General Kernel Spectral Methods for Equilibrium Measures

MMSC Dissertation

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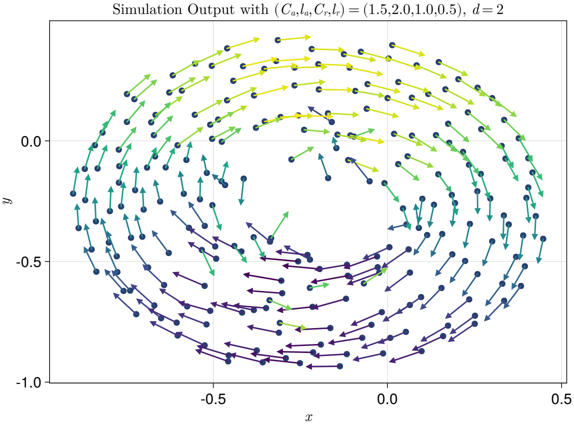

Figure: $N_p = 120$ particles in $d = 2$ dimensions. Morse potential, friction and self-propulsion terms are as given in [1], this figure reproduces their results.

Definition (Equilibrium Measure)

For a given pairwise interaction potential $K : \mathbb{R} \to \mathbb{R}$, the equilibrium measure $\hat{\rho} : D \to \mathbb{R}$ with $D \subseteq \mathbb{R}^d$ is a measure chosen such that

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

is minimised, where $\mathrm{d}\hat{\rho} = \hat{\rho}(\hat{\boldsymbol{x}})\mathrm{d}\hat{\boldsymbol{x}}$.

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is minimised, where $\mathrm{d}\hat{\rho} = \hat{\rho}(\hat{\boldsymbol{x}})\mathrm{d}\hat{\boldsymbol{x}}$.

For example: in a two-particle system, $\hat{\rho}(\hat{\boldsymbol{x}}) = \delta(\hat{\boldsymbol{x}} - \hat{\boldsymbol{p}}_{\mathbf{1}}) + \delta(\hat{\boldsymbol{x}} - \hat{\boldsymbol{p}}_{\mathbf{2}})$ to see that $U_K[\hat{\rho}] = K(0) + K(\|\hat{\boldsymbol{p}}_{\mathbf{1}} - \hat{\boldsymbol{p}}_{\mathbf{2}}\|_2)$, and hence, the total energy becomes

$$E = \frac{m}{2}\left(\|\hat{\boldsymbol{v}}_{\mathbf{1}}\|_2^2 + \|\hat{\boldsymbol{v}}_{\mathbf{2}}\|_2^2\right) + K(0) + K(\|\hat{\boldsymbol{p}}_{\mathbf{1}} - \hat{\boldsymbol{p}}_{\mathbf{2}}\|_2).$$

Definition (Particle Density Distribution Problem)

Given an interaction kernel $K : \mathbb{R}^+ \to \mathbb{R}$, the density distribution problem is to find the equilibrium measure $\hat{\rho} : B_R(\mathbf{0}) \to \mathbb{R}$ of mass $M = 1$ on a d-dimensional ball of radius $R \in \mathbb{R}^+$ that minimises the total potential $U_K[\hat{\rho}]$.

Problem Formulation

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We then consider a spectral method with the following ansatz

$$\rho[\boldsymbol{\rho}](\boldsymbol{x}) = \rho(\boldsymbol{x}) := \left(1 - \|\boldsymbol{x}\|_2^2\right)^{m-\frac{\alpha+d}{2}} \sum_{k=0}^{N-1} \rho_k P_k^{\left(m-\frac{\alpha+d}{2}, \frac{d-2}{2}\right)}\left(2\|\boldsymbol{x}\|_2^2 - 1\right), \tag{1}$$

with $P_k^{(a,b)}$ and ρ_k the kth Jacobi polynomial and its corresponding coefficient.

Definition (Power Law Operator $\mathcal{Q}^\beta$)

The power law operator $\mathcal{Q}^\beta : \mathcal{L} \to \mathcal{L}$ is given by

$$\mathcal{Q}^\beta[\rho](\boldsymbol{x}) := \int \|\boldsymbol{x} - \boldsymbol{y}\|_2^\beta \, \mathrm{d}\rho(\boldsymbol{y}) = \int_{\mathrm{supp}(\rho)} \|\boldsymbol{x} - \boldsymbol{y}\|_2^\beta \, \rho(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} \,.$$

Applied to the ansatz given in Equation (1), we can evaluate the appearing integrals explicitly. For the attractive-repulsive interaction kernel $K_{\alpha,\beta}(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta}$, the matrix representation of the operator becomes

$$Q_{\alpha,\beta} := \frac{R^{\alpha+d}}{\alpha} Q^\alpha - \frac{R^{\beta+d}}{\beta} Q^\beta \,. \tag{2}$$

Analysis: The Attractive-Repulsive Operator

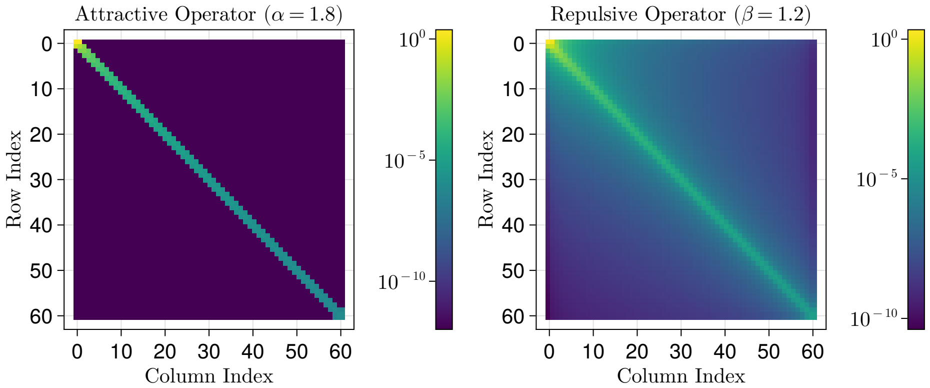

Figure: The attractive and repulsive operators (matrices), the (absolute) matrix values are shown in a $\log_{10}$ colour scale. Due to the choice of basis, the attractive operator is exactly banded.

Analysis: Comparison with Analytic Solution

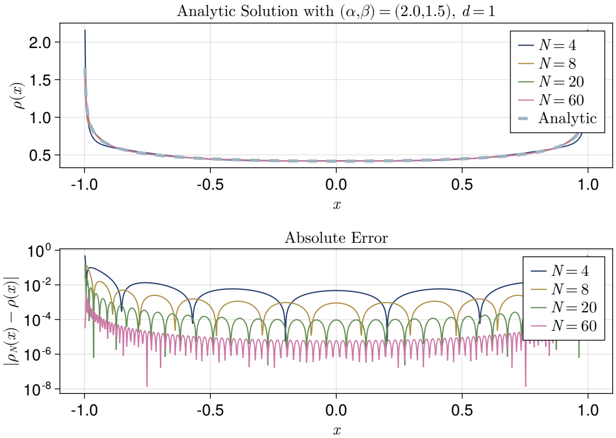

Figure: The analytical solution $\rho(x)$ compared to the (spectral method) solutions $\rho_N(x)$ of different order.

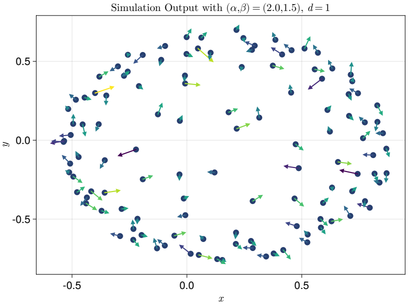

Figure: Simulation output with $N_p = 150$ particles using the same attractive-repulsive kernel $K_{\alpha,\beta}(r)$.

Results: Simulation and Solver Comparison

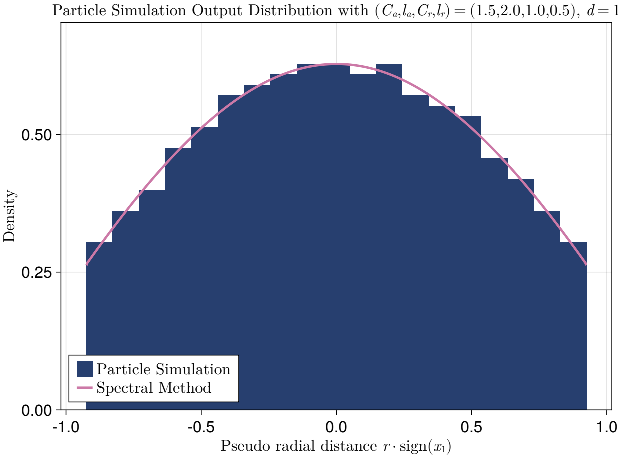

Figure: Comparison of the radial distance histogram from the simulation output with the $G = 8$ general kernel solver's equilibrium measure $\rho_{12}(r)$ at R given by th

Original Contribution: General Kernel Spectral Method

We express the general kernel as a polynomial, through reprojection from the Jacobi polynomials,

$$K_G(r) = \sum_{l=0}^{G-1} g_l r^l \approx K(r)\,, \quad \boldsymbol{g} := (g_0, \ldots, g_{G-1})^T \in \mathbb{R}^G\,. \tag{3}$$

The operator can then be expressed as

$$\mathcal{Q}_G[\hat{\rho}](\hat{\boldsymbol{x}}) = \int_{B_R(\boldsymbol{0})} \sum_{l=0}^{G-1} g_l \left\|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}\right\|_2^l \hat{\rho}(\hat{\boldsymbol{y}})\,\mathrm{d}\hat{\boldsymbol{y}} = \sum_{l=0}^{G-1} g_l R^{l+d} \mathcal{Q}^l[\rho](\boldsymbol{x})\,.$$

Contributions, Challenges Faced & Future Work

Contributions:

- An original implementation.
- General kernel spectral method + implementation.
- Lemma for initial guess of R.

Challenges:

- Synchronisation of simulator and solver.

Future Work:

- Describing phase-space distributions in a self-propulsion setup.

Thank you.

Bibliography I

[1] M. R. D'Orsogna, Y. L. Chuang, A. L. Bertozzi and L. S. Chayes. 'Self-Propelled Particles with Soft-Core Interactions: Patterns, Stability, and Collapse'. In: *Phys. Rev. Lett.* 96.10 (Mar. 2006), p. 104302. ISSN: 1079-7114. DOI: 10.1103/PhysRevLett.96.104302.