Finding hyperuniform structures using a Machine Learning based method

Roger Arnau[1], Jose M. Calabuig[2], Mario Lázaro, Lluis M. Garcia, Vicente Romero-García and Enrique A. Sánchez-Pérez[2]

UNIVERSITAT POLITÈCNICA DE VALÈNCIA

[1] PhD student, [2] PhD supervisors. Programa de Doctorado en Matemáticas (UPV).

ararnnot@posgrado.upv.es, jmcalabu@mat.upv.es, malana@mes.upv.es, lmgarciaraffi@gmail.com, virogar1@mat.upv.es, easancpe@mat.upv.es

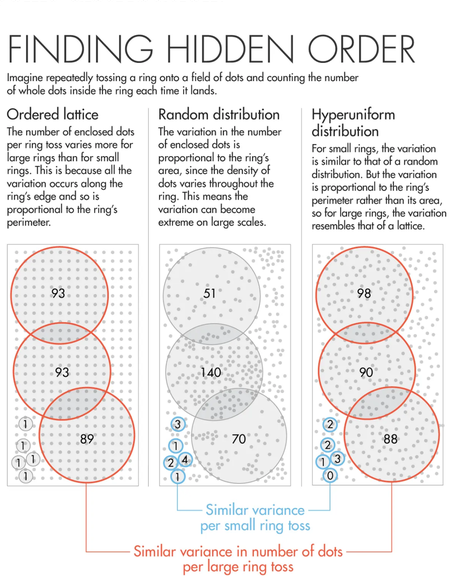
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Abstract

The aim of this work is to use a Machine Learning approach to find hyperuniform structures. The methodology is based on the work of Yu et al. [4] for disordered structures, which uses a composition of two convolutional networks as in an autoencoder architecture.

Introduction

Hyperuniformity is a mathematical property of a point spatial distribution where the variance in the number of points within a spherical window of a specified radius divided by the volume of the observation window tend to 0, when increasing the radius. As illustrated in the figure below, hyperuniformity can be conceptualized as an intermediary state between a random and a periodic point distribution.



Hyperuniformity example. Image from [2].

An equivalent definition could be given in therms of the *structure factor* of a point distribution $\{\vec{r_1}, \vec{r_2}, \ldots, \vec{r_n}\}$:

$$S(\vec{q}) = \frac{1}{N} \sum_{j=1}^{N} \sum_{l=1}^{N} \exp(-i\vec{q}(\vec{r_j} - \vec{r_l})),$$

saying that is a hyperuniform distribution if $\lim_{\vec{q}\to 0} S(\vec{q}) = 0$.
For that reason, we are interested in the study of scatterers satisfying that $S(\vec{q}) = 0$ for $0 < |\vec{q}| < \chi$. The value (maximum) value of χ for which it is satisfied is called stealthiness.

Applications

If we consider the points as scatterers in a homogeneous medium, hyperuniformity allows us to design heterogeneous medium with properties ad hoc to the control and manipulation of waves, such as:

1. total transparency in a frequency band,
2. full isotropic bandgaps, or
3. equiluminosity (equal diffusion in all directions) for a frequency band.

For a detailed example of these structures, we refer to the previous works of the research group such as [3].

Methodology

We follow the work in [4], in which a neural network approach is implemented to find disordered structures with fixed properties for waves.

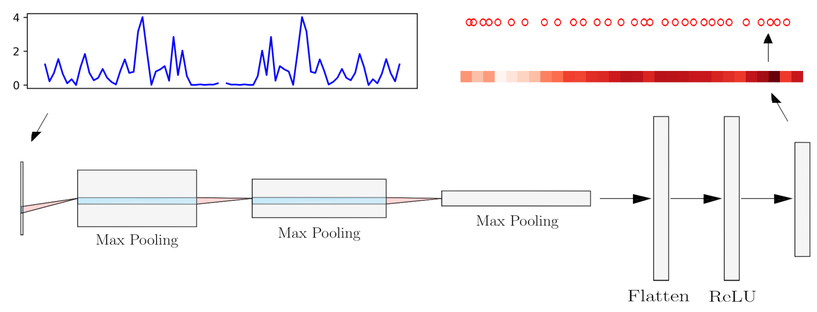
Processing of the data

Our dataset is composed by one dimensional near-hyperuniform point distributions obtained by previous works of V. Romero-García and complemented with randomly generated data.
Each observation consists of 30 non-overlapped points distributed on the domain $[0, 1]$ and the corresponding first 40 structure factor values. The point distribution is codified as a 1D image of one channel, that is, an $\mathbb{R}^{30}$ vector in which each entry represents the deviation of each point from a uniformly spaced distribution.

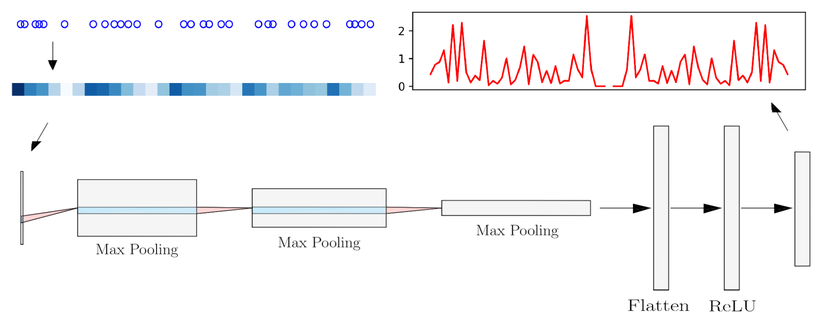
Model architecture

Our model is composed by two modules:

1. Points to Structure Factor ($P2S$): given a distribution of 30 points, it must predict its 40 first structure factor values.



2. Structure Factor to Points ($S2P$): must find a distribution on 30 points that has a fixed structure factor.

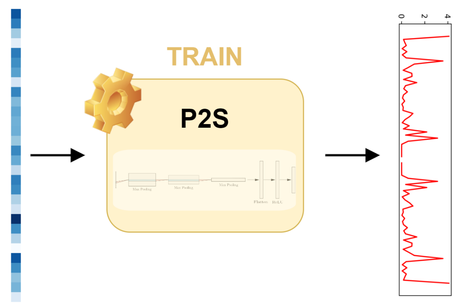


Both modules are composed by the same architecture (three 1D-convolution layers with two fully connected layers at the end), only differing on the input and output sizes.

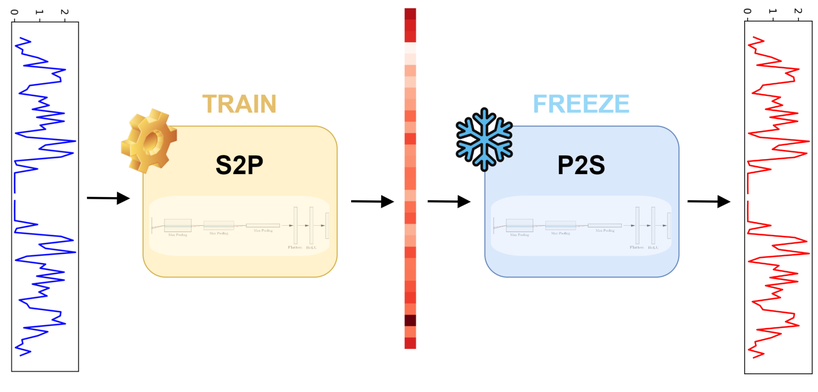
Trainning process

The network trainning is divided into two steps, one of each with the purpose of training one module.

1. First, the $P2S$ network is trained using the mentioned dataset.



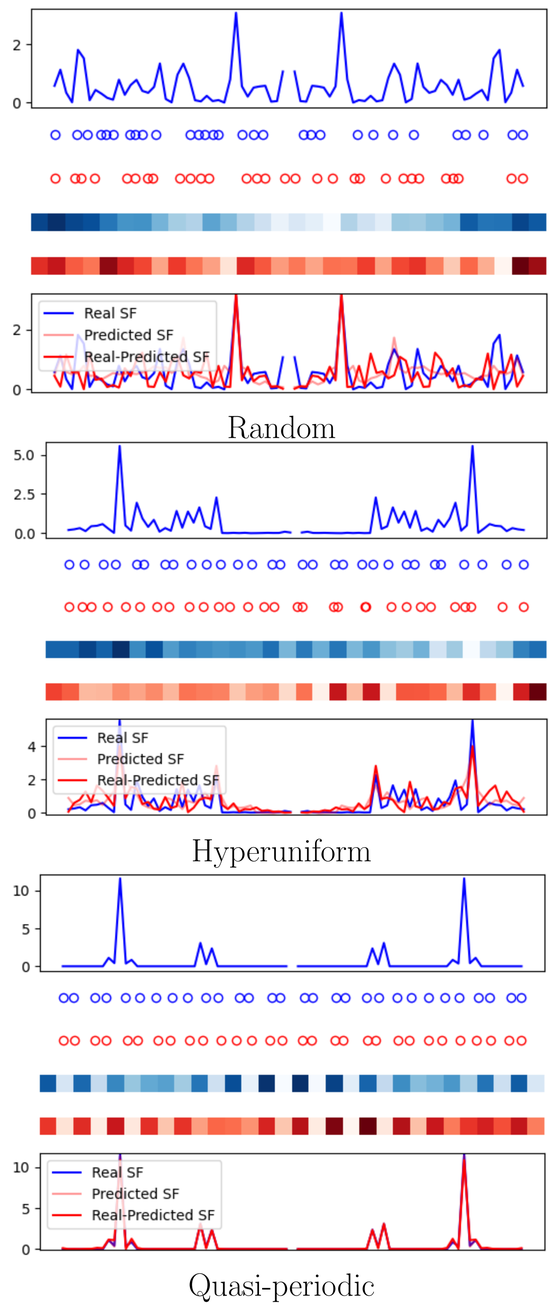
2. Once the $P2S$ network is trained, all its weights are fixed, and it is assumed that, given any point distribution, its output is the associated structure factor. Now, the $S2P$ network is trained using each structure factor as inputs, and its outputs pass through the $P2S$ network, yielding a structure factor that must be as similar as the input one.



These two steps are implemented to avoid training the $S2P$ network to map structure factors to point distributions, which could lead to instability problems due to the degeneration of the $P2T$ network. This is because different point distributions could lead to the same structure factor, see [1]. In that case, the $S2P$ will only be able to find one point distribution with the given structure factor.

Preliminary results

The results are tested in observations of hyperuniform scatterers for χ values up to 0.45, and some results are shown below for different distributions.



As one can see, the model is capable to find a point distribution with a given structure factor in the quasi-periodic. We notice that, as we assumed, the scattering is different of the given one, but it fits perfectly its structure factor.
For the hyperuniform case, the model finds a distribution with a structure factor near to 0 (but not 0) for the same amplitudes and also the bigger peaks.
On the random example, also the more relevant peaks are replicated, but one can see that the predicted structure factor tends to the mean for large values of $|\vec{q}|$.

Conclusions and further work

The presented model is able to find point distributions given its structure factor which haven't been used in the training process. While it is capable to find point distributions with small values of $S(\vec{q})$ near the origin and the most relevant peaks, the reconstruction is not perfect in most of the cases. The $P2S$ network seems to lack of precision for large $\vec{q}$ with a trend to the mean, wich makes impossible for the $S2P$ module to find structures with exactly the same structure factor.
We will continue the research on the topic with the aim to improve the results, since the problem of finding hyperuniform structures in higher dimensions become more difficult and takes a huge computational time.

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