

# General Kernel Spectral Methods for Equilibrium Measures

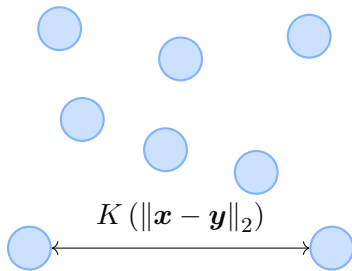
## An MMSC Dissertation Project



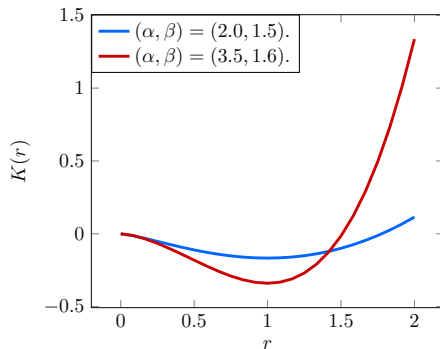
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- Find the Equilibrium Distribution  $\rho(\mathbf{x})$  of a Many-Particle-System.



$N = 8$  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  $\alpha, \beta$ .

- Interactions through (power-law) Attraction-Repulsion Potentials<sup>1</sup>

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

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

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



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

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

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

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

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

- ▶ 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  $\rho$ , 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 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

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

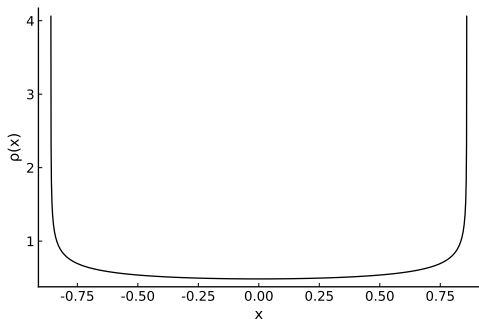
so they satisfy

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

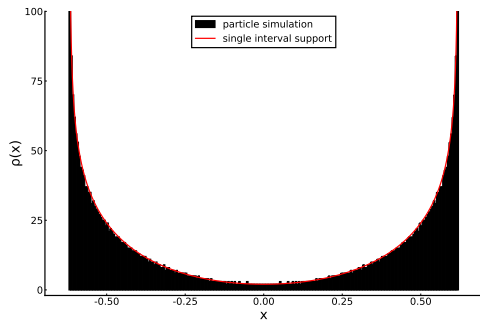
with  $a, b > -1$ , which uniquely determines  $P_n^{(a,b)}(x)$ . The special case of  $a = b$  corresponds to the ultraspherical or Gegenbauer polynomials, while the case  $a = b = 0$  corresponds to the Legendre polynomials [3].

► 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).



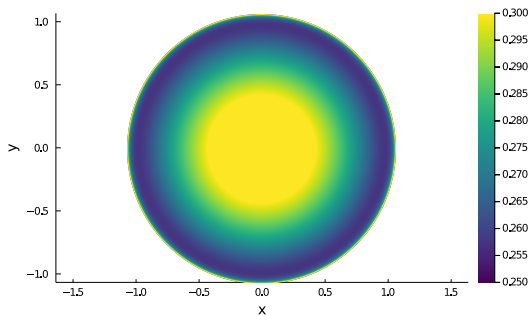
Equilibrium distribution  $(\alpha, \beta) = (2, 1.5)$  [1].



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



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 [2].

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  $\rho(\mathbf{x})$  using a fully implemented spectral solver<sup>2</sup>.
- ▶ 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  $V(\mathbf{x})$ .
- ▶ Optionally: Extending to l-Morse potentials  $K(r) = C_1 e^{r/l_1} - C_2 e^{r/l_2}$ .

<sup>2</sup>This is the first numerical method for particle distribution problems!

Questions?

- [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](https://doi.org/10.1090/mcom/3740). eprint: [2011.00045](https://arxiv.org/abs/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](https://doi.org/10.1007/s00365-022-09606-0). eprint: [2109.00843](https://arxiv.org/abs/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](https://doi.org/10.1017/S0956792514000126).