General Kernel Spectral Methods for Equilibrium Measures

An MMSC Dissertation

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Project Motivation and Goal

- Simulate Many-Particle-Systems and find their Equilibrium Distribution.
- Interactions through (power-law) Attraction-Repulsion Potentials[1]

$$K(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta} \quad \text{with parameters} \quad \alpha, \beta \in \mathbb{R}\backslash\{0\}\,.$$

- Each particle $i = 1, \dots, N$ at position $\boldsymbol{x_i} \in \mathbb{R}^n$ and time $t \in \mathbb{R}^+$ follows

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

for reference see, for example, [2, 1].

[1] If the repulsive part is larger (so $\beta > \alpha$), there is no equilibium distribution as particles simply continue repelling one another out to infinity.

An Integral Equation

The total energy is

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

which, in the continuous limit ($N \to \infty$), becomes

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

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

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

Simulation Results

Figure: The positional distribution approached by $N = 250$ particles.

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

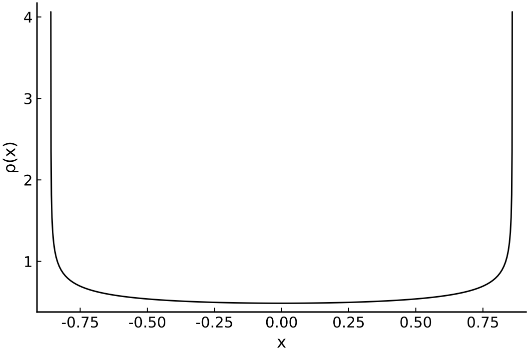
$$\rho(\boldsymbol{x}) = \sum_{n=0}^{\infty} f_n p_n(\boldsymbol{x})$$

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

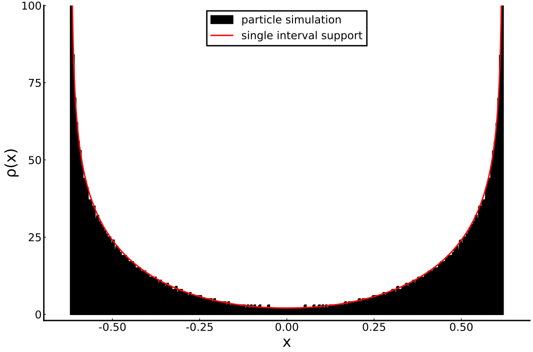
- Using the Jacobi polynomial basis.
- Minimization routine of E over coefficients in ρ, as a subroutine of outer minimisation over a and b the bounds of the box (simpler: $a = b = r$).
- We see that we do not need the inner optimisation routine, because TODO.
- Yields a banded operator.

Results from the Spectral Solver

Using the spectral method, we try to immediately solve for the distribution function in the continuous limit.



Equilibrium distribution for $\alpha = 2$, $\beta = 1.5$



Equilibrium distribution for $\alpha = 3.5$, $\beta = 1.6$

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.

Questions?

Bibliography I

[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.