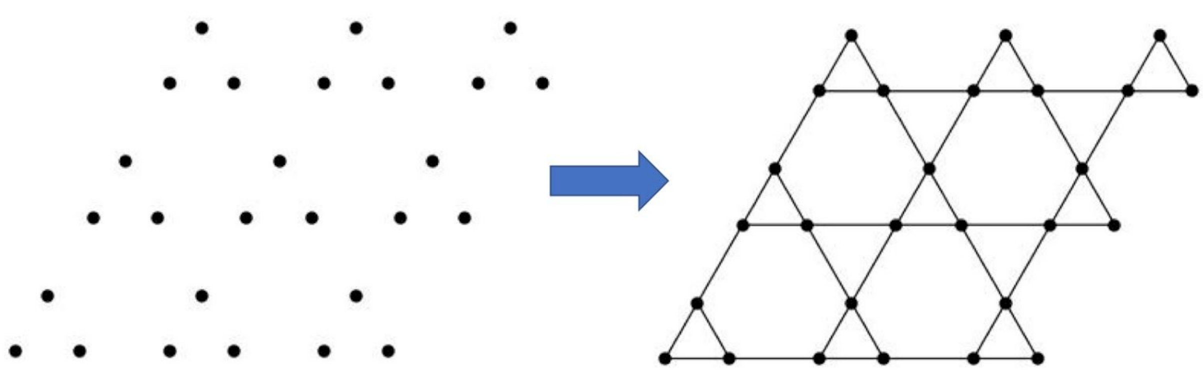
Capstone Project Proposal - Develop a Image-to-Image Translation Model to Capture Local Interactions in Mechanical Networks

Introduction

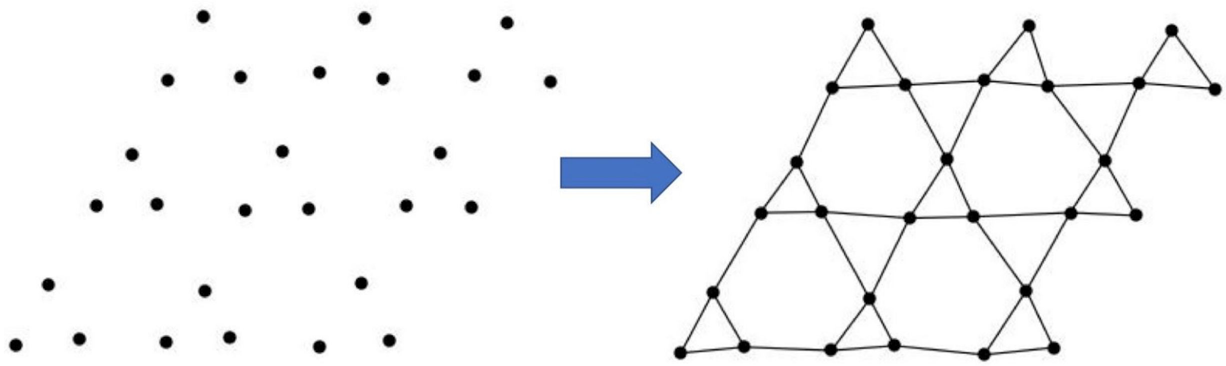
This project is intensively related to my research work in physical sciences at the Georgia Institute of Technology. As a Ph.D. student, my work consists in studying metamaterials, engineered systems with functional mechanical properties. These properties arise from the underlying structure of the material, precisely how things connect with one another. Whether it is at the human or nano scale, the typical structural model of a metamaterial is the same: free sites (also known as nodes, or balls) are spread out in a roughly periodic structure and they are connected by springs (also known as edges). These **balls / springs networks** (also known as lattices) aim to represent either the intermolecular forces between the atoms of a material or the structure of an artificial mechanical system . The bond connectivity, which is how the sites connect with one another, is critical to the nature of the mechanical properties of the system, whether it is entirely rigid or possesses flexible regions.

Motivation / Goal

This project aims to design a neural network model that will plot the bond connections between the sites of a given system. Consider the following situation: if one were to observe a material via an electron microscope, they would be able to easily detect its particles, but not the intermolecular forces (the bonds) which yet govern its mechanical properties. The goal of this project is to design a **Image-to-Image Translation** model which inputs the image of the particles and outputs the same image with the bonds drawn:



A reference system where it is useful to draw the bond connectivity (solid lines) is the Kagome lattice. The Kagome lattice drawn above is ordered, in that the sites (black dots) are ordered periodically in space in groups of three. Each set of three neighboring sites constitute what we call a cell. However, in general, the systems encountered will be a bit more disordered, like in the following.



As you can see, the input image here appears identical to one I shared earlier, at least to the human eye.. But despite appearing their apparent similarities, when the bonds are plotted, it becomes clear each image represents two very different systems. This “bond-plotting” model can facilitate the classification of these mechanical systems and could be very enriching for the scientific community that studies such materials.

Data

The data I’ll use is one I generate for my research work, using the program Mathematica. The input and output images will be similar to those already shared: about 30 sites and as many edges. Each jpg image will roughly be 5 KB in size and 350x250 pixels in dimension. The practical advantage here is the potential to easily generate 1000s of pictures, or more if the model needs it.

Methodology

Image-to-Image models start to become more and more common among deep learning algorithms. For this project, I will use the Pix2Pix Generative Adversarial Network (GAN) developed by Jason Brownless Ph.D. and referenced here:
https://machinelearningmastery.com/how-to-develop-a-pix2pix-gan-for-image-to-image-translation/

Also, I plan to use Google’s Colab and take advantage of their GPU in order to run the GAN, as it seems like computer power may be an issue here. I am also considering using the Pro version of Colab if needed.