Interplay of rearrangements, strain, and local structure during avalanche propagation

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Abstract

We demonstrate how a machine-learned quantity can give new insight into a challenging physical sciences problem. Jammed soft disks exhibit avalanches of particle rearrangements under quasistatic shear. These avalanches consist of localized rearrangements that trigger rearrangements elsewhere, and result from a complicated interplay between local structure, rearrangements and elasticity. To date, there has not been a useful variable for characterizing local structure that could be used to describe the avalanche process. We show how a machine-learned quantity, softness, that characterizes local structure and is designed to be highly correlated with rearrangements, enables us to disentangle the interplay for the first time. Our findings form a firm microscopic foundation for a coarse-grained model for plasticity that includes local structure.

1 Introduction

Machine learning has been used as a tool for approximation and classification in physics, but applications to develop new theories of phenomena have been rare. One class of problems in which a machine-learned quantity has been proven to yield insight is in the dynamics of systems near glass transitions (1; 2; 3; 4). Here we use a similar approach to build a new theoretical framework for describing plastic flow in disordered solids.

All disordered solids respond elastically at low strain but flow plastically at sufficiently high strain. As strain increases beyond the elastic regime, disordered solids partially relax via intermittent localized rearrangements until they reach the yield strain, where they begin to flow. Beyond the yield strain, many systems exhibit avalanche behavior (5; 6; 7; 8). An avalanche consists of a series of rearrangements. A class of models known as elastoplastic models describes the courses of avalanches in terms of the interplay of rearrangements and elastic stress (9): an increase of elastic stress can cause a local region to yield and rearrange, while conversely, a local rearrangement can increase stress elsewhere. It has become increasingly clear, however, that rearrangements and elasticity do not tell the whole story. Systems with identical microscopic interactions can show ductile or brittle behavior depending on preparation history (10; 11). This bolsters approaches postulating that certain local structures are prone to rearrange (12; 13), but also points to the need for microscopic understanding of the connection between local structure and the physics included in elasto-plasticity models. While it has been shown that certain local structural environments are much more likely to rearrange than others (1; 14; 15), the effects of rearrangements on local structure have not been established, even though it is clear that they must exist (1). It is also clear that elastic stresses can distort the structural environment surrounding a particle. These considerations point to the need for detailed understanding of the interplay of local structure, rearrangements and elasticity.

Third Workshop on Machine Learning and the Physical Sciences (NeurIPS 2020), Vancouver, Canada.

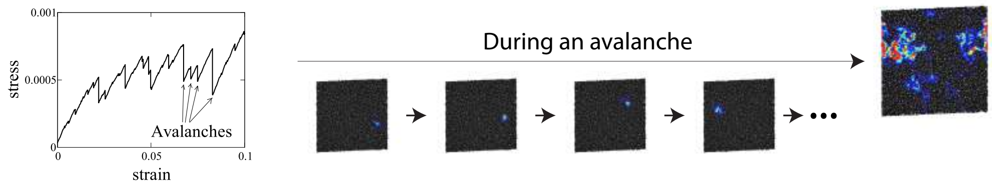

Figure 1: As strain increases, avalanches occur during stress drops. During an avalanche, some constituent particles rearrange, triggering other localized rearrangements far away in the depicted system of $N = 4000$ particles, which is smaller than the ones used in the rest of the paper for improved visual clarity. Here, the non-affine displacement of particles, indicative of particle rearrangements, is represented on a black-to-blue-to-red scale with red corresponding to high values of displacements. The rightmost plot depicts the cumulative non-affine displacement measured over the entire stress drop.

Here we untangle the interplay of local structure, rearrangements and strain in athermal, quasistatically sheared jammed packings of soft disks. We capture local structure via a machine-learned quantity, softness (1; 2; 3; 16). Following Ref. (1), we describe softness as the weighted sum of a set of structural quantities based on the local pair correlation function, where the weights are chosen to maximize the correlation with rearrangements that occur during avalanches. To tease out the interplay between softness, rearrangements and stress, we look at the effects of each of these factors on the others to develop a “structuro-elasto-plasticity" framework for avalanches in disordered solids.

2 Simulation details and softness

We generate two-dimensional packings of $N = 10^5$ soft disks, which repel each other if they overlap and have no interaction otherwise. Such a large N allows us to study the effect of a rearrangement at a large distance ($r = 100$). We chose such a simple model not only because it enables this large N, but also because more complicated models are not necessary for our purpose since there is likely a common mechanism behind avalanches in all kinds of disordered materials (9). To avoid crystallization, we use a $1 : 1$ mixture of particles with radii $\sigma = 0.5$ and $\sigma = 0.7$. Such a composition and radii ratio are chosen to minimize the tendency to from crystals (17). Starting from random initial conditions, we minimize the potential energy to find the initial zero-temperature jammed state. We then repeatedly apply a small shear-strain step of $\delta\epsilon$ and minimize the energy after each step. The stress-strain relation for a single configuration, shown in Fig. 1, confirms the existence of avalanches. We focus only on these stress drops, using steepest descent with adjustable step sizes to capture the over-damped relaxation process from the beginning of the energy drop to the end. We save intermediate configurations that are equidistant in configuration space, so that the sum over particles of particle displacement squared is fixed between successive frames.

To identify rearranging particles, or “rearrangers," we calculate D^2_{min} (18), which is the local average non-affine displacement around a particle. A particle with $D^2_{\text{min}} > 0.0025$ between two adjacent frames is a rearranger. The rest of the paper presents results for rearrangers that are small particles in our binary mixture, but we have verified that results for large-particle rearrangers are qualitatively the same.

We draw from the sets of rearrangers and non-rearrangers to train a linear support vector machine (SVM) to obtain softness, a structural quantity that indicates the propensity of a particle to rearrange (1). The SVM's input (i.e., feature set) is the local pair correlation function $g_i(r)$ at different rs. As in Ref. (1), the trained weights is highly negative at the first peak of $g(r)$, implying that particles with fewer neighbors have higher softness, consistent with intuition based on the cage picture.

3 The avalanche process

In Fig. 1, we confirm that during avalanches, rearrangements are indeed localized and sequential, as assumed in elastoplastic models (9). Moreover, consecutive rearrangements can be very far apart.

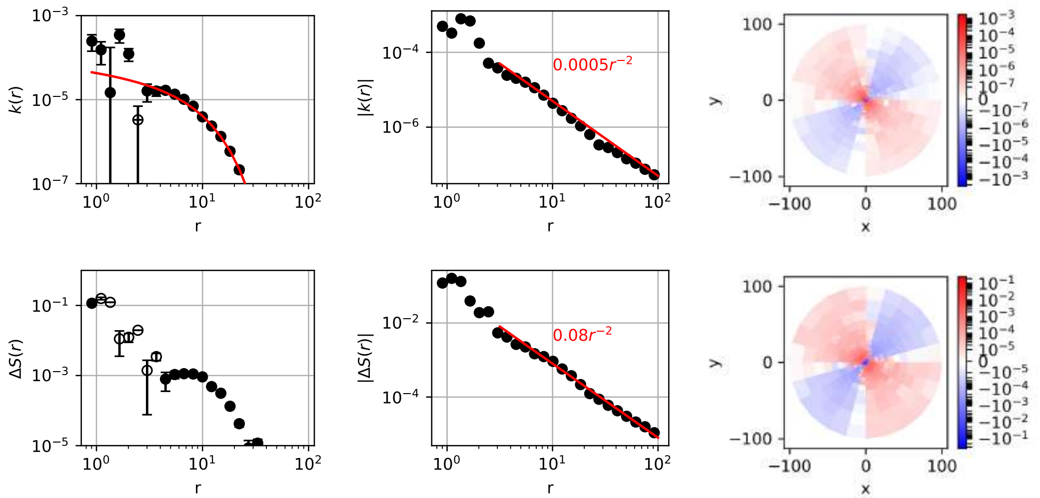

Figure 2: Mean volumetric strain k (top row) and softness change (bottom row) per frame caused by a rearranging particle at the origin. Angular-averaged (left), angular-averaged absolute value (middle), and angular (right) versions are shown. In the left two plots, solid circles represent positive values of $k(r)$, while open circles represent negative values. Red lines are fits to continuum-elasticity predictions.

3.1 Interplay of rearrangements with strain

We begin our study of the interplay between rearrangements, softness and strain by examining the effect of a rearrangement at the origin on strain at $\mathbf{r}$, averaged over many rearrangements. We calculate the local-fit deformation tensor about each particle and extract three different strain components: the volumetric (isotropic) strain k, total deviatoric strain $\tilde{\epsilon}$, and shear strain in the xy direction (the direction of the global shear), ϵ_{xy}. We extract these by comparing two consecutive frames when a rearrangement is occurring. Of these three strain components, $\tilde{\epsilon}$ and ϵ_{xy} have been well studied in analytical derivations (19), numerical measurements (20), and experiments (21). Both quantities have an r^{-2} radial dependence. While ϵ_{xy} has quadrupolar angular dependence, $\tilde{\epsilon}$ is isotropic. We confirm that our results match previous studies.

The volumetric strain $k(r)$, however, is typically neglected but as we will show, plays an important role because softness is strongly dependent on local density. The left plot of Fig. 2 shows that the angular-averaged volumetric strain $k(r)$ is positive at most r and does not exhibit a power-law decay. The middle plot shows that the absolute value of $k(r)$ is dominated by the first term and shows an r^{-2} decay. The right plot shows that for $r > 5$, k has the dipolar angular dependence. Our results indicate that there are two contributions to the local volumetric strain, a term arising from the point shear strain dominates but angle-averages to zero due to its dipolar angular dependence so that the second term is revealed in the angular-averaged $k(r)$.

These induced strains cause future rearrangements (9). While many elasto-plastic models only takes into account ϵ_{xy} when determining next rearrangement, others also considered $\tilde{\epsilon}$. We studied this by computing the frame-dependent pair correlation function of rearrangers $g_2(\mathbf{r}, \delta f)$, namely the probability of finding a rearrangement at $\mathbf{r}$ δf frames later, given a rearrangement at the origin at frame $\delta f = 0$. We find a $g_2(r, \delta f)$ that is isotropic and decays as r^{-3}. This suggests that the next rearrangement is triggered by $\tilde{\epsilon}$.

3.2 Interplay of softness with rearrangements and strain

In training the machine-learning algorithm to obtain softness, we find that 90% of rearrangers have $S > 0$, while 84% of non-rearrangers have $S < 0$. Moreover, Fig. 3 shows that the softness distribution for rearrangers is very different from that of the whole population, and that the probability that a particle rearranges increases by four orders of magnitude as softness increases. These results verify that softness affects the propensity to rearrange very strongly.

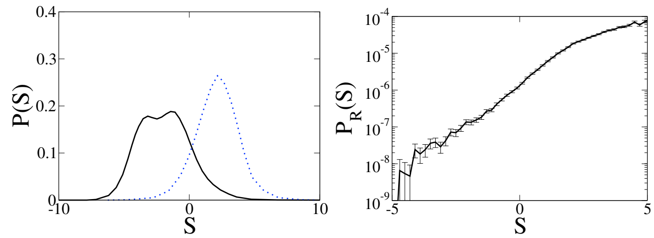

Figure 3: Performance of machine-learned softness. (left) The distribution of softness for all particles (black solid) and for rearrangers only (blue dotted). There is a pronounced difference between the two distributions. (right) The probability that a particle is rearranging, P_R, as a function of its softness. As the softness increases, P_R increases by four orders of magnitude, verifying the high correlation between softness and rearrangements.

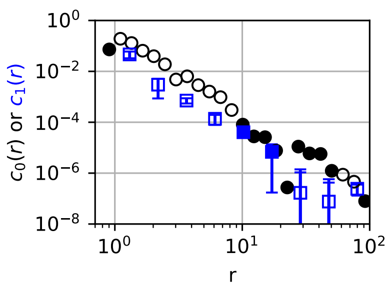

Figure 4: Parameters c_1 (squares) and c_0 (circles) defined in Eq. (1), at different distances r. Solid symbols represent positive values, while open ones represent negative values.

In turn, rearrangements can affect softness. The average difference in softness of a rearranger immediately before and after the rearrangement is $\langle \Delta S \rangle_R = -0.75$; the softness of a rearranger drops significantly when it rearranges. Rearrangements can also affect the softness of other particles. The mean softness change per frame, $\langle \Delta S \rangle$, at $\mathbf{r}$ when a particle at the origin rearranges, shown in Fig. 2, is very similar to the volumetric strain field for $r > 5$. We find that the mean softness change of a particle with softness S at $\mathbf{r}$ when a particle at the origin rearranges is:

$$\Delta S(\mathbf{r}, S) = c_0(r) + c_1(r)(S - \langle S \rangle) + bk(\mathbf{r}) \tag{1}$$

where $c_0(r)$ and $c_1(r)$ are given in Fig. 4 (b), and $b \approx 207$. We do not find any angular dependence in c_0 or c_1. We plot their r-dependence in Fig. 4. Clearly, c_0 and c_1 exhibit similar power law decays; we find $|c_0(r)| = 0.3r^{-3.1}$ and $|c_1(r)| = 0.06r^{-3.2}$. Their fast decay makes the third term $[bk(\mathbf{r})]$ dominate for $r \geq 5$.

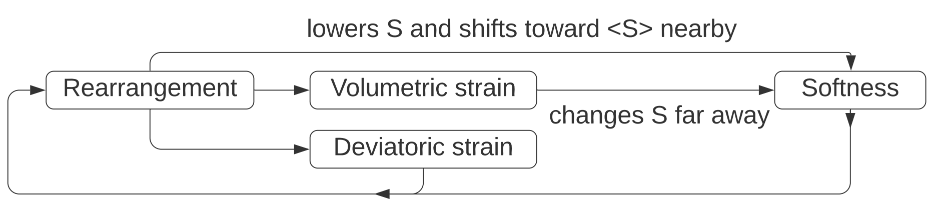

Figure 5: Summary of the interplay between rearrangements, strains, and softness we identified. A rearrangement decreases the softness of nearby particles, alters the softness of far-away particles through volumetric strain, and exerts a deviatoric shear strain on all particles. The local deviatoric strain and softness together determine future rearrangements.

4 Discussion

In this paper, we study avalanches that occur during energy drops when a jammed binary Hertzian disk packing is sheared quasistatically, using steepest descent to follow the minimization process. We find that (1) a rearrangement alters the softness of a nearby particle according to the difference between its softness and the mean softness. This behavior was first observed for 3D Lennard-Jones systems above the glass transition (1), indicating that it is quite general. (2) A rearrangement alters the softness of distant particles through volumetric strain. The fact that local dilation/compaction increase/decrease the softness is consistent with the previously observed dependence of softness on local density in 3D Lennard-Jones mixtures and with our physical understanding of softness (1), and is therefore also quite general. (3) A rearrangement exerts a deviatoric strain on the rest of the system. This should be generally true for isotropic systems in any dimension.

Our results point to a few factors that may contribute to the ductile behavior observed. Future rearrangements are triggered by the total deviatoric strain rather than the xy-shear strain. As a result, rearrangements trigger successive rearrangements that are isotropically distributed, not concentrated in the direction of maximum xy-strain. In addition, a rearranger lowers the softness of nearby particles, discouraging them from rearranging, while on average raising the softness of distant particles, facilitating their rearrangement. Third, rearrangements tend to push the softness of nearby particles towards the mean, which is quite high for the ductile system.

Due to the generic nature of our findings, the summary of our results in Fig. 5 should hold generally for avalanches in ductile disordered solids. Our results are summarized in Fig. 5, which constitutes a structuro-elasto-plastic model. This model goes beyond previous approaches by describing how the local structural environment of a particle affects and is affected by rearrangements and strain. It is the first coarse-grained model for describing plasticity that includes local structure and is based firmly on microscopic physics.

Broader Impact

This work establishes a theoretical framework for understanding plasticity in disordered solids. Our approach can be applied directly to systems that exhibit shear-banding and brittle failure to see whether the interplay is different in such systems. Earlier papers have shown that softness is readily identified in experimental systems for which the positions of particles can be tracked with time (3; 22; 23). Our analysis for disentangling the interplay of softness, rearrangements and strain can therefore be applied directly to experiments as well as simulations. It is likely that the key to understanding ductile vs. brittle behavior is encapsulated in this interplay. Brittle failure bedevils applications of disordered solids in multifunctional coatings, micro- and nano-devices, biomedicine and manufacturing. An understanding of the microscopic origins of brittle failure could potential lead to new strategies for avoiding it. There are no negative ethical or societal consequences of this work that are apparent to us.

Acknowledgments and Disclosure of Funding

We thank Hongyi Xiao, Robert J. S. Ivancic, Douglas J. Durian and Robert A. Riggleman for helpful discussions and their careful reading of the manuscript. This work was supported by the UPenn MRSEC NSF-DMR-1720530 (GZ), the Simons Foundation for the collaboration "Cracking the Glass Problem" award #454945 to AJL (GZ,SR,AJL), and Investigator award #327939 (AJL), the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE- FG02-05ER46199 (GZ), and NSERC via a PGS-D fellowship (SR).

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