General Kernel Spectral Methods for Equilibrium Measures

MMSC Dissertation

Peter Julius Waldert

Mathematical Institute
University of Oxford

- Simulate Many-Particle-Systems and find their Equilibrium Distribution.
- Interactions through (power-law) Attraction-Repulsion Potentials

$$K(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta}\,, \quad \alpha, \beta \in \mathbb{R}\,.$$

- Each particle $i = 1, \ldots, N$ at position $\boldsymbol{x_i}$ and time t follows

$$\frac{\mathrm{d}^2 \boldsymbol{x_i}}{\mathrm{d}t^2} = f\left(\left\|\frac{\mathrm{d}\boldsymbol{x_i}}{\mathrm{d}t}\right\|_2\right)\frac{\mathrm{d}\boldsymbol{x_i}}{\mathrm{d}t} - \frac{1}{N}\sum_{j=1, i\neq j}^{N} \nabla K\left(\|\boldsymbol{x_i} - \boldsymbol{x_j}\|_2\right)\,,$$

(Gutleb, José A. Carrillo and Olver 2020; Gutleb, José A. Carrillo and Olver 2021).
- Add tikzpicture of particle box with interaction
- If repulsive part is larger (so $\beta > \alpha$), there is no equilibium distribution: particles simply continue repelling one another out to infinity

An Integral Equation

The total energy is

$$E = \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} K\left(\|\boldsymbol{x_i} - \boldsymbol{x_j}\|_2\right) \,,$$

which can be equivalently expressed as

$$E = \frac{1}{2} \iint K\left(\|\boldsymbol{x} - \boldsymbol{y}\|_2\right) \mathrm{d}\rho(\boldsymbol{x})\, \mathrm{d}\rho(\boldsymbol{y}) \,,$$

where $\mathrm{d}\rho = \mathrm{d}\rho(x)\mathrm{d}x$ is a measure chosen such that

$$M = \int \mathrm{d}\rho = \int_{\mathrm{supp}(\rho)} \rho(x)\, \mathrm{d}x = 1 \,.$$

Simulation Results

What we expect:

[Plots of simulator equilibium measure]

- In order to find $\rho(x)$, we consider the following Ansatz

$$\rho(\boldsymbol{x}) = \sum_{n=0}^{\infty} f_n p_n(\boldsymbol{x})$$

  by which we construct a spectral method for the solution of the above integral equation.

- Using the Jacobi polynomial basis.
- Minimization routine of E over coefficients in ρ, as a subroutine of outer minimisation over a and b the bounds of the box (simpler: $a = b = r$).
- We see that we do not need the inner optimisation routine, because TODO.

Results from the Spectral Solver

Here are some plots

If too ambitious, just use those from paper

Project Goals

- Establish theory behind spectral methods in the Jacobi basis.
- Use kernel expansions to construct an equilibrium measure method on $[-1, 1]$.
- Consider the d-dimensional unit ball.
- Numerically solve for $\rho(x)$ using a fully implemented spectral solver.
- Implement a particle simulator for the same kernel K.
- Compare results of the two methods.
- First numerical method on continuous space problems!! (we are the fastest anyway!).
- Optional: Potentially, extend to l-Morse potentials.
- Spread Open Source!

Questions?

[1] Andrea L. Bertozzi, Theodore Kolokolnikov, Hui Sun, David Uminsky and James von Brecht. 'Ring patterns and their bifurcations in a nonlocal model of biological swarms'. In: *Comm. Math. Sci.* 13.4 (2015), pp. 955–985. ISSN: 1945-0796. DOI: 10.4310/CMS.2015.v13.n4.a6.

[2] J. A. CARRILLO, Y. HUANG and S. MARTIN. 'Explicit flock solutions for Quasi-Morse potentials'. In: *European Journal of Applied Mathematics* 25.5 (2014), pp. 553–578. DOI: 10.1017/S0956792514000126.

[3] José A. Carrillo and Yanghong Huang. 'Explicit equilibrium solutions for the aggregation equation with power-law potentials'. In: *Kinetic and Related Models* 10.1 (2017), pp. 171–192. ISSN: 1937-5093. DOI: 10.3934/krm.2017007.

[4] Timon S. Gutleb, José A. Carrillo and Sheehan Olver. 'Computation of Power Law Equilibrium Measures on Balls of Arbitrary Dimension'. In: *arXiv* (Sept. 2021). DOI: 10.1007/s00365-022-09606-0. eprint: 2109.00843.

[5] Timon S. Gutleb, José A. Carrillo and Sheehan Olver. 'Computing Equilibrium Measures with Power Law Kernels'. In: *arXiv* (Oct. 2020). DOI: 10.1090/mcom/3740. eprint: 2011.00045.