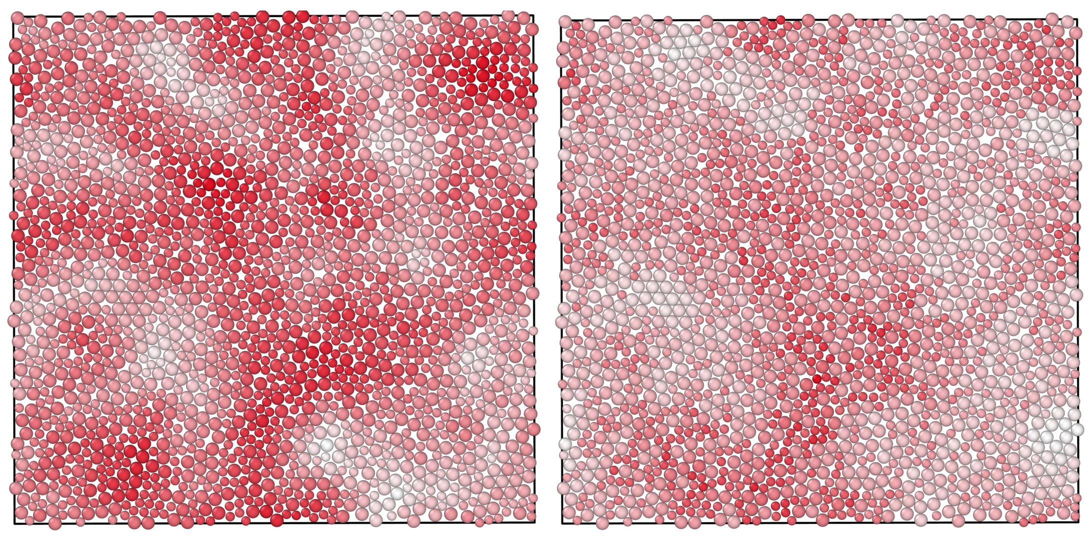


Fig.1 Snapshots of a 2D glass former. Particles are coloured by their machine-learned membership probability $\bar{P}_{red}$ (left) and by the dynamic propensity D_i (right).

METHODS

- Event driven molecular dynamics generates 2D binary hard disk liquids.
- Bond-orientational order parameters describe the local structure.
- Neural network based autoencoder implemented with PyTorch [3].
- Gaussian mixture model clustering algorithm

RESULTS

- The UML approach separates the particles into two clusters according to their local structure.

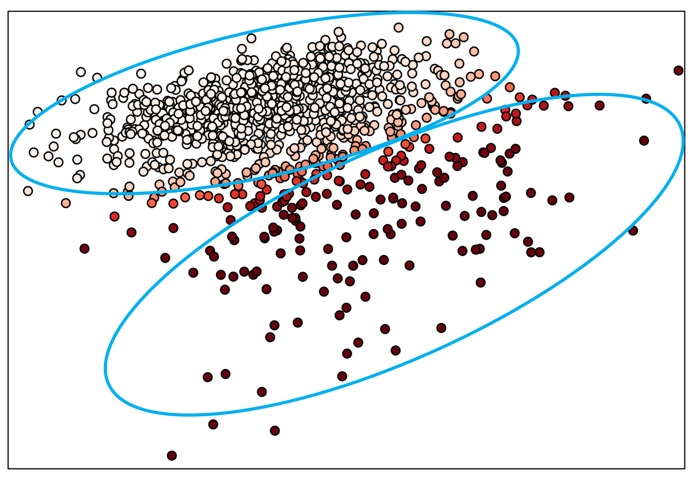


Fig. 2 Large particles are clustered on the reduced dimensional space. Red points correspond to faster particles a posteriori.

- Average membership probability correlates with dynamic propensity.

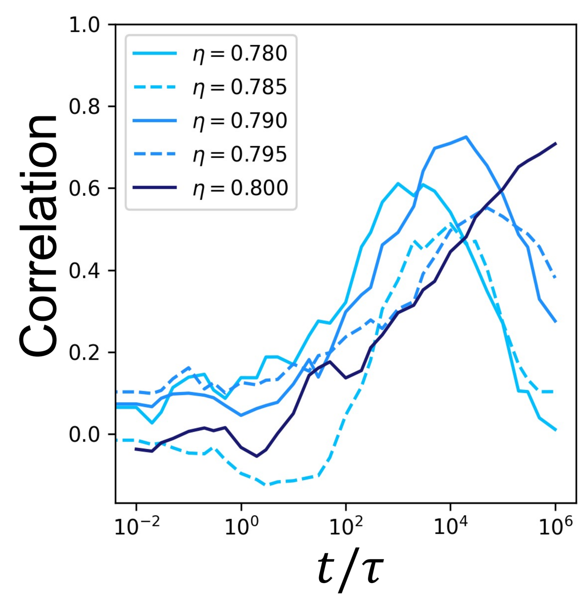


Fig. 3 Spearman's rank correlation between the particles' membership probability and their dynamic propensity. The probability values are predicted by UML.

DISCUSSION

- 2D correlations are comparable to their 3D equivalents [1].
- We can improve the correlation between the machine-learned order parameter and dynamics by also considering structural descriptors that only consider particles of the same species.

Scan to see this poster and related animations

Supplementary Information

Bond orientational order parameters

$$\phi_k(i) = \frac{1}{n}\sum_j^n e^{ik\theta_{ij}}$$

Locally averaged bond order parameters

$$\bar{\phi}_k(i) = \frac{1}{n}\sum_j^n \phi_k(j)$$

Input to the autoencoder

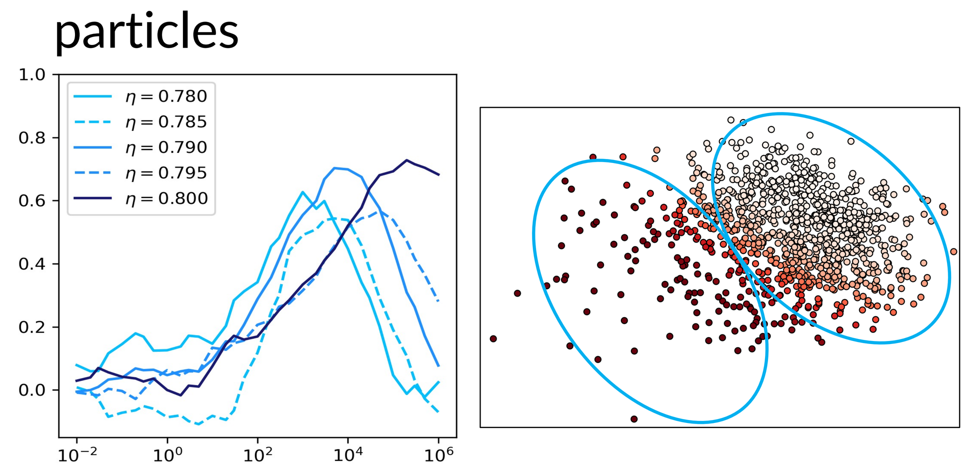
$$\bar{\Phi}(i) = \left(\{\bar{\phi}_k(i)\}, \{\bar{\phi}_k^{ss}(i)\}\right)$$

Dynamic propensity

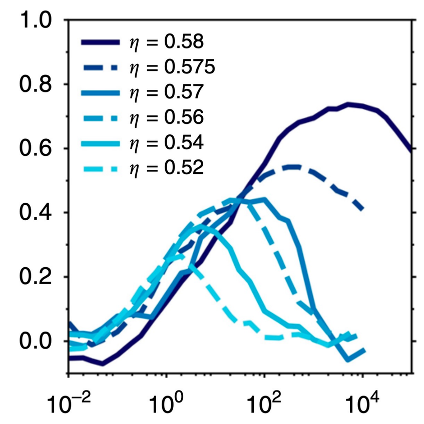
$$D_i(\delta t) = \langle |\mathbf{r}_i(\delta t) - \mathbf{r}_i(0)| \rangle_c$$

Autoencoder architecture
Linear input layer dimension: d=16
Nonlinear encoder layer dimension: 10d
Bottleneck dimension: c=2
tanh activation function is used in both nonlinear layers

Correlations and clustering of small particles



Correlations in 3D taken from [1]



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