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Quantifying force networks in particulate systems

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HIGHLIGHTS

- We present mathematical models for analyzing force distributions in particulate systems.
- Persistent homology is used to compare the force networks in different granular systems.
- We consider the stability of the persistence diagrams with respect to experimental error.

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ABSTRACT

We present mathematical models based on persistent homology for analyzing force distributions in particulate systems. We define three distinct chain complexes of these distributions: *digital*, *position*, and *interaction*, motivated by different types of data that may be available from experiments and simulations, e.g. digital images, location of the particles, and the forces between the particles, respectively. We describe how algebraic topology, in particular, homology allows one to obtain algebraic representations of the geometry captured by these complexes. For each complex we define an associated force network from which persistent homology is computed. Using numerical data obtained from discrete element simulations of a system of particles undergoing slow compression, we demonstrate how persistent homology can be used to compare the force distributions in different systems, and discuss the differences between the properties of digital, position, and interaction force networks. To conclude, we formulate well-defined measures quantifying differences between force networks corresponding to the different states of a system, and therefore allow to analyze in precise terms dynamical properties of force networks.

1. Introduction

Particulate systems consisting of a large number of particles have attracted significant attention in the last decades. Despite significant research on these systems, their properties are still not well understood and some of them appear to be rather elusive. The fact that the forces do not propagate uniformly in systems made of interacting particles has been established in a number of different systems, including granular matter, colloids, gels, emulsions and foams, see, e.g., [1–4]. It is well accepted that the interparticle forces play a key role in determining the mechanical properties of static and dynamic systems; see e.g. [5] for an extensive review of the role of interaction networks in the context of amorphous solids. However there are no universal methods for describing and quantifying relevant aspects of the interparticle forces. For example, even the commonly used notion of 'force chain' – which we take to mean a connected set of particles interacting by a larger than average force – is not generally defined. One important goal of this paper is to present a method that can be used to describe precisely the global properties of force networks in both static and dynamic settings.

Forces between interacting particles have been considered extensively from statistical point of view, in particular in the context of dense granular matter (DGM). For example, the works by Radjai and collaborators, see, e.g. [6,7], discussed the differences in the probability density functions of strong and weak forces (distinguished by the forces being larger or smaller than the average one) arising in simulations; Behringer and collaborators explored these forces in the experimental systems built from photoelastic particles, see e.g. [4]. Possible universality of the force distributions has been considered [8], as well as the connections between force and contact networks [9]. These works have provided a significant insight into the statistical properties of the force distributions but

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by design do not focus on the structural properties of force networks.

Only recently, attempts have been made to move beyond purely statistical description and consider in more detail the properties of these networks. Examples of recent studies include works by Tordesillas and collaborators, see [10–12] and the references therein. These studies include extensive discussion of local properties of networks of forces based on the forces that particles experience and on their connectivity, including appropriately defined force chains and force cycles with a particular emphasis on cycles of length 3 and 4. Furthermore, these studies introduce mesoscopic network properties such as degree, clustering coefficient and centrality which describe particle arrangements. Averaging these properties over the entire network allows to discuss the connection between the changes observed in the macroscopic network properties to the underlying structural rearrangements of the material.

Alternative approaches use network-type of analysis to discuss the properties of force networks [13–15]. These works provide a significant new insight and confirm that the properties of force networks are relevant in the context of propagation of acoustic signals [13], fracture [14], and compression and shear [15]. Topology based approach has been considered as well, with focus on the contact network topology in isotropically compressed [16] and tapped granular media [17]. A similar approach is considered in our recent work [18], where we discuss connectivity of force networks, including the dependence of the number of connected components and holes/loops (quantified by the Betti numbers), on the (normal) force between the particles. While that work uncovered some intricate properties of force networks and allowed to connect the results of topology based analysis to the ones obtained using standard percolation-based approach, it was still based essentially on counting components and loops at fixed magnitudes of force. As such, it thus does not provide an understanding of how these geometric structures persist through different magnitudes of the force.

In [19] we introduced the use of persistent homology [20,21] to DGM. More recently, these ideas have been employed in the context of tapped systems [22]. Conceptually persistent homology is preferable to the above mentioned Betti number analysis. By design persistent homology measures the same geometric structures as the Betti number analysis, but simultaneously records how these structures appear, disappear or persist through different magnitudes of the force. Thus, two networks of forces could produce identical information on the level of Betti numbers, i.e., the number of connected components and loops, but still have distinct global structures in the sense that as one varies the magnitudes of the forces the relationships between the connected components and loops are different. Therefore, the results presented in [19] provide better quantification of the properties of considered force networks and shed new light on the differences between the systems that differ by their frictional properties and particle size distributions.

It should be noted however, that persistent homology is an abstract tool. Hence, there is considerable freedom as to how it can be employed. In this paper we provide a firm mathematical background for using persistent homology in the context of DGM. In addition, we discuss different concepts for constructing and comparing the persistence diagrams. This allows us to compare the features of different force networks both locally and globally and hence is complementary to the approaches, discussed above, that consider local properties of force networks. Furthermore, the ability to compare different force networks is crucial for quantifying the dynamical properties of DGM.

In the next section we give an overview of persistence homology and the structure of the paper.

2. Overview

In this paper we introduce the concept of a force network, which is designed to model force interactions between the particles. The definition varies depending on available form of the data, but every force network is described by a scalar function $f : D \to \mathbb{R}$. The domain D models the particles and the function f models the forces. Persistent homology is used to reduce the function f to a collection of points in the plane. This collection of points is called a *persistence diagram* and denoted by $\mathrm{PD}(f)$. Each point in the persistence diagram encodes a well defined geometric feature of f.

It is useful to view persistent homology as a mapping from scalar functions to persistence diagrams, e.g. $f \mapsto \mathrm{PD}(f)$. Stated more formally, persistent homology can be viewed as a function from a space of scalar functions to a space of persistence diagrams. A fundamental result is that with appropriate metrics on the space of functions and on the space of persistence diagrams, persistent homology is a continuous function [21]. At least theoretically this implies that bounded noise or small errors in the measurement of the DGM will lead to a small change in the associated persistence diagram.

This theoretical potential combined with the successful applications presented in [19] suggests the need for a careful analysis of the practical details of applying persistent homology to DGM. There are at least three specific issues that need to be addressed:

1. Given a particular form of the experimental or numerical data, how can one perform the persistent homology computations?
2. Having chosen a method by which the persistent homology computations are being performed, how robust is the resulting persistence diagram as a function of experimental or numerical noise or errors?
3. How can the information provided by the persistence diagrams be used to analyze DGM?

Addressing these issues in the context of DGM is the main focus of this paper.

The first step in the construction of the force network is to establish the domain D on which the function f representing the force interactions is defined. A contact network seems to be a natural candidate for the domain D. Indeed, if positions and shapes of the particles are known, then one can construct a contact network. If the data is in the form of a digital image, then building a contact network is more complicated. In Section 3 we start by introducing *digital* and *position* networks that are closely related to contact networks. We investigate their stability with respect to measurement errors and show that their topology can considerably differ from the topology of the physical system they represent. Therefore we propose an alternative domain, the *interaction* network. This is an abstract mathematical concept and its topology is not related to the topology of the physical system it represents. However, it provides a fixed domain for describing the force networks in DGM.

Section 4 introduces homology, which can be crudely interpreted as a tool for counting connected components, loops and cavities. The advantages of homology are that it supports efficient algorithms, can be used in higher dimensions, and allows one to compare components, loops, and cavities over different spaces. Section 5 introduces force networks, clarifying the connection between the type of available data and formulation of appropriate network. Section 6 focuses on persistence homology, our principal tool for analyzing the force networks. The interaction network can be used in the setting of numerical simulations or experiments (see, e.g., [4]), where complete information about the forces between adjacent particles is known. However, for many experiments only the total force experienced by a particle may be available [23]. This necessitates the use of a digital or position network.