Can we detect order in disorder?

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I. THE CHALLENGE

Glass is one of the least understood states of matter. If you look at an image of the particles in a glass on the microscopic level, it looks almost the same as a liquid. However, if you watch its dynamics – it acts more like a crystal (see Figure 1).

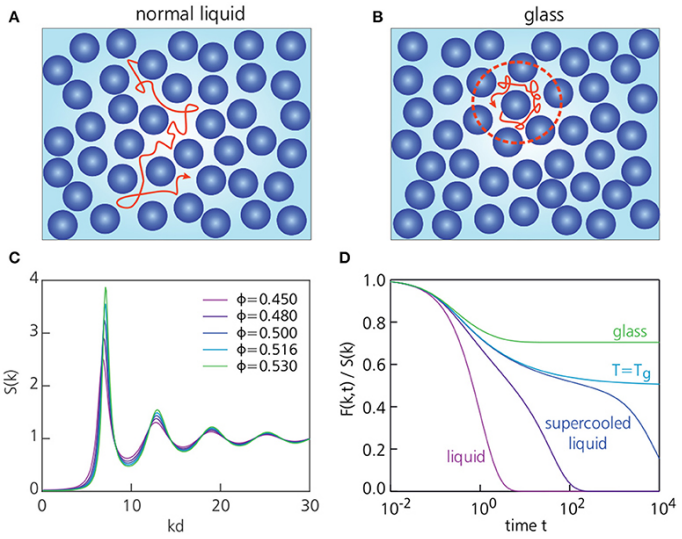

FIG. 1. Structure and dynamics in glassy systems. a) A cartoon of a liquid, b) A cartoon of a glass, c) The structure factor of a hard sphere glass at different densities. As the density increases, the system should become more glassy. Note that nearly no changes are visible in the structure factor. d) The self-intermediate scattering function which gives information on the dynamics of the system. Note that while the structure barely changed the dynamics depends strongly on the density. Taken from Ref. 1.

In order to better understand this behaviour, physicists have dug deeper into both the structure and dynamics of glassy systems. An important realization has been that the dynamics in glassy systems is highly heterogeneous – with some largish regions more mobile than others[?] . This leads to another important question – is there a structural origin for this difference in dynamics?

An ideal tool to address such a question is machine learning. In this project you will explore whether unsupervised machine learning identifies different structural regions in a glass (is there order in the disorder?), and explore whether there is any connection between these structural regions and the dynamics.

To do this we require two elements:

- a description of the local environment of each particle. For this we will use a vector of bond order parameters, as described in Ref.
- a "measure" of the dynamics per particle at different future times. For this we will use the so-called dynamic propensity. The dynamic propensity $\Delta r_i(t)$ of each particle i is obtained by averaging its absolute displacement over a set of simulations starting from the same configuration, i.e.

$$\Delta r_i(t) = \langle |\mathbf{r}_i(t) - \mathbf{r}_i(0)| \rangle_{\text{conf}} \,, \tag{1}$$

  where the subscript 'conf' indicates the isoconfigurational average. Note that an isoconfigurational average is determined by running many molecular dynamics simulations of the system starting with the same positions for each particle but with different velocities (where the velocities are chosen via the Maxwell Boltzmann distribution). Hence, the dynamic propensity can be seen as the "average" distance a particle in a specific environment would travel in a give time t.

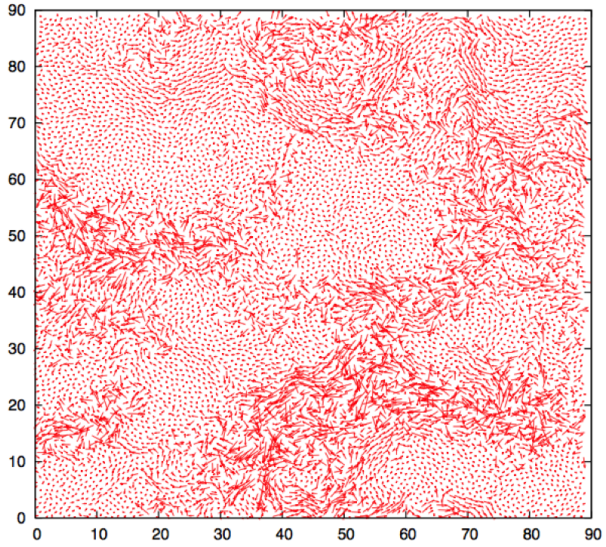

FIG. 2. In this image the dynamics of particles in a glass are drawn with arrows. Note that in some regions particles move a lot, while in other they basically stay still over this time window. This is what is referred to as dynamic heterogeneity. Taken from Ref. 2

II. PROJECT

The data set provided includes both the local descriptors and the dynamic propensity at different times. Your project is to design an unsupervised ML algorithm that explores the differences in local structure in this glassy system, and compares them to the dynamic propensity. Note that the data package contains data for three separate glassy systems: i) binary hard spheres[3], ii) Kob Andersen[4], and iii) harmonic spheres[5,6]. A short description of each model system can be found in Ref. 7. Start with one model, but if you have time check out what happens when you explore the others.

A useful background reference on glassy systems is Ref. 8. For the machine learning a good starting point are Refs. 9 and 7.

III. REFERENCES

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