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Hands-on Graph Neural Networks with Pytorch

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For a few years now, deep learning researchers have been talking a lot about Graph Neural Networks (GNNs). Understanding how to use GNNs practically on real datasets has proven challenging because of the large variety of tools available and the inherent complexity of working with graphs. Here, we'd like to provide a quick overview of how to build a GNN and train it with a real dataset using the PyTorch framework.

Monotonicity of Centralities in Undirected Networks

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Is it always beneficial to create a new relationship (have a new follower/friend) in a social network? This question can be formally stated as a property of the centrality measure that defines the importance of the actors of the network. Score monotonicity means that adding an arc increases the centrality score of the target of the arc; rank monotonicity means that adding an arc improves the importance of the target of the arc relatively to the remaining nodes. It is known that most centralities are both score and rank monotone on directed, strongly connected graphs. In this talk, I will show that, surprisingly, the situation in the undirected case is very different and that, while it is always a good thing to get a new follower, it is not always beneficial to get a new friend.

Fungal-fungal interactions: A study of three *Trichoderma* strains against plant-associated fungi, isolated from Northern Italy

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Soil microbial communities form complex networks of interaction with each other or with other living organisms. In this complex picture, soil fungi play essential roles in ecosystems through their relationships mostly with soil bacteria, other fungi, and plants. Interactions within these ecological networks may be inhibitory, stimulatory, mutualistic, or neutral for each participating partner. In this research, we used three strains of the *Trichoderma* genus (i.e., *Trichoderma simmonsii* EXF-17015, *Trichoderma* sp. EXF-17016, and *Trichoderma* sp. EXF-17020) as models to study fungal-

fungal interactions. The behavior of *Trichoderma* strains was examined with each other and against eight plant-associated fungi, including plant pathogens. All strains were isolated from vineyards in Northern Italy and identified according to morphological features and genome sequencing. Studies have been performed using the dual culture method in Petri dishes. According to the results, different types of behavior have been observed depending on the *Trichoderma* strain or the other fungal partner used. Specifically, all *Trichoderma* strains showed neutral behavior (symbiosis or proto-cooperation) between themselves and *Aspergillus aculeatus*, competition against *Alternaria* sp., and inhibition by *Rhizopus arrhizus*. However, the stains EXF-17016 and EXF-17020 of *Trichoderma* sp. were inhibited by *Penicillium oxalicum*, but *T. simmonsii* showed antagonistic behavior against the same strain, suggesting that fungal interactions are also strain-dependent. Since strains of the *Trichoderma* genus are used as microbial biological control agents in the new management techniques for plant diseases, studies on their interaction with other soil microflora partners could clarify the impact of the biological fungicides better.

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Predicting microclimate conditions with a mechanistic model supported by AI

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Microclimate mapping and monitoring are of fundamental importance to manage natural resources and to optimize agricultural procedures. Nowadays, precision agriculture is based on the management of spatial-temporal microclimatic variation in fields monitored by IoT systems. Networks of microclimate sensors provide point-based measurements that can be used as input data for mechanistic and artificial intelligence (AI) models to study variations of microclimatic conditions over several spatial and temporal scales. Mechanistic models aim to describe the physical processes which drive microclimatic variations by determining the effects of terrain and vegetation on energy and water fluxes. Artificial intelligence provides powerful algorithms which can capture complex nonlinear relationships hidden in data. While the mechanistic models can be often reduced to too simplistic forms due to the complexity of the phenomena, AI produce black-box models which hamper a clear view and comprehension of the problem. Here, I propose a hybrid model which combines physical laws of energy fluxes with AI algorithms to describe the spatial-temporal variation of temperature over a study area. This combination avoids the complexity and computational costs of a model which fully resolves the physics of atmospheric processes, but without reducing the model to a black box. This approach allows also to extend the microclimatic predictions over field zones where sensors are absent creating a continuous spatial-temporal monitoring of the target area. This can be very useful in precision agriculture to optimize the positioning of monitoring sensors networks.

Rigidity of cellular structures

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In this study we consider a database of more than 17,000 cellular structures with known elastic moduli and their dependence from the structure density. The goal of this study is to obtain a relation between the density scaling of the moduli and the rigidity of the structure. We considered the adjacency matrix and the Hessian matrix which describes elastic properties of the structures and used numerical algorithms to compute their eigenvalues, focusing on the non-trivial zero values which are known to describe loss of rigidity. We studied the role of periodic boundary conditions and of tensile stress on the eigenvalue spectra.

Designing Mechanical Metamaterials for Industries

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Metamaterials in general are the materials which are engineered to have exceptional properties that are not found in naturally occurring materials. These properties come from the geometric structure of material and not from the substance of which they are made. Usually metamaterials consist of sets of elementary cells arranged in a regular way. The particular shape, size, orientation and arrangement of these cells is what gives the material its properties. Mechanical metamaterials are one of the many types of metamaterials, they are designed to have values of mechanical properties that are not found in nature like negative poisson's ratio. They are characterised by unique deformation properties when compressed, pulled, twisted, or subjected to other efforts. They consist of functional areas where elementary cells are periodically repeated. Each elementary cell responds in an appropriate way to supplied inputs. In this way, the metamaterial deforms according to a programmed pattern to produce the required functionality. Metamaterials provide an answer to the demand for greater environmental sustainability in the development of industrial components. By optimising the meso-structure instead of the chemical composition, it is possible to minimise the use of environmentally harmful materials, replacing them with environmentally sustainable materials without loss of performance for the finished component. In industries mechanical metamaterials can replace actuators and thus remove the need for assembling different structural components. But designing mechanical metamaterials manually is very time consuming and not very efficient, therefore there is a need for Automatic design (see Bonfanti et al. Automatic design of mechanical metamaterial actuators», Nature Communications 11, 4162 (2020)). Currently we are trying to design different products for industries using the principles in the above-mentioned work. We are working on designing a Strip Ejector using metamaterials. Our approach is, first design the initial structure, then apply metropolis and other algorithms to get efficient structures, then obtain a realistic simulation by Finite Element Method using COMSOL Multiphysics and finally proceed for 3D printing of samples. Metamaterials have potential to revolutionise the

industry as they have countless applications especially in Automation, Aerospace, medicinal implants, safety devices, cancer diagnosis textile, design, etc

Low-Frequency Vibrational Modes in High Entropy Alloys

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Understanding the vibrational features of amorphous materials is the key to rationalize their peculiar properties. It has been reported that low-frequency vibrational modes in glassy systems at low temperatures are expected to present a universal density of states which depends on the fourth power of the frequency. This law is observed in computer simulations mainly in a toy model of amorphous systems, suggesting that this universal form is a generic consequence of the atomic positional disorder or glassiness. However, a recent work has shown that, remarkably, the quartic law extends also to models of disordered crystals, where the level of disorder can be controlled. Here we study the vibrational properties of a novel class of metallic alloys which are the so-called High Entropy Alloys, varying the positional disorder systematically from disordered crystal to amorphous glass. Our results show the universal quartic trend typical of nonphononic excitations in high entropy alloys across various levels of disorder, while their amplitude is suppressed in disordered crystals compared to their glassy counterpart. Our work offers a unified perspective to describe the vibrational properties of high entropy alloys.