

General Kernel Spectral Methods for Equilibrium Measures

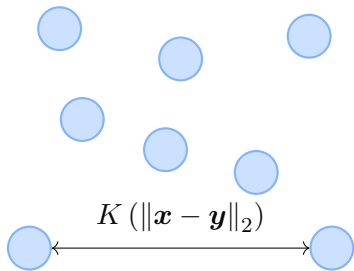
An MMSC Dissertation



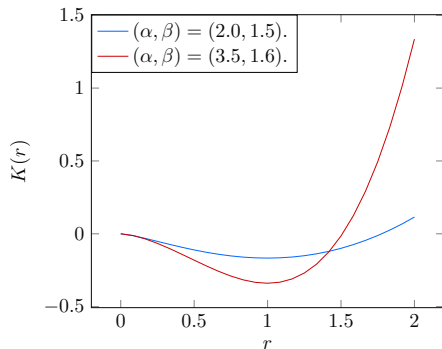
Peter Julius Waldert
Mathematical Institute
University of Oxford

22nd May 2023

- Find the Equilibrium Distribution $\rho(\mathbf{x})$ 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 .

- Interactions through (power-law) Attraction-Repulsion Potentials¹

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

- Each particle $i = 1, \dots, N$ at position $\mathbf{x}_i \in \mathbb{R}^d$ and time $t \in \mathbb{R}^+$ follows

$$\frac{d^2 \mathbf{x}_i}{dt^2} = f \left(\left\| \frac{d\mathbf{x}_i}{dt} \right\|_2 \right) \frac{d\mathbf{x}_i}{dt} - \frac{1}{N} \sum_{j=1, i \neq j}^N \nabla K(\|\mathbf{x}_i - \mathbf{x}_j\|_2),$$

for reference see, for example, [2, 1]. For now, we only consider the case without an external potential $V(\mathbf{x})$.

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

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

$$E = \sum_{i=1}^N \sum_{j=1, j \neq i}^N K(\|\mathbf{x}_i - \mathbf{x}_j\|_2),$$

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

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

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

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



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

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

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

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 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

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

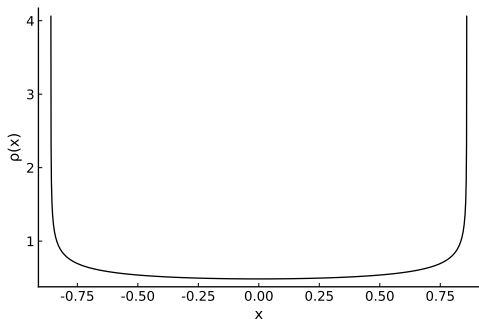
so they satisfy

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

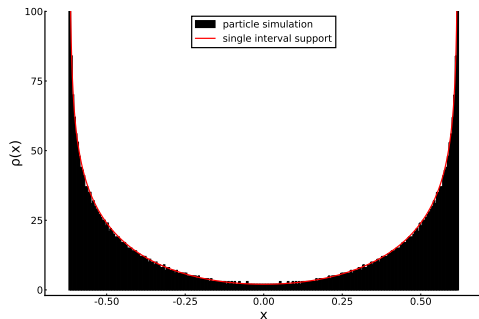
with $a, b > -1$, which uniquely determines $P_n^{(a,b)}(x)$. The special case of $a = b$ corresponds to the ultraspherical or Gegenbauer polynomials, while the case $a = b = 0$ corresponds to the Legendre polynomials [3].

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

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

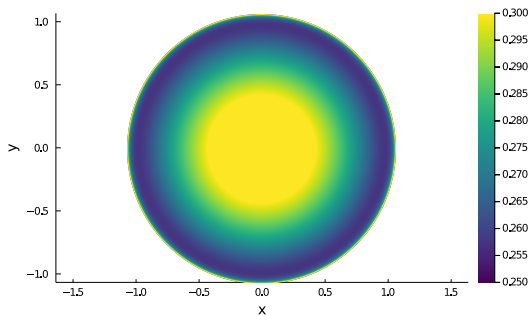


Equilibrium distribution $(\alpha, \beta) = (2, 1.5)$ [2].



Equilib. distribution $(\alpha, \beta) = (3.5, 1.6)$ [2].

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



The radially symmetric equilibrium distribution $\rho(\mathbf{x})$ for $\alpha = 1.2$, $\beta = 0.1993$ in $d = 2$ dimensions, obtained using a spectral method [1].

- ▶ Establish theory behind spectral methods in the Jacobi basis.
- ▶ Use kernel expansions to construct an equilibrium measure method on $[-1, 1]$.
- ▶ Numerically solve for $\rho(\mathbf{x})$ using a fully implemented spectral solver².
- ▶ 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: Considering external potentials $V(\mathbf{x})$.
- ▶ Optionally: Extending to l-Morse potentials $K(r) = C_1 e^{r/l_1} - C_2 e^{r/l_2}$.

²This 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](https://doi.org/10.1007/s00365-022-09606-0). eprint: [2109.00843](https://arxiv.org/abs/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](https://doi.org/10.1090/mcom/3740). eprint: [2011.00045](https://arxiv.org/abs/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*. <http://dlmf.nist.gov>. Dec. 2018. (Visited on 11/11/2020).