General Kernel Spectral Methods for Equilibrium Measures

MMSC Dissertation

Peter Julius Waldert

Mathematical Institute
University of Oxford

Project Motivation and Goal

- 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 $i = 1, \dots, N$ 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, Carrillo and Olver 2020; Gutleb, Carrillo and Olver 2021).

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

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

- 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.

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.
- Potentially, extend to l-Morse potentials.

Questions?

[1] 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.

[2] 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.