Supplemental Material to "Predicting Defects in Soft Sphere Packings Near Jamming Using The Force Network Ensemble"

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Predicting Breakable Contacts

In this section we elaborate on the process of finding sets of breakable contacts and critically jammed systems. The states of self stress of the system are the left singular values of $\mathcal{R}$. In practice we find them by computing the eigenvectors with zero eigenvalues of the square matrix $\mathcal{R} \cdot \mathcal{R}^T$. We remove unstable particles (rattlers) from $\mathcal{R}$ before doing this calculation, as they contribute only empty rows to $\mathcal{R}$ and will thus contribute additional trivial zero modes. We construct a force space plot of the loads (see Fig. 1) in which each plotted point corresponds to a contact within the system and the point's coordinates are the loads applied to that contact in each normalized state of self stress. We compute the convex hull of all of these points in force space, including the origin. Most facets of this convex hull do not intersect the origin, but some will contain the origin as well as $N_{SSS}-1$ contacts. These facets intersect sets of contacts which can be brought to zero force while the system still retains a purely compressive force network. Thus, each facet represents a stably jammed system with the force on that facet's contacts brought to zero (i.e. broken). The loads for the system in which these contacts are broken are given by the distance from each contact to the hyperplane intersecting the $N_{SSS}-1$ breakable contacts and the origin.

For a system with exactly two states of self stress, this is geometrically constrained to return exactly two facets, which will typically each contain just one breakable contact. We note that while it is theoretically possible that the convex hull could not return any facets containing the origin this would only happen when the system requires both compressive and tensile forces to be stable. In practice, we find that there are always facets containing the origin and thus there are some contacts which are unnecessary for the mechanical stability of the system. We therefore declare that these contacts are "breakable."

Angular Consistency

In this section we elaborate on our process for comparing systems as they decompress. In each step of decompression, we find two arbitrary basis vectors (i.e. states of self stress) that span the space of possible (with both tension and compression) force networks for the spring system representation of the contact network. We call those two arbitrary basis vectors F_1' and F_2'. When we compute them, they are randomly oriented as any two orthogonal vectors spanning the same space are equally valid. We thus are free to define new basis vectors, F_1 and F_2 as $F_1 = F_1' cos(\zeta) + F_2' sin(\zeta)$ and $F_2 = -F_1' sin(\zeta) + F_2' cos(\zeta)$. We choose ζ to maximize the sum of the individual elements in F_2. While maximizing the elements in F_2 is a completely arbitrary choice, doing so allows us to obtain basis vectors that remain comparable even as the space which they span evolves slightly under decompression. We considered iteratively projecting the basis vectors onto the force space of the system at each subsequent pressure iteration, but we find that maximizing elements in F_2 effectively achieves the same result while additionally allowing for the analysis at each pressure to be completely independent.

Number of Critically Jammed Systems and Number of Breakable Contacts

We include here the data for the scaling of N_{cj} as well as the scaling of the number of breakable contacts, N_{bc}. In Fig. S1, we show how N_{bc} and N_{cj} scale as a function of the dimensionality of the normalized SSS, d_{SSS}. At 2SSS, the force network ensemble can be understood as a line which encompasses the set of allowed mixing angles. In this case, $N_{cj} = 2$ as there are exactly two endpoints to a line. This typically also results in two breakable contacts, one at each endpoint, but may instead result in $N_{bc} \geq 5$ by creating a rattler at one endpoint (i.e. four or more contacts are broken to form one of the critically jammed systems). We rarely find $N_{bc} = 3, 4$ which can only arise from degeneracies or numerical instabilities in the 1SSS force network. At 3SSS, the boundaries of the allowed force space are the edges of a polygon, and at higher SSS the facets of a polytope. The vertices of these polytopes represent

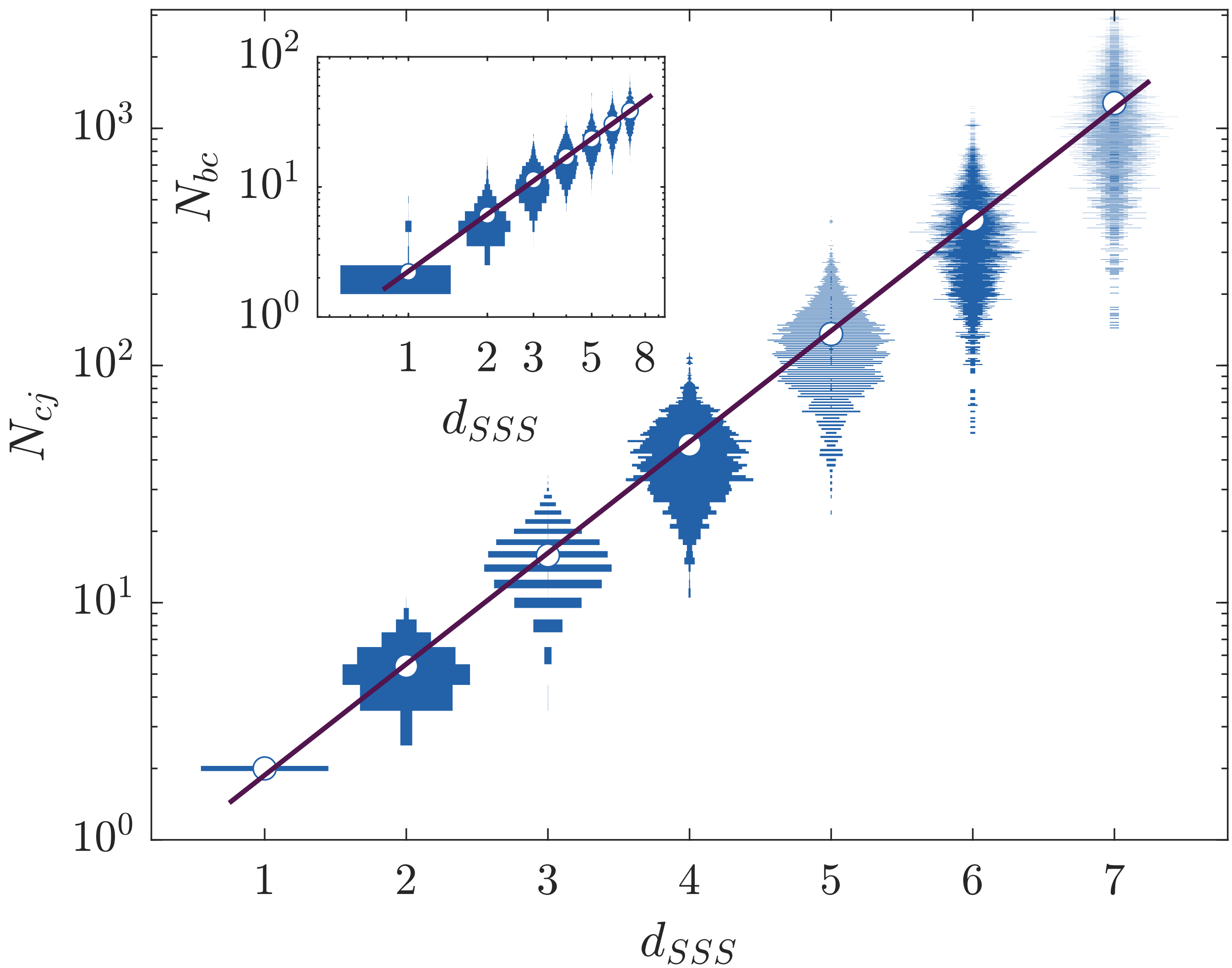

Figure S1. Violin plot of the number of critically jammed systems, N_{cj}, versus dimension of the normalized space of SSS, d_{SSS}, for $N = 128$. Purple line shows the empirical fit of the means (white circles), $\bar{N}_{cj} \approx 0.64 \cdot 2.94^{d_{SSS}}$. We note that in odd d_{SSS}, only even numbers of N_{cj} are allowed, which is geometric in nature and holds also for convex hulls of random points. Inset, the number of breakable contacts, $\bar{N}_{bc}$ with d_{SSS}. Purple line shows the empirical fit of the means (white circles), $N_{bc} \approx 2.25(d_{SSS})^{1.46}$.

the predicted critically jammed systems, and the $d_{SSS}-1$ dimensional facets represent the sets of breakable contacts. These polytopes must have at least d_{SSS} facets, but may have arbitrarily many facets and thus arbitrarily many breakable contacts. We find the means of N_{cj} and N_{bc} to have the following scalings:

$$\bar{N}_{bc} \approx 2.25(d_{SSS})^{1.46} \tag{S1}$$

$$\bar{N}_{cj} \approx 0.64 \cdot 2.94^{d_{SSS}} \tag{S2}$$

Correlations Between Breakable Contacts

As shown in Figures S2 and S3, we examine the real space correlations between pairs of breakable contacts in systems at 2SSS and find no correlation in position or angle subtended between contact vectors. In Figure S4, we examine the distribution of contact numbers in systems at 2SSS and find that breakable contacts are more likely to occur between particles with higher than average contact number ($z \sim 6.4$). Such particles are thus more likely to have a contact that is unnecessary for system stability. This stands in contrast to the soft spot literature, in which particles with fewer contacts are identified as more likely to rearrange [S1–S4]. This difference arises because soft spots exclusively identify instabilities, but the FNE also predicts the more numerous stable contact changes involving more highly coordinated particles.

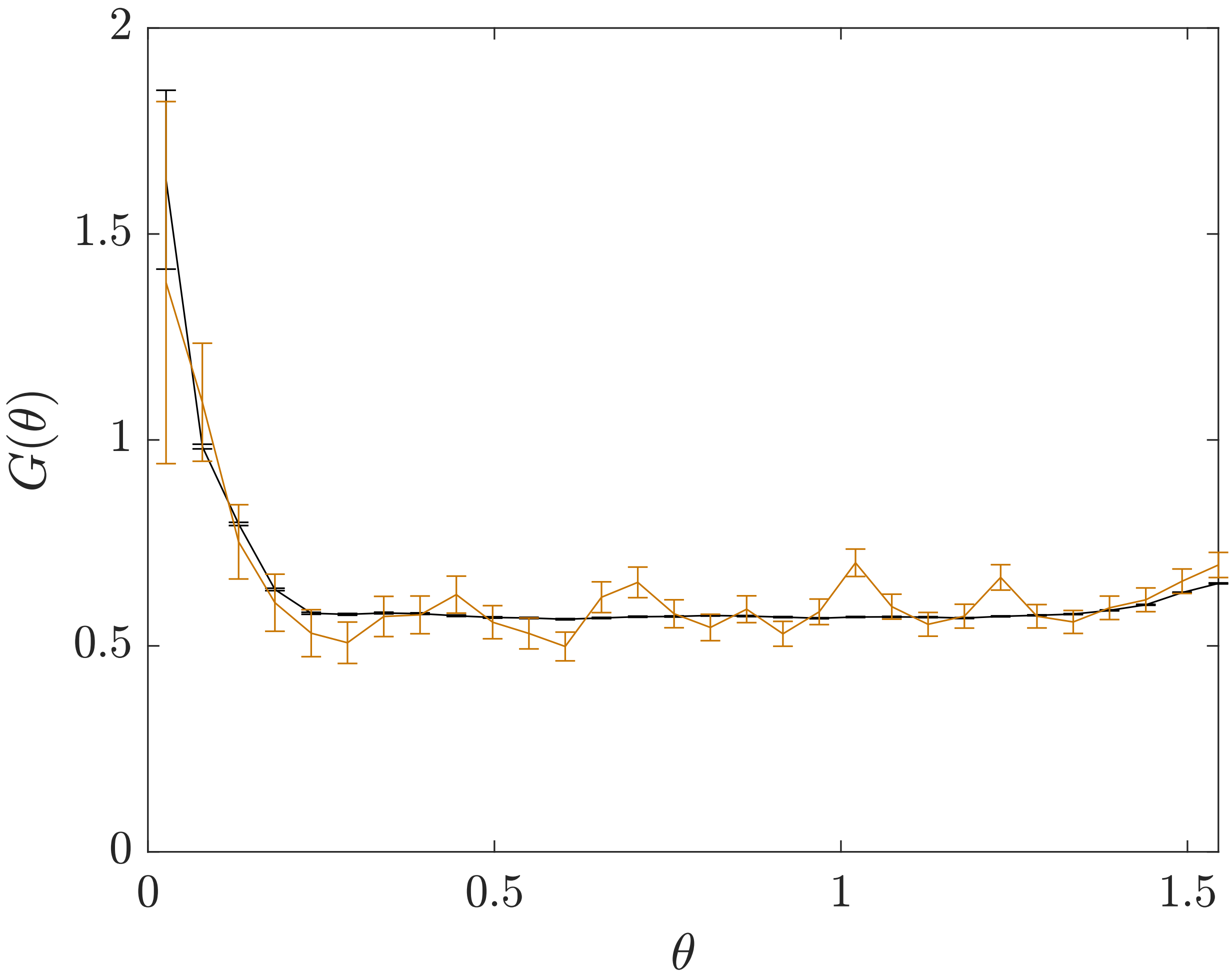

Figure S2. Correlation function $G(\theta)$ of angles θ between pairs of breakable contacts in all systems, orange, and between all pairs of contacts in a system, black. Pairs of breakable contacts are similar in correlation to a randomly selected pair.

[S1] M. L. Manning and A. J. Liu, Vibrational Modes Identify Soft Spots in a Sheared Disordered Packing, Physical Review Letters **107**, 108302 (2011).

[S2] S. A. Ridout, J. W. Rocks, and A. J. Liu, Correlation of plastic events with local structure in jammed packings across spatial dimensions, arXiv:2011.13049 [cond-mat] (2020), arXiv: 2011.13049.

[S3] J. W. Rocks, S. A. Ridout, and A. J. Liu, Learning-based approach to plasticity in athermal sheared amorphous packings: Improving softness, APL Materials **9**, 021107 (2021).

[S4] D. Richard, M. Ozawa, S. Patinet, E. Stanifer, B. Shang, S. A. Ridout, B. Xu, G. Zhang, P. K. Morse, J.-L. Barrat, L. Berthier, M. L. Falk, P. Guan, A. J. Liu, K. Martens, S. Sastry, D. Vandembroucq, E. Lerner, and M. L. Manning, Predicting plasticity in disordered solids from structural indicators, Physical Review Materials **4**, 113609 (2020).

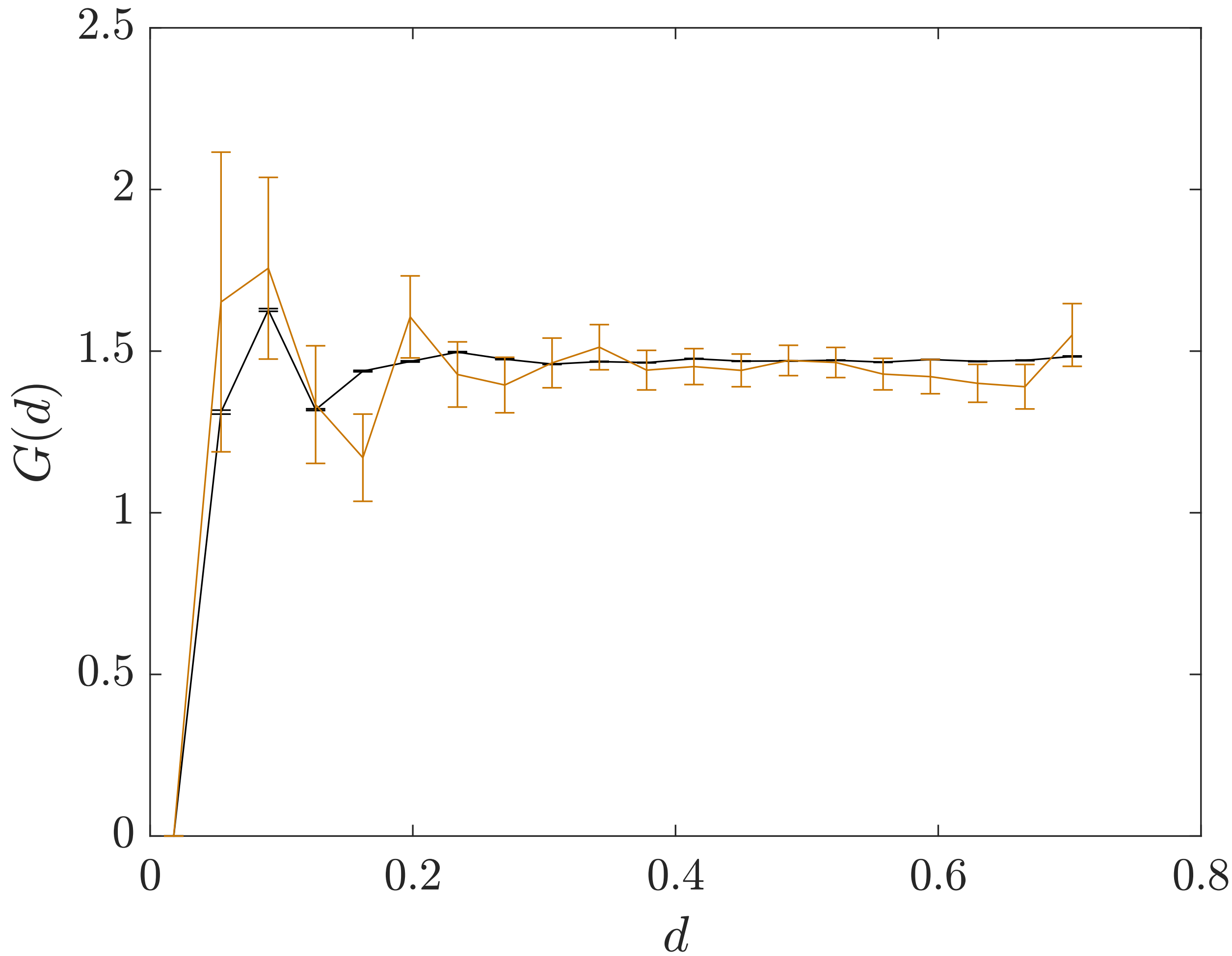

Figure S3. Pair correlation function $G(d)$ between pairs of breakable contacts at a distance d, orange, and between all pairs of contacts, black. Pairs of breakable contacts are not correlated in position.

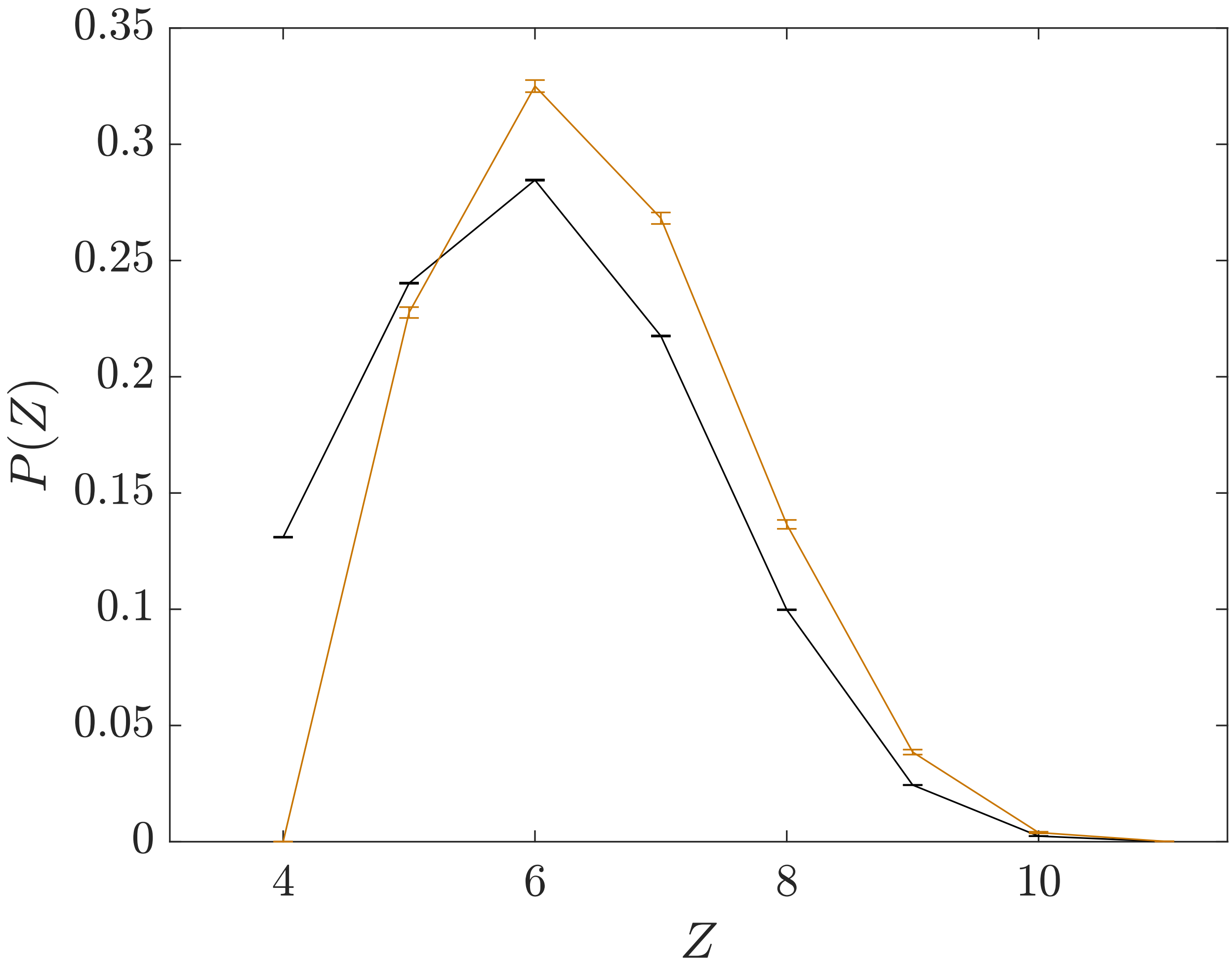

Figure S4. Probability distribution of contact number Z for all particles, black, and for particles that have a breakable contact, orange. No particles with a breakable contact have 4 (i.e. the minimum $d+1$) contacts, and the distribution is skewed towards higher number of contacts, with an average value of ~ 6.45 rather than 6 (i.e. $2d$).