

## Potential Symmetry Motivation and Definition

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Awhile ago I was thinking about artificial intelligence and creativity. Computers are great at certain things like finding and producing patterns. It seemed to me that, as the development of intelligent machines progresses, the only remaining advantage that humans will have is the ability to create outside of patterns ("creativity" for the purpose of this thread). This means not only being random (because random events can also form patterns accidentally) but consciously avoiding patterns. On the other hand, maybe even creativity, by this definition, has a pattern. If I am avoiding all known possible patterns, then will my resulting creation not also follow a sort of pattern?

As a more concrete example of what we mean by "pattern", consider 2 points on a plot (black dots on Fig.1): If we were to place a 3rd point somewhere, where would we place it to maximize the symmetry of the resulting 3-point object? Perhaps we would continue the first 2 points to form a line of 3 points, or perhaps we would use the 3rd point to form an equilateral triangle. These options are shown in the Fig.1, with the original 2 points in black and the (in my opinion) high-symmetry points in red. If you were pushed further, what would you say were the next-highest symmetry positions for the 3rd point? I'd say the orange points but who knows.



Figure 1

The red points seem like the obvious choices, but how do we formalize this idea of potential symmetry, PS? We would need an algorithm that can pick out regular patterns like lines and grids, as well as amorphous patterns such as rings of  $n$  points. The way I've decided to do this is by using a simulation of NEXAFS (Near Edge X-Ray Absorption Fine Structure). NEXAFS works by diffracting X-rays off of a cluster of atoms. These X-ray photons which have scattered off of at least one atom each reach some detector where their intensity is measured. If the distance between atoms is roughly the same as the photon wavelength, then the photons will interfere constructively, while they will interfere destructively if the inter-atomic distance is roughly half a wavelength. The scattering is performed with a range of wavelengths, and the resulting wavelength dependence of the detected NEXAFS spectrum

represents information pertaining to the  $n$ th-nearest neighbor distances, which in turn represent structural symmetries of the system. So, to the point, I use a calculation inspired by NEXAFS to calculate the PS (i.e. the symmetry resulting from adding a point) over a 2D range. This is the result (red is high symmetry, blue is low symmetry):

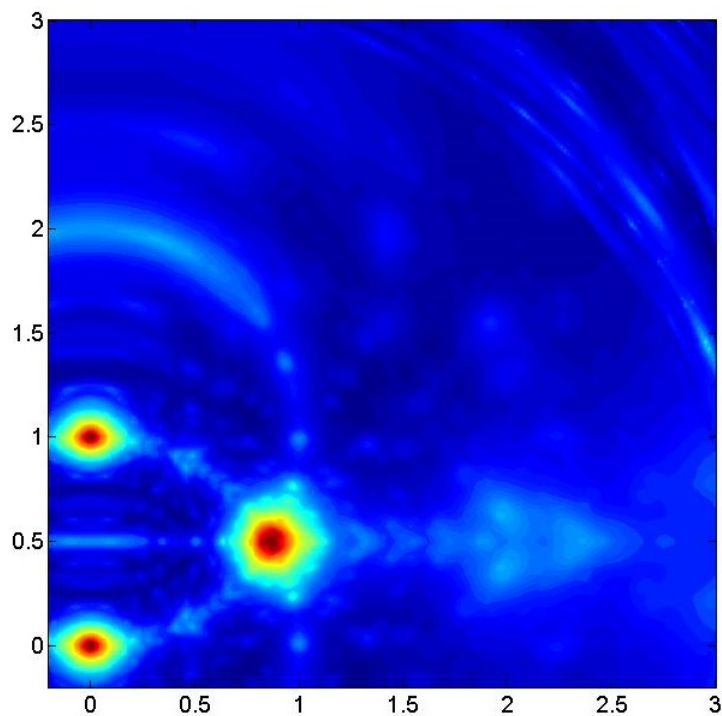


Figure 2

The initial 2 points are at  $(0,0)$  and  $(0,1)$ . As you can see, the PS is high at the expected 3rd-point locations (equilateral triangle and 3-point line), but the PS plot is far more rich than I could have predicted. I might have guessed that there would be PS peaks at the points forming a square with the first 2 points, but to my surprise that is not the case. At least one aspect (the sharp boundary at  $\text{radius}=3$ ) is probably an artifact of the calculation method. This calculation of PS will work with any combination of starting points. As another example, here is a PS plot for 3 initial points at  $(0,0)$ ,  $(0,1)$ ,  $(1,0)$  (an L shape) (again, red is high symmetry, blue is low symmetry):

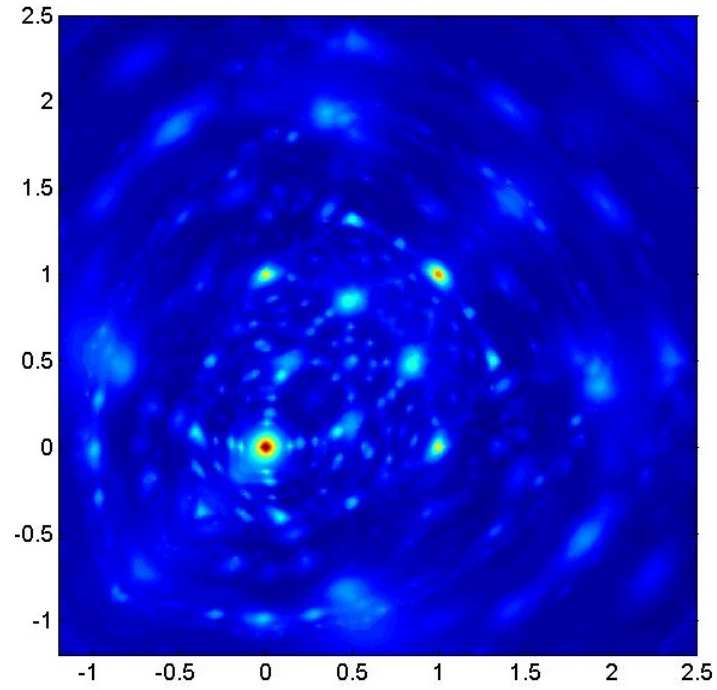


Figure 3

So, to address my original question, if I wanted to make a computer program that produces a collection of points that *avoids* geometrical patterns, I would pick two random points and calculate the PS plot, then I would pick a 3rd point from a low-symmetry (blue) region of the plot and calculate the PS plot for the 3 current points, then I would pick a 4th point from the low-symmetry regions... and so on.