Anisotropic Extensions of Nonlocal Interaction Models

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Abstract

In this project, we investigated pattern formations which arise from self-organizing mathematical models significant to physical, biological, and engineering systems. The mathematical problems examined in our research have applications in models of materials science and in collective behavior of multi-agent systems such as superconductor vortices, robotic swarms, and biological aggregations. These patterns can be described as minimal energy configurations N interacting particles.

Most nonlocal interaction models in the literature consider only *isotropic* interaction energies where the interaction kernel is radially symmetric. In this project, we first examined pattern formations induced by several *smooth and crystalline anisotropies*. The results of our numerical experiments showed significant quantitative differences in the properties of the energy-optimal configurations between smooth and crystalline anisotropies.

Introduction and Discussion

We have the Hamiltonian of a particle interaction system given by

$$E(\boldsymbol{x_1},\dots,\boldsymbol{x_N}) = \sum_{\substack{i,j=1\\ i\neq j}}^{N} K(\|\boldsymbol{x_i}-\boldsymbol{x_j}\|),$$

where $\boldsymbol{x_1},\dots,\boldsymbol{x_N}$ are vectors (x_1,x_2) in 2-dimensional Euclidean space $\mathbb{R}^2$ and $K:\mathbb{R}\to\mathbb{R}$.

To determine the ground state of this system, we solve the following ODE system

$$\frac{d\boldsymbol{x_i}}{dt} = -\frac{1}{N}\sum_{\substack{i,j=1\\ i\neq j}}^{N} \nabla K(\|\boldsymbol{x_i}-\boldsymbol{x_j}\|).$$

Our initial results involved a spherical kernel $K_s:\mathbb{R}^2\to\mathbb{R}$ where for $p,q\in\mathbb{R}$ with $q>p>-2$:

$$K_s(\boldsymbol{x_i}-\boldsymbol{x_j}) = K_s(x_1,x_2) = \frac{(x_1^2+x_2^2)^{\frac{q}{2}}}{q} - \frac{(x_1^2+x_2^2)^{\frac{p}{2}}}{p}$$

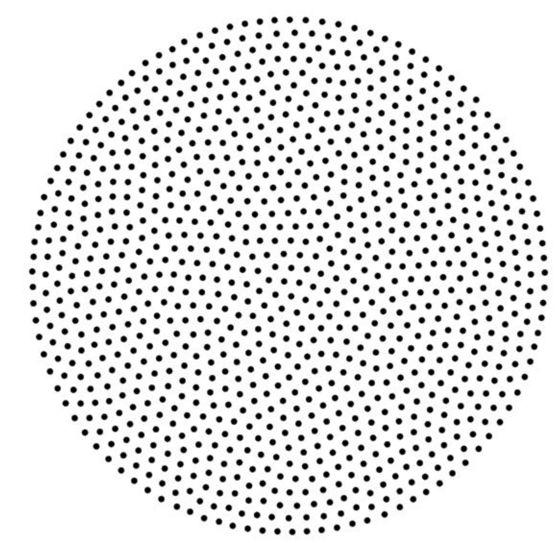
We later examined elliptical kernels $K_{e,c}:\mathbb{R}^2\to\mathbb{R}$ with norm c and parameters $a,b\in\mathbb{R}$. For $c\geq 1$, we have

$$K_{e,c}(x_1,x_2) = \frac{(a^c|x_1|^c+b^c|x_2|^c)^{\frac{q}{c}}}{q} - \frac{(a^c|x_1|^c+b^c|x_2|^c)^{\frac{p}{c}}}{p}.$$

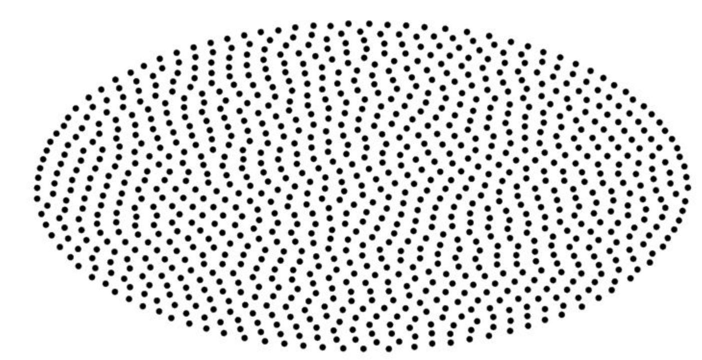
In our kernels, if $p=0$ or $q=0$, the p or q expressions were treated as logarithms. For the elliptical norm, this would therefore be

$$\frac{(a^c|x_1|^c+b^c|x_2|^c)^{\frac{0}{c}}}{0} = \log\left((a^c|x_1|^c+b^c|x_2|^c)^{\frac{1}{c}}\right)$$

Numerical Results

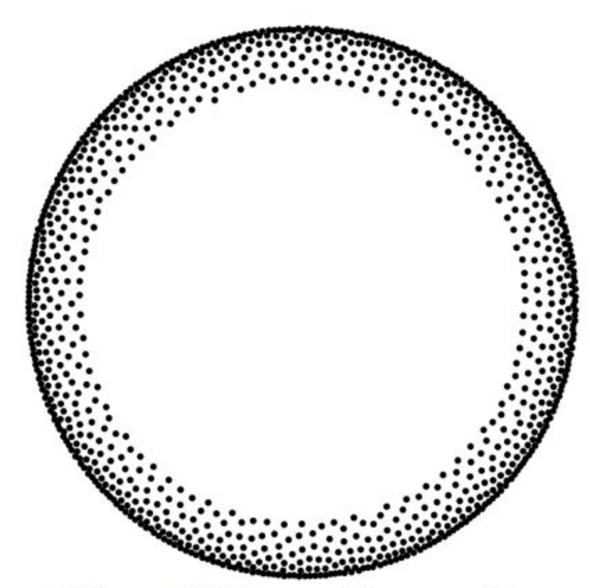


K_s with $p=0$, $q=2$, and $N=1000$

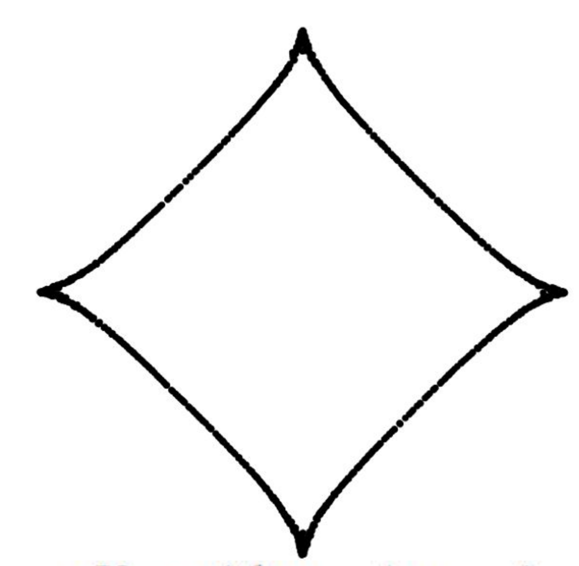


$K_{e,2}$ with $p=0$, $q=2$, $a=0.5$, $b=1$, and $N=1000$

For $p=0$, $q=2$, K_s gives a uniform distribution of points throughout a circle. However, when using $K_{e,2}$, changing a and b away from 1 results in uniform distribution throughout an ellipse. As described in the Analytic Results section, we are able to describe this change through a change of variables.

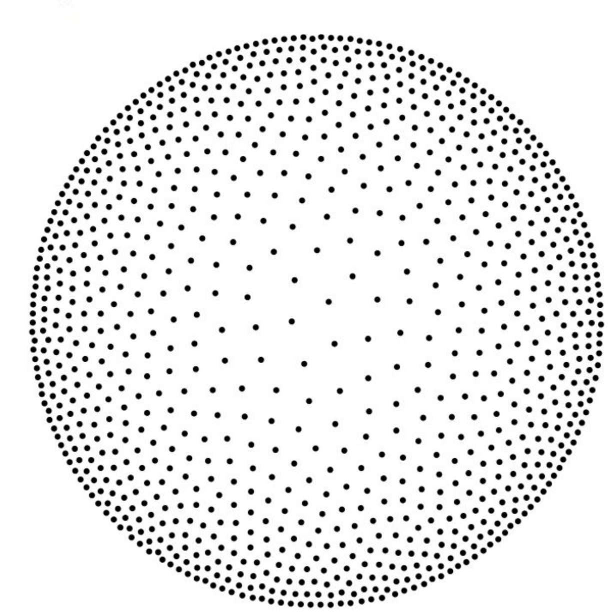


$K_{e,2}$ with $p=1$, $q=4$, $a=1$, $b=1$, and $N=1000$

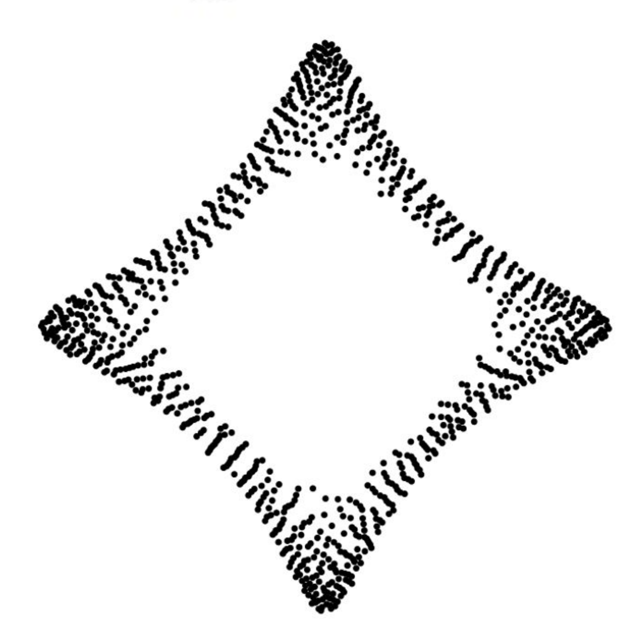


$K_{e,1}$ with $p=1$, $q=4$, $a=1$, $b=1$, and $N=1000$

For $p=1$, $q=4$, $K_{e,1}$ gives a 1 dimensional curve (an astroid), while $K_{e,2}$ gives a 2 dimensional distribution. This difference in dimensionality reveals significant quantitative differences between these two types of kernels.



$K_{e,2}$ with $p=0.5$, $q=4$, $a=1$, $b=1$, and $N=1000$



$K_{e,1}$ with $p=0.5$, $q=4$, $a=1$, $b=1$, and $N=1000$

Even though $p=1$, $q=4$ led to differences in dimensionality, other parameters such as $p=0.5$, $q=4$ led to minimizers of the same dimension. We attempted to describe this behavior using an inequality described in the Analytic Results section.

Analytic Results

We can write K using K_s as

$$K_s(\boldsymbol{x}-\boldsymbol{y}) = K(\|\boldsymbol{x}-\boldsymbol{y}\|_2)$$

and we can represent the elliptical behavior using $f_{*,c}:\mathbb{R}^2\to\mathbb{R}$ given by

$$f_{*,c}(\boldsymbol{x}-\boldsymbol{y}) = \left(\left(\frac{x_1-y_1}{a}\right)^c + \left(\frac{x_2-y_2}{b}\right)^c\right)^{1/c}$$

to write

$$K_{e,c}(\boldsymbol{x}-\boldsymbol{y}) = K\left(f_{*,c}(\boldsymbol{x}-\boldsymbol{y})\right).$$

Consider a density function, ρ, which models the distribution of particles. For $\rho\geq 0$, we have

$$\int_{\mathbb{R}^2}\rho(\boldsymbol{x})d\boldsymbol{x} = m.$$

For K_s, ρ is given by

$$\rho(\boldsymbol{x}) = \frac{m}{\pi}\chi_{B(0,1)}(\boldsymbol{x}).$$

Our energy functional is given by

$$\mathcal{E}[\rho] = \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} K(\|\boldsymbol{x}-\boldsymbol{y}\|_2)\rho(\boldsymbol{x})\rho(\boldsymbol{y})d\boldsymbol{x}d\boldsymbol{y}.$$

Using

$$\widetilde{\boldsymbol{x}} = \left(\frac{x_1}{a},\frac{x_2}{b}\right),\quad \widetilde{\boldsymbol{y}} = \left(\frac{y_1}{a},\frac{y_2}{b}\right),\quad \widetilde{\rho}(\boldsymbol{x}) = ab\rho(\boldsymbol{x}),$$

we were able to represent the minimizer of the $p=0$, $q=2$ case of K_s in terms of the $p=0$, $q=2$ case of $K_{e,2}$.

We also attempted to compare the energies of minimizers of $K_{e,1}$ and $K_{e,2}$ analytically. Our calculations revealed the following relation

$$\begin{aligned}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} K(\|\boldsymbol{x}-\boldsymbol{y}\|_1)\rho(\boldsymbol{x})\rho(\boldsymbol{y})d\boldsymbol{x}d\boldsymbol{y} &\leq \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} K(\|\boldsymbol{x}-\boldsymbol{y}\|_2)\rho(\boldsymbol{x})\rho(\boldsymbol{y})d\boldsymbol{x}d\boldsymbol{y}\\ &\leq 2^{\frac{q}{2}}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} K(\|\boldsymbol{x}-\boldsymbol{y}\|_1)\rho(\boldsymbol{x})\rho(\boldsymbol{y})d\boldsymbol{x}d\boldsymbol{y}\\ &\quad + \frac{2^{\frac{A}{2}}}{p}\int_{\mathbb{R}}\int_{\mathbb{R}^2}\|\boldsymbol{x}-\boldsymbol{y}\|_1^p\rho(\boldsymbol{x})\rho(\boldsymbol{y})d\boldsymbol{x}d\boldsymbol{y},\end{aligned}$$

where

$$A = \frac{2\log\left(2^{\frac{q}{2}}-2^{\frac{p}{2}}\right)}{\log(2)}.$$

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