General Kernel Spectral Methods for Equilibrium Measures

An MMSC Dissertation Project

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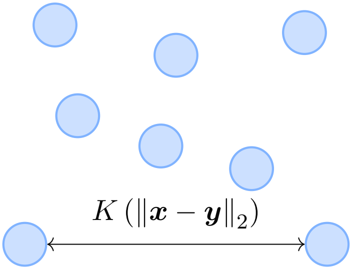
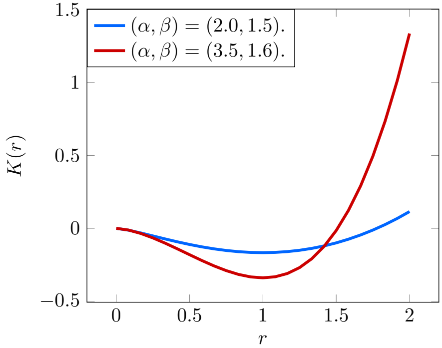
Problem Setting

- Find the Equilibrium Distribution $\rho(\boldsymbol{x})$ of a Many-Particle-System.





$N = 8$ particles interacting with one another through the potential $K(r)$.

Plot of attractive-repulsive potential functions $K(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta}$ for different α, β.

Project Motivation and Goal

- 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 $i = 1, ..., N$ at position $\boldsymbol{x_i} \in \mathbb{R}^d$ 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, [1, 2]. For now, we only consider the case without an external potential $V(\boldsymbol{x})$.

[1] If the repulsive term is stronger (so $\beta > \alpha$), there is no equilibium distribution as particles simply continue repelling each other out to infinity.

Simulation Results

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

An Integral Equation

The total potential energy of an N-particle system is then given by

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

which, in the continuous limit as $N \to \infty$, 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 (the equilibrium distribution) chosen such that

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

- In order to find $\rho(\boldsymbol{x})$, we consider the following ansatz

$$\rho(\boldsymbol{x}) = \sum_{n=0}^{\infty} c_n P_n^{(a,b)}(\boldsymbol{x}) \,, \quad c_n \in \mathbb{R} \,,$$

  with which we construct a spectral method for the numerical solution of the above integral equation.
- Minimization routine of E over coefficients in ρ, as a subroutine of outer minimisation over the bounds of the box (simpler case: use $[-r, r]$, $r \in \mathbb{R}^+$).
- By construction, we find that we do not need an iterative approach for the inner optimisation routine.
- The outer minimisation can be performed using known methods from continuous optimisation.

Jacobi polynomials $P_n^{(a,b)}(x)$ are orthogonal on $[-1,1]$ w.r.t. the weight function

$$w^{(a,b)}(x) = (1-x)^a(1+x)^b\,,$$

so they satisfy

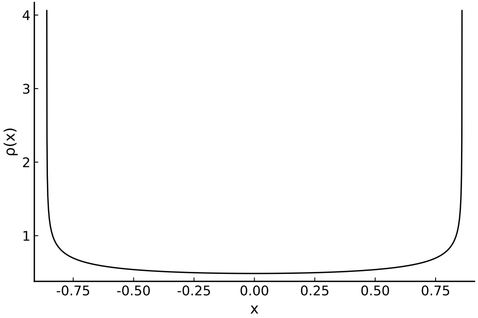
$$\int_{-1}^{1}(1-x)^a(1+x)^b P_n^{(a,b)}P_m^{(a,b)}\,\mathrm{d}x = \frac{2^{a+b+1}\Gamma(a+n+1)\Gamma(b+n+1)}{n!(a+b+2n+1)\Gamma(a+b+n+1)}\delta_{n,m}\,,$$

with $a, b > -1$, which uniquely determines $P_n^{(a,b)}(x)$. The special case of $a = b$ corresponds to the ultraspherical or Gegenbauer polynomials, while the case $a = b = 0$ corresponds to the Legendre polynomials [3].

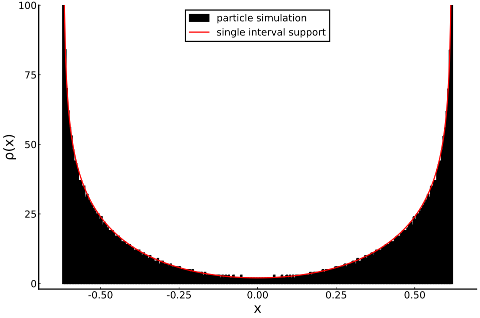
- This basis yields a **sparse**, and in particular, **banded** operator.

Results from the Spectral Solver

Using the spectral method, we try to immediately solve for the distribution function in the continuous limit (here, $d = 1$ dimension).



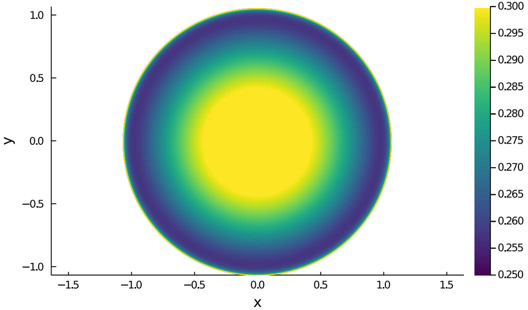
Equilibrium distribution $(\alpha, \beta) = (2, 1.5)$ [1].



Equilib. distribution $(\alpha, \beta) = (3.5, 1.6)$ [1].

Two Dimensional Results

The same is possible for $d = 2$ or more dimensions.



The radially symmetric equilibrium distribution $\rho(\boldsymbol{x})$ for $\alpha = 1.2$, $\beta = 0.1993$ in $d = 2$ dimensions, obtained using a spectral method [2].

Upcoming Work

In this MMSC dissertation project, we will:

- Establish theory behind spectral methods in the Jacobi basis.
- Use kernel expansions to construct an equilibrium measure method on $[-1, 1]$.
- Numerically solve for $\rho(\boldsymbol{x})$ using a fully implemented spectral solver[2].
- Implement a particle simulator for the same kernel K (mostly done).
- Compare results of the two methods and analytic solutions of special cases [4].

Further goals include:

- Considering the d-dimensional unit ball domain $(d > 1)$.
- Optionally: Considering external potentials $V(\boldsymbol{x})$.
- Optionally: Extending to l-Morse potentials $K(r) = C_1 \mathrm{e}^{r/l_1} - C_2 \mathrm{e}^{r/l_2}$.

[2] This is the first numerical method for particle distribution problems!

Questions?

Bibliography I

[1] 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.

[2] 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.

[3] F.W.J. Olver, A.B.O. Daalhuis, D.W. Lozier, B.I. Schneider, R.F. Boisvert, C.W. Clark, B.R. Miller and B. V. Saunders (eds.) *NIST Digital Library of Mathematical Functions*. http://dlmf.nist.gov. Dec. 2018. (Visited on 11/11/2020).

[4] J. A. Carillo, 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.