# General Kernel Spectral Methods for Equilibrium Measures

An MMSC Dissertation


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21st May 2023

- 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 $i = 1, ..., N$ 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, [2, 1]. For now, we only consider the case without an external potential $V(\boldsymbol{x})$.

[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.

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, 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

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


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

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

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

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

- Minimization routine of $E$ over coefficients in $\rho$, 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 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

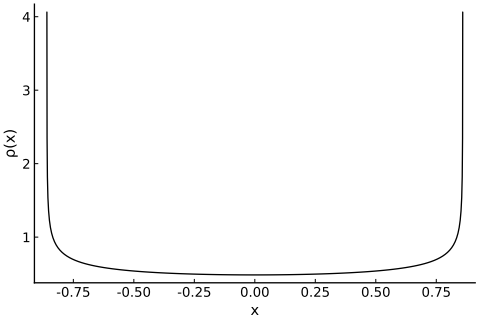
$$\int_{-1}^{1}(1-x)^a(1+x)^b P_n^{(a,b)}P_m^{(a,b)}\mathrm{d}x = \frac{2^{a+b+1}\Gamma(a+n+1)\Gamma(b+n+1)}{n!(a+b+2n+1)\Gamma(a+b+n+1)}\delta_{n,m},$$

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, Table 18.3.1].

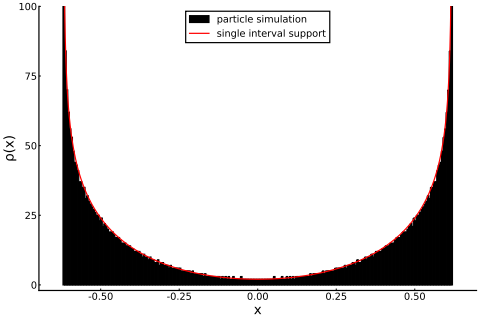
- This basis yields a **sparse**, and in particular, **banded** operator.

# 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).



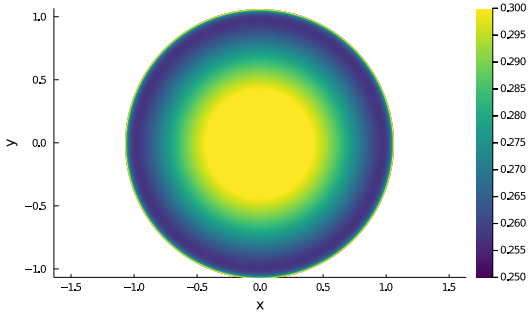

Equilibrium distribution for $\alpha = 2$, $\beta = 1.5$




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

# 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.

# Upcoming Work

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

Further goals include

- Considering the $d$-dimensional unit ball domain ($d > 1$).
- Optionally: Extend to l-Morse potentials.

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

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.

[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*. en. http://dlmf.nist.gov. Dec. 2018. (Visited on 11/11/2020).