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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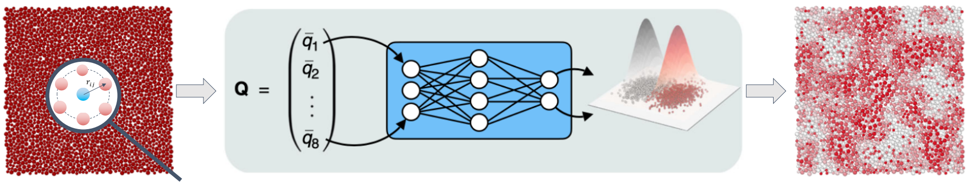


INTRODUCTION

- Glassy systems remain one of the unsolved problems of condensed matter physics [1].
- Unsupervised machine learning proves useful in predicting the dynamics of 3D glass formers from their structure [2].
- We extend this technique to a 2D glass former composed of binary hard disks.

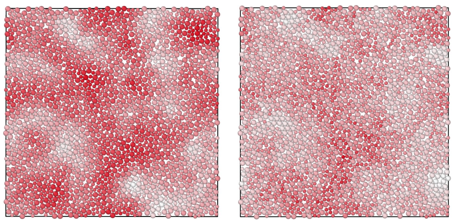


Fig.1 Snapshots of a 2D glass former. Particles are coloured by their membership probability P_{red} obtained by machine learning algorithms (left) and by the dynamic propensity D_i (right).

METHODS

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

RESULTS

- Particles cluster according to their membership probability

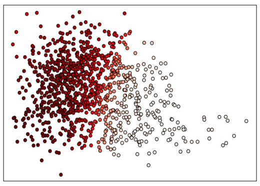


Fig. 2 Large particles are clustered on the reduced dimensional space. Red points correspond to faster particles a posteriori

- Average membership probability correlates with dynamic propensity

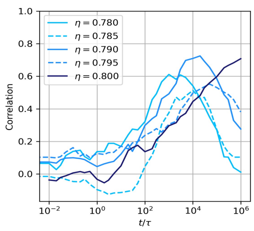


Fig. 3 Spearman's rank correlation between the particles' membership probability and their dynamic propensity. The probability values are predicted by UML

DISCUSSION

- 2D correlations are comparable to their 3D equivalents
- Calculating a particle's order parameter by also considering its same species neighbours improves correlations and it is not observed in 3D.

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

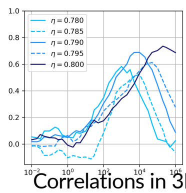
$$\bar{\Phi}(i) = \left(\{\bar{\phi}_k(i)\}, \{\bar{\phi}_k^{ss}(i)\}\right)$$

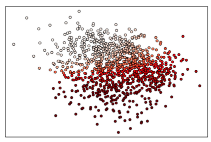
Dynamic propensity

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

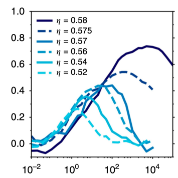
Autoencoder architecture
Linear input layer dimension: d=16
Nonlinear encoder layer dimension: 10d
Bottleneck dimension: c=2
tanh activation function is used in both nonlinear layers

Correlations and clustering of small particles





Correlations in 3D



REFERENCES

[1] L. Berthier et al. Rev. Mod. Phys. 83, 587 (2011)

[2] E. Boattini et al. Nat. Commun. 11, 5479 (2020)