Examining evolving structural networks using minimal cycle similarity networks: applications to stick-slip granular dynamics

David M. Walker†, Antoinette Tordesillas‡ and Gary Froyland‡

†Department of Mathematics & Statistics, University of Melbourne, Parkville, VIC 3010, Australia
‡School of Mathematics and Statistics, University of New South Wales, Sydney NSW 2052 Australia
Email: dmwalker@unimelb.edu.au, atordes@ms.unimelb.edu.au, g.froyland@unsw.edu.au

Abstract—A complex network consisting of nodes and links evolves through time by destroying old links and creating new links. Existing nodes can also be destroyed and new nodes can be created. We introduce a framework based on the evolution of the minimal cycle topology whereby the changes in the network can be characterized through properties of a new similarity network. We demonstrate the methodology by focussing on the local mesoscopic cycle evolution within structural contact networks of quasistatically deforming dense granular materials. At each stage of a prescribed loading program (e.g. biaxial compression subject to constant confining pressure boundary conditions) the assembly of granular particles is represented by a contact network. This complex network is rich in cycle topologies and for each particle we compare the changes to its local mesoscopic cycle topology across a specified strain (or temporal) interval. A similarity network constructed using close topological distance of cycle changes between particles summarizes the structural evolution. Properties of the similarity network including centrality measures and motif structures help to reveal deformation associated with stick-slip behaviour.

1. Introduction

Complex networks are used to characterize and model the behaviour of a variety of systems in the social, biological and physical sciences [1]. Systems typically vary through time and so a complex network representation consisting of network nodes and network links reflect these changes by creating new nodes and new links as well as removing old nodes and associated links. In addition connections between existing nodes can be created or destroyed through rewiring of the network to reflect changing relationships between agents represented by nodes. It is therefore of interest to develop methods which can capture these changes so that models describing such processes can be better informed or formulated. The subject of this paper is to introduce such a framework and we do so with respect to a specific application from granular physics.

Granular materials span a broad spectrum of substances including minerals, soils, powders and grains [2]. When these materials are subjected to different stresses they exhibit properties and complex behaviour in common with other forms of matter (e.g. self-organized pattern formation, scale invariance and co-existing multiphase behaviour). It is important to develop methods in order to characterize and model such behaviour. Many experiments and simulations have been devised to probe the rheological response of granular materials to different stresses including compression and shearing tests [3, 4, 5, 6]. These tests can generate vast quantities of data across different spatial and temporal scales which must be processed in an advantageous manner. The techniques of complex network theory have recently been shown to be of use in analyzing such data and a purpose of this paper is to introduce a novel way of using similarity networks to study the functional role granular particles play in the structural and rheological evolution of dense granular materials through deformation.

The properties of, and structures within, complex networks have been used in the past to study granular rheology. The majority of work has concentrated on characterizing the topology of structural contact and contact force networks at different stages of loading and force thresholds (e.g. [7, 8, 9]). More recently, efforts have been made to construct more functional networks of granular properties using kinematical measurements over short strain intervals [10] and even longer temporal behaviour of particle structures [11]. Here, we propose a method whereby the rheology of a dense granular material can be studied which examines the evolution of the local topology of structural contact networks. The role each particle plays within such evolution is summarized in a similarity network. Properties and motif structures within these networks reveal important temporal and spatial zones throughout loading and within the material where deformation is paramount (e.g. shear bands and periods of stick, or jamming behaviour is identified). More broadly, the method allows the dynamical evolution of complex networks to be studied by tracking how a node’s local motif or n-cycle topology evolves.

The remainder of this paper is organized as follows: in Sec. 2 we give information of the specific granular system we use to develop our methods. The system is a discrete element method (DEM) simulation of biaxial compression and we outline key kinematical features of the rheological response of the material throughout its deformation history. In Sec. 3 we briefly introduce the concept of the contact network and discuss the n-cycle topology of such
networks. Sec. 4 introduces our framework for summarizing the evolution of the contact networks n-cycle population using similarity metrics and similarity networks constructed based on topological distance. The results of the application of the methods to the DEM test system is shown in Sec. 5 by relating similarity network properties, in particular closeness centrality and connected 4-node motifs, to the rheology of the physical material. A summary is presented in Sec. 6 to close the paper.

2. DEM Test System

An excellent arena to test and advance the development and extend the reach of complex network application is the physics and engineering of granular media. Granular materials are a paradigm for complexity exhibiting self-organized pattern formation, emergence and co-existing multiphase behaviour. Furthermore, because the physics of granular materials is tangible it is often the case that any abstract measure, or construction, of a complex network can be translated back meaningfully to the physical domain thus facilitating a deeper understanding of a concept in the two fields. A useful sandpit then for development of new network methods is to consider well-studied granular systems where important events and responses (e.g. formation of persistent shear bands, stick-slip or jamming-unjamming periods of particle rearrangements) are known so that such feedback to interpretation is possible.

We are primarily interested in the rheological response of assemblies of dense granular materials to different loading programs. To this end we consider a sample of 5098 poly-disperse particles in a DEM simulation of biaxial compression subject to constant confining pressure from the lateral boundaries [12]. Contact laws describing the interaction of two particles are modelled by a combination of springs, dashpots and sliders [6]. In this simulation a coefficient of rolling friction is introduced to better model the effects of particle shape, thus making the simulation a more realistic analogue to real sand [13]. This particular sample exhibits multiphase behaviour observed by a change from a solid-like to a liquid-like response regime through the formation of a persistent shear band. This transition-like behaviour is seen in the marked drop in the standard soil mechanics measure of shear stress ratio which reaches a peak then drops at around 4% axial strain (see, Figure 1 upper).

The prevailing kinematics at the scales of interacting particles, particle clusters and the macroscopic bulk are as follows: throughout the entire loading history quasi-linear force chains of particles bearing the majority of the load are present [12]. Force chains are laterally supported by a weaker network of neighbouring particles with local topologies taking the form of different length cyclic structures. From the onset of loading we see an almost linear increase in macroscopic shear stress ratio as force chains have enough support to bear more and more load. During this period we also see a reduction in another standard soil mechanic measure, the volumetric strain (see, Figure 1 lower). This reflects the initial contraction of the material due to the compression further highlighting the strong support the member particles of the force chain network are receiving. As the increase in shear stress ratio begins to slow down, associated with the local minimum of the volumetric strain being realized and this quantity increasing, reflecting the dilatation of the material as the confining pressure is overcome, we observe within the material particle rearrangements continually occurring including so-called local microbanding. Eventually, the lateral support afforded to force chains lessens to such an extent that the force chain can no longer support the increased load. At this point failure is triggered through the mechanism of force chain buckling and load gets redistributed onto existing force chains and newly formed force chains. The region of the material where this occurs is strain localized in what becomes the persistent shear band. As the load increases towards peak shear stress the rate of force chain failure reaches the point where we see collective buckling of force chains in a fully formed shear band [12]. The material can no longer support a significant load and the prevailing dynamics is one of birth and death of force chains in the high strain region manifest as oscillations in the shear stress ratio reflecting the localized stick-slip or jamming-unjamming kinematics and a levelling off of the volumetric strain. Throughout the entire loading so-called rattlers are present. These are particles that for a given observed strain state have zero or one contact and no surrounding lateral support (i.e. they sit in cages of particles). The proportion of rattlers, or non-rattlers, within samples have been recognized to be of importance in the formulation of a phase diagram for granular materials [14] and statistical mechanic formalisms of granular matter [15].

We are interested in developing a method to track the contact topology evolution of each particle across strain intervals throughout loading as such changes in network structure reveal the formation of new links, destruction of old links and as rattlers change status to non-rattlers the growth and shrinkage of general complex networks is captured.

3. Contact Network and Minimal Cycle Motifs

The compression test described above has previously been analyzed and characterized using complex network measures applied to the evolving structural contact network [7, 8]. The contact network of an assembly of particles is a representation of the physical arrangement of particles where each particle is a node and a link connects two nodes if the corresponding particles are in physical contact with each other. The aforementioned rattlers are recognized within these network representations as having zero degree, or degree equal to one. As such for a given observed strain state of the loading they bear insignificant load and they are also not a part of n-cycle topologies. The
response of the material to loading manifests as changing network properties of the evolving contact networks (e.g. degree, clustering coefficient, centrality measures etc.). In this DEM system the rise to peak shear stress corresponds to a drop in average contact network degree and a drop in average clustering coefficient \[7\]. So, despite the material seemingly being capable of carrying increased load the local structural topology within is one of loss of contacts (i.e. lower degree) and also loss of tight triangle topologies (i.e. lower clustering coefficient).

The change in the population of network motifs is also revealing of the grain rearrangement and deformation apparent in the material. In particular the membership of minimal cycle motifs of the contact networks, i.e., 3-cycles, 4-cycles and longer length cycles can reveal the onset of dilatation. Figure 2 shows the population of different length \(n\)-cycles throughout loading. We note that 3-cycles are dominant throughout but the amount of these structures present reduces through to failure at approximately 4% axial strain. Three-cycle topologies die due to cleaving into larger length cycles because of dilatative particle rearrangements, and we see a corresponding rise in higher-order cycles, in particular 5- and 6-cycles. As we can see rattlers are present throughout loading comprising 2% to 5% of the particle population at any stage of the deformation.

In addition, the interplay of mesoscopic scale low-order cycles with the load-bearing force chain structures within the material is of relevance to force chain stability and failure of force chains through buckling \[16\]. We are interested in characterization of the mesoscale evolution of the cycle topology of a particle across a strain interval, or more generally, how the local cycle motifs of a network node changes as a network grows or shrinks.

For example, consider the small network structures in Figure 3 which can be regarded as the network topology at the beginning and end of a strain interval, or snapshots of a network at the beginning and end of an observation window \([t, t + \delta t]\). The local cycle topology of the central particle \(A\) at time \(t\) consists of four 3-cycles and one 4-cycle. At the end of the interval, time \(t + \delta t\), particle rearrangements perhaps due to an increase of strain results in a local cycle topology consisting of one 3-cycle, and two 4-cycles. Particle \(B\), in contrast has changed from being part of one 4-cycle to become a rattler and a part of no cycle topologies. Clearly a suitable network and resulting network property capable of measuring such deviation is of great interest. Likewise, a measure capable of capturing the reverse rearrangement where particles that are rattlers become a part of the global cycle topology is of use. A purpose of this paper is to search for such a property within similarity networks to enable the study of the whole system.

4. Similarity Network Construction

The principle of designing a second network to describe the functionality of an existing network is not new but is still a rarity. For example, role-similarity networks have been proposed to summarize the importance of roles nodes in a directed network play with respect to shortest in and out path lengths \[17\]. Here, we take a different approach inspired by these methods whereby a node’s role with respect to functional changes in the network cycles structural topology is of interest. In particular, we modify the role-similarity technique for directed networks to examine the mesoscopic scale deformation of cycles in an evolving contact network. The basic idea is to construct a set of coordinates which represents a node’s role within a network.
Figure 3: The evolution of the local mesoscopic cycle topology of a particle/nodes rearrangement across a strain interval \([t, t + \delta t]\). Particle \(A\) loses 3-cycle membership but increases its 4-cycle membership. In contrast the particle denoted \(B\) loses all cycle participation and becomes a rattler.

As mentioned, in a directed networks this can be based on the number of shortest in (out) paths of a given length terminating (originating) at a node. A row vector for each node is constructed by augmenting this “in” and “out” information. The pairwise distance between all of these row vectors can be calculated to produce a matrix which can be considered as a network weight matrix. Subject to appropriate thresholding this weight matrix is converted to an adjacency matrix to form an undirected complex network. Node and larger scale properties of this similarity network reveals relationships between nodes hitherto unclear based on their role with respect to shortest path lengths in the original network.

In our case we have different structural contact networks for increasing strain. Each of these networks can be described by its minimal cycle basis which changes character through loading (see, the cycle populations in Figure 2). By considering the cycle structure of a contact network across a strain interval we can create a coordinate vector for each node which represents its local mesoscopic cycle evolution. That is, we consider a particle’s cycle membership at two equilibrium strain states – the start and end of a given strain interval – to construct a similarity matrix \(C\) where each row corresponds to a particle and the first \(n\) columns list the number of individual 3, 4, 5, …, \(n\)-cycles the particle is a participant of at strain state \(t\). The remaining \(n\) columns list the number of 3, 4, 5, …, \(n\)-cycles the particle is a part of in the contact network at strain state \(t + \delta t\). For a particle \(A\), a row of \(C\) takes the form

\[ C^A = [c^A_t, c^A_{t+\delta t}] \]  

where \(c^A_t\) represents a census of the cycles in the contact topology of particle \(A\) at strain \(t\). We recall that it is possible for a particle to not be a part of any cycle at a given strain state (i.e. a rattler) and also after at the end of strain interval may remain a rattler. In this case \(C^A\) would be a zero-vector. The distance function we use to compare cycle evolution is cosine distance and a zero vector clearly causes problems. Thus we append \(c^A_t\) with an extra entry which is equal to one if the particle is a rattler and is zero otherwise.

To be more specific, consider the central particle in Figure 3. At time \(t\) we see that particle \(A\) is a part of four 3-cycles and one 4-cycles. Similarly, particle \(B\) is a part of one 4-cycles, and so, for cycles up to length 6, we have

\[ c^A_t = [r c 3 \ c 4 \ c 5 \ c 6] = [0 \ 4 \ 1 \ 0 \ 0], \]  

\[ c^B_t = [r c 3 \ c 4 \ c 5 \ c 6] = [0 \ 0 \ 1 \ 0 \ 0]. \]  

At time \(t + \delta t\) we see that particle \(A\) now participates in one 3-cycle but has increased its 4-cycle membership to two. Particle \(B\), in contrast, has lost all participation in \(n\)-cycles and has become a rattler. So, at time \(t + \delta t\) we now have

\[ c^A_{t+\delta t} = [r c 3 \ c 4 \ c 5 \ c 6] = [0 \ 1 \ 2 \ 0 \ 0], \]  

\[ c^B_{t+\delta t} = [r c 3 \ c 4 \ c 5 \ c 6] = [1 \ 0 \ 0 \ 0 \ 0]. \]  

Thus

\[ C^A = [0 \ 4 \ 1 \ 0 \ 0 | 0 \ 1 \ 2 \ 0 \ 0], \]  

\[ C^B = [0 \ 0 \ 1 \ 0 \ 0 | 1 \ 0 \ 0 \ 0 \ 0]. \]

A (weighted) similarity network \(W\) is constructed by calculating the pairwise distance between each \(C^A\). Cosine similarity is used for distance and is defined as

\[ d_C(x, y) = 1 - \frac{x \cdot y}{||x|| ||y||}. \]

\(k\)-network construction A distance threshold can be applied to convert \(W\) to the form of an adjacency matrix of a complex network. The distance threshold can be classed as one of two types: metric distance and topological distance. The concept of metric distance is easy to describe as each node is connected to every other node within a prescribed distance. This distance is typically chosen to be the same for all nodes. Topological distance on the other hand connects each node to a fixed number \(k\) of close neighbours. Since it is possible that a node, say \(A\), can be a \(k\)-closest neighbour of a node \(B\), but node \(B\) is not a \(k\)-closest neighbour of node \(A\), nodes can end up being connected to more than \(k\) neighbouring nodes. This aspect is crucial to the eventual usefulness of characterization through different network properties.

Connecting nodes using topological distance has found useful application in the construction of complex networks from time series data. In this application a reconstructed phase space is built using the method of time-delay embedding and each embedded state space point represents a network node. Links in this network, coined a Phase Space Network (PSN), are specified by connecting each
node to their $k$-closest neighbours in phase space. Properties of these PSN’s, in particular the ranking of prevalence of certain motif structures have been shown to exhibit a superfamilial structure related to the character of the underlying dynamics generating the observed time series [18]. We have also had success in the past when analyzing the rheology of sand specimens using functional kinematical networks by connecting nodes representing particles through topological distance [10, 11]. In these works we selected the value of $k$ to be the minimum integer such that the resulting network forms one connected component. This results in each node being connected to every other node in the network by a finite shortest path length. We follow this method of network connection here as a way of thresholding the weighted similarity matrix $W$ to produce a $k$-similarity complex network. The properties of this network, including closeness centrality can be calculated to characterize the functional role of particles in the evolving structural contact networks representing the granular assembly throughout its deformation. Furthermore, since physical particle information is available these network properties can be mapped back to the physical domain so that the spatial effect of these temporal changes can be examined.

5. Network Metrics and Structures

We have introduced a framework to study the evolution of the minimal cycle topology of changing complex networks. The method can account for the creation and destruction of network nodes by considering them as rattlers at the appropriate ends of the observation window. Our interest is primarily concerned with the application of the method to the study of contact networks of deforming granular materials. In this case the observation window to track the changes in the cycle topology is a suitable strain interval. From earlier studies from a different perspective – modelling deformation using Markov transition matrices [19] – we have found that a strain interval $\delta t = 4$ observation time steps is reasonable and in the analysis to follow we fix the observation window to be this long. In [20] we proposed a prescription for determining suitable lengths of strain interval and an interval of 4–6 steps for the major deformation slip event – the big drop in shear stress from peak (Figure 1) – is consistent with our choice here. Throughout loading, we examine all strain intervals of length 4 and construct $k$-similarity networks using cycles up to a maximum cycle length of 10. This results in 295 different similarity networks whose network topology can be examined using appropriate complex network statistics. As alluded to above we are able to map local node quantities back to the particles in the physical domain to determine their usefulness for analyzing the effect of particle rearrangements in response to loading at the local mesoscopic scale as well as the macroscopic scale.

The character of a complex network is typically described by local properties of degree, clustering coefficient and more global properties such as shortest path lengths. In [10] we found that when mapped back to the physical domain the local properties of degree and clustering coefficient within kinematical networks connected using topological distance were less effective than properties based on shortest path lengths. Although, degree and clustering coefficient are more informative in the present situation it appears that shortest path length measures, in particular closeness centrality, remains as effective. As such we present the closeness centrality properties of the $k$-similarity networks. The closeness centrality of a node in a network is a local summary of global information and we contrast this by also considering a global summary of local information through the rank-ordering of specific local network motifs.

**Figure 4:** The value of closeness centrality in the $k$-similarity networks for each node/particle throughout each deformation strain interval. For qualitative comparison and reference to important events scaled versions of the shear stress ratio (solid) and volumetric strain (dashed) are shown in black. Higher values of closeness centrality appear to be related to drops in shear stress ratio and corresponding rises in volumetric strain due to dilatative rearrangements.

**Closeness centrality** The property of closeness centrality ($cc$) is a node property which quantifies the location of the node within the network with respect to shortest path lengths. Explicitly, $cc$ is calculated for a node $A$ in a network $N$ by

$$cc(A) = \frac{1}{\sum_{(A,B) \in N} d_{AB}},$$

where $d_{AB}$ is the shortest path length between nodes $A$ and $B$ and the sum is over all node pairs $(A, B)$ in the network $N$. We note that by construction the $k$-similarity networks form a single component graph and so $d_{AB}$ is finite for all node pairs. In Figure 4 we show the calculated value of closeness centrality for each $k$-similarity network of the loading history. The changing structure of each network as axial strain increases is evident from the banding of colours
in this figure. For strain intervals at peak shear stress – scaled versions of shear stress ratio and volumetric strain are overlaid for reference – where the major failure structure of the persistent shear band is forming we typically see a k-similarity network with higher node closeness centrality values. This appears typical of failure events as can be seen from 4% axial strain onwards where the higher (yellow) valued bands are associated with slip events. This is also marked by the increase in volumetric strain indicative of the overwhelming dilatative rearrangements responsible for the slip events. Stick periods after failure where shear stress ratio increases are typically associated with lower values of closeness centrality in k-similarity networks.

In addition to observations of the temporal evolution of network quantities we can map each network property back to the physical domain and examine the spatial distribution of node properties. In Figure 5 we show the spatial distribution of closeness centrality values in the physical domain of the sample for 12 strain intervals starting at peak stress through to the end of the successive big slip events at 4% axial strain. The assemblies are plotted according to the particle positions at the beginning of each strain interval. Recall, each strain interval spans 4 observation strain steps and therefore intervals span slip (unjamming) events, stick (jamming) events and a mixture of both. The drop from peak stress is indicative of failure of the material and in this sample is associated to failure by strain localization (i.e. shear banding). In this sample the persistent shear band extends diagonally from the bottom left of the sample to the top right of the sample. In all strain intervals shown the shear band is apparent. The first and second strain intervals encompasses the first big slip event but also the beginning of the small period of stick behaviour (recall, Figure 1).

We see that the k-similarity networks have higher closeness centrality values compared to the strain intervals spanning the stick period. The major slip events during intervals of strain 3.77% – 4.00% are associated to k-similarity networks exhibiting relatively high closeness centrality and the highest values are present within the shear band. We see that the similarity networks then capture the relative quiescent period of stick starting at 3.92% strain before the final interval shown once again extends towards the onset of another period of slip or unjamming.

Motifs  Our methodology has been concerned with the evolution of the rheological relevant n-cycle motifs within a contact network. The n-cycles are also of significance in other complex networks. Indeed the population and density of 3-cycles, or triad motifs, are of such a status that the complex network measure of clustering coefficient is introduced to solely quantify their presence in a network. More generally, motifs are sub-networks, usually consisting of a small number of connected nodes, whose prevalence in a network is higher than would be expected within an equivalent random network [21]. A special set of motifs consisting of the six possible configurations of 4-node sub-networks have been shown to make up a superfamily characterization of nonlinear dynamical behaviour within so-called Phase Space Networks [18]. The rank-ordering of the prevalence of these motifs within such a network helps to classify whether the underlying dynamical system is operating in a chaotic, hyper-chaotic, or periodic regime. The structure of these 4-node motifs, denoted by the nomenclature A, B, C, D, E, and F are shown in the inset of Figure 6. We have calculated the prevalence of each of these structures within the similarity networks for all strain intervals considered. We have recorded the rank ordering of these motifs and found 8 distinct rankings. Figure 6 redraws the evolution of shear stress ratio coloured by 4-node motif rank order. The most prevalent ordering through loading is DCABFE (orange) and from 4% axial strain onwards, i.e., in the so-called critical state regime in the presence of a persistent shear band, it appears this motif persists through stick, or jamming periods (i.e. rises in the shear stress ratio). Towards the peaks of these shear stress rises, or the onset of slip or unjamming events, we see that the motif ranking typically changes to either ABDCFE or ADBCFE (blue/cyan coloured). Similarly, although less convincing at the end of a slip period and the beginning of another rise in shear stress the motif ranking within the similarity networks cascades through DABCFE and DACBF before reverting to the dominant ranking of DCABFE. Of note, is the rank ordering of motifs at peak shear stress and the onset of the large slip events which signal failure of the material and the ultimate formation of the persistent shear band. The dominant motif orderings in this strain period is consistent with the orderings observed during the small slip events seen later in the loading history. It appears that in addition to the macroscopic network quantities such as closeness centrality, the local structure of the similarity networks are capable of revealing the stick-slip behaviour of the material.

6. Summary

We have introduced and developed a novel application of similarity metrics to study the changes in complex networks as they grow or shrink in size and re-organize their contact topology. We developed the methods with reference to a specific application, namely, the study of the rheology of dense granular materials during deformation. By constructing a similarity network based on topological distance we showed that important stick-slip (jamming-unjamming) mechanisms are reflected in the properties of the networks. The temporal evolution and spatial distribution of the value of closeness centrality in these networks revealed the local evolution of mesoscopic cycle topologies in the structural contact networks due to particle rearrangements. In particular the shear band failure zone could be distinguished. Furthermore, the rank-ordering of connected 4-node motifs revealed the presence of 8 superfamilies with the dominant set (DCABFE) being closely asso-
Figure 5: Twelve successive strain intervals from peak shear stress (left to right and down from top left) showing the values of node closeness centrality within the \( k \)-similarity networks mapped back to the physical domain. Particles are coloured by relative values of closeness centrality with respect to these twelve intervals to aid the visualization and obtain a better contrast of colours. Blue is low with values increasing through green, yellow to high valued red colours.

Associated with stick and jamming behaviour. Our method of describing the functional evolution of the \( n \)-cycle motifs in a network through a similarity metric is useful for investigating the rheology of dense granular materials and should also be of interest more generally to researchers analyzing other systems with evolving complex networks.

Figure 6: The rank ordering of 4-node sub-network motifs within the similarity networks throughout loading. Inset: the structure and nomenclature of the 4-node sub-networks.

Acknowledgments

This work was supported by US Army Research Office (W911NF-11-1-0175), the Australian Research Council Discovery Projects 2012 (DP120104759) and the Melbourne Energy Institute.

References


