PDE Workshop in Stability Analysis for Nonlinear PDEs

18th August 2022

Computing power law equilibrium measures

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Talk structure

1. Banded spectral methods

2. Computing power law equilibrium measures

3. Numerical experiments

Core idea of spectral methods

Obtain numerical solutions to mathematical problems by approximating functions in simpler basis function spaces.

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approximate

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Obtain **numerical** solutions to **mathematical problems** by approximating functions in **simpler** basis function spaces.

- Monomials $\{x^0, x^1, x^2, \dots\}$
- Fourier series $\{e^{i2\pi nx/P}\}$
- Orthogonal Polynomials ⟵

in 1D: e.g. Jacobi, Hermite, Laguerre

in 2D: e.g. Proriol (◣), Zernike (●)

A primer on sparse spectral methods

A set of polynomials $P_n(x)$ is orthogonal w.r.t. a weight $w(x)$ if

$$\int_\Omega w(x) P_n(x) P_m(x) \mathrm{d}x = c_{n,m} \delta_n^m$$

We can then expand sufficiently well-behaved functions

$$f(x) = \sum_{n=0}^{\infty} P_n(x) f_n = \mathbf{P}(x)^\mathsf{T} \mathbf{f}$$

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$$f(x) = \sum_{n=0}^{\infty} P_n(x) f_n = \mathbf{P}(x)^\top \mathbf{f}$$

$$\mathbf{P}(x) := \begin{pmatrix} P_0(x) \\ P_1(x) \\ \vdots \end{pmatrix}, \quad \mathbf{f} := \begin{pmatrix} f_0 \\ f_1 \\ \vdots \end{pmatrix}$$

Banded sparse operators via orthogonal polynomials

Multiplication operators can be defined using **recurrence relations** of the orthogonal polynomial basis of choice:

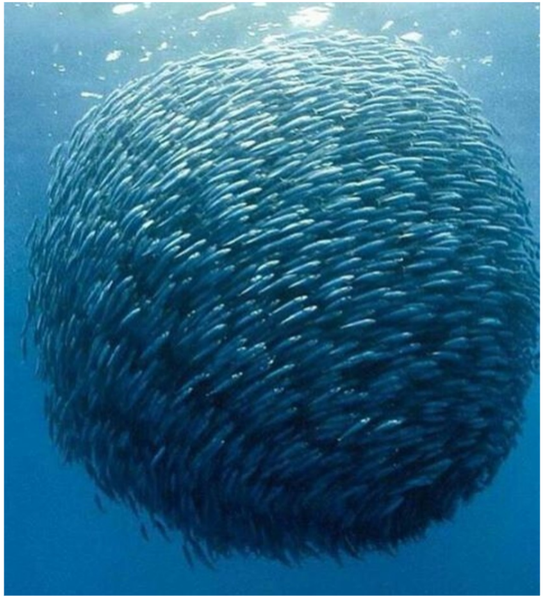
$$P_{n+1}(x) = (A_n x + B_n)P_n(x) - C_n P_{n-1}(x)$$

$$\mathbf{P}(x)^{\mathsf{T}}\mathrm{X}\mathbf{f} = x f(x)$$

And similarly for integration, differentiation and other operators.

Olver, S., Slevinsky, R.M., & Townsend, A. (2020). Fast algorithms using orthogonal polynomials. Acta Numerica.

Motivating power law equilibrium measures (I)



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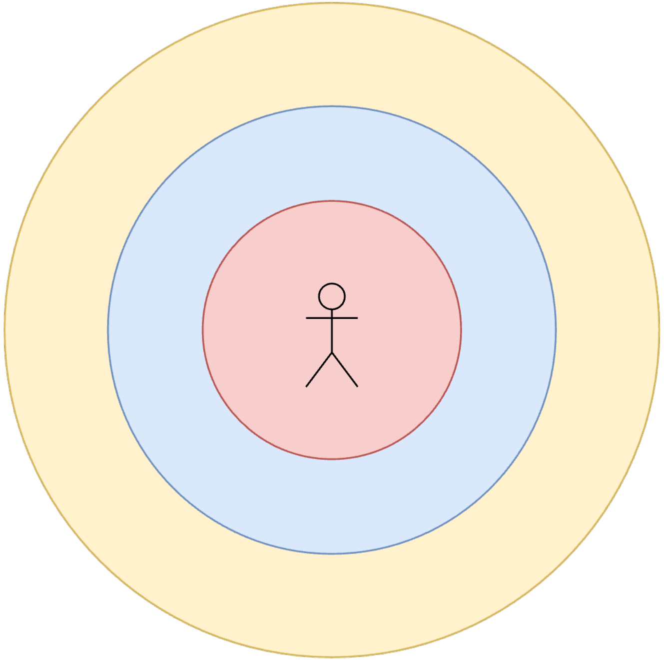

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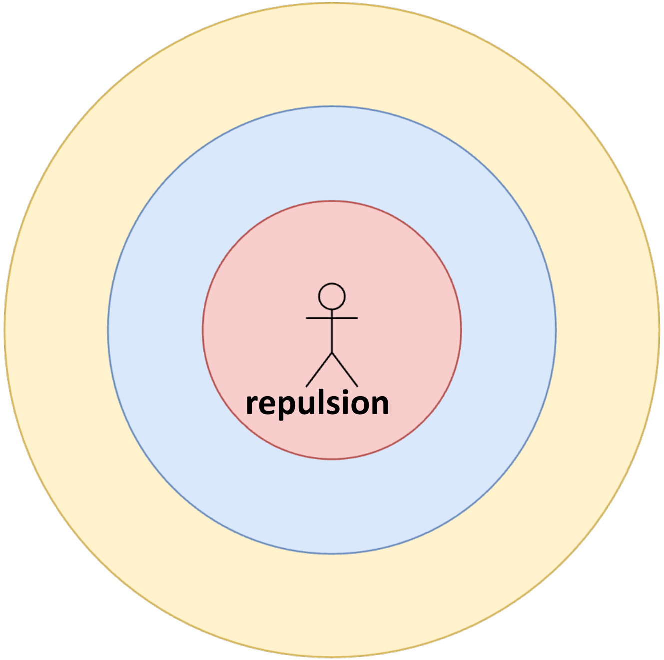

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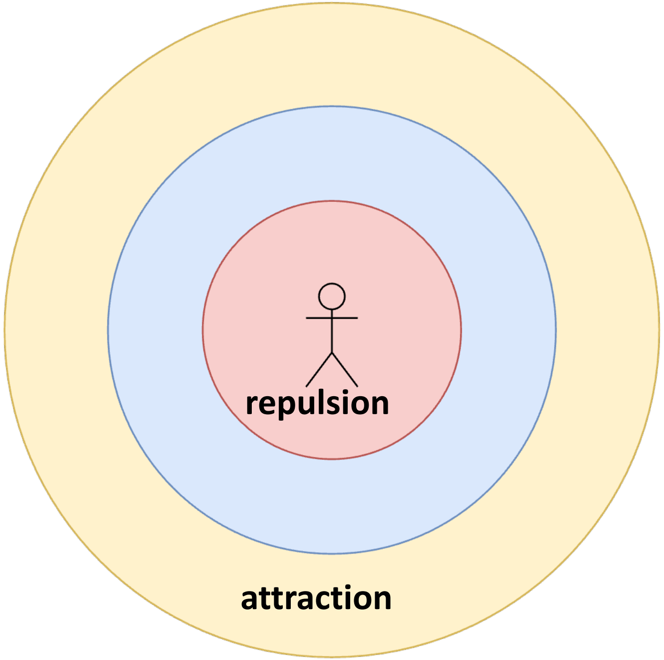

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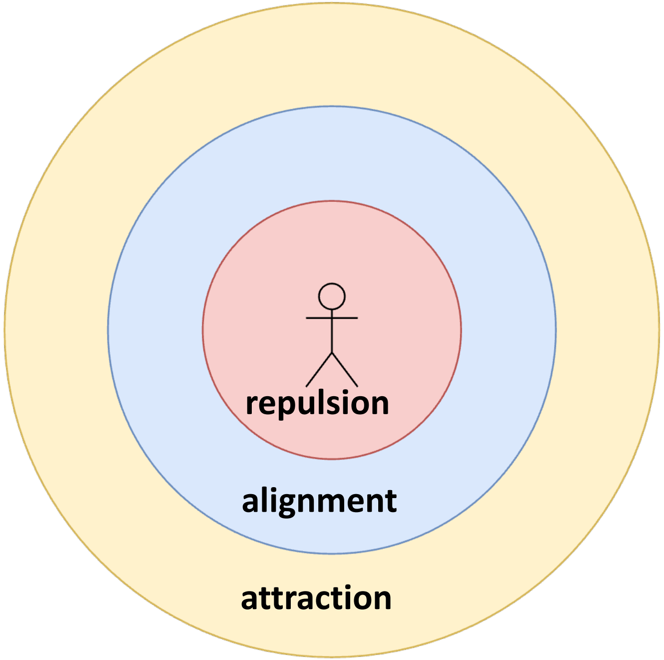

Motivating power law equilibrium measures (I)

Discrete N particle dynamics described by Newtonian dynamics:

$$\frac{\mathrm{d}^2 x_i}{\mathrm{d}t^2} = f\left(\left|\frac{\mathrm{d}x_i}{\mathrm{d}t}\right|\right)\frac{\mathrm{d}x_i}{\mathrm{d}t} - \frac{1}{N}\sum_{j\neq i}\nabla K(|x_i - x_j|)$$

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self-propulsion and friction forces

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particle acceleration

pair-wise interaction potential

Motivating power law equilibrium measures (II)

The equilibrium states of the continuous problem minimize

$$\iint K(x-y)\mathrm{d}\rho(x)\mathrm{d}\rho(y) + \int V(y)\mathrm{d}\rho(y).$$

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We consider attractive-repulsive power law kernels of the form

$$K(x,y) = \frac{1}{\alpha}|x-y|^{\alpha} - \frac{1}{\beta}|x-y|^{\beta}$$

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An Euler-Lagrange approach shows we can instead find minimizers of

$$E + V(x) = \frac{1}{\alpha}\int_{\mathrm{supp}(\rho)} |x-y|^{\alpha}\rho(y)\mathrm{d}y - \frac{1}{\beta}\int_{\mathrm{supp}(\rho)} |x-y|^{\beta}\rho(y)\mathrm{d}y.$$

Connection to fractional calculus

DEFINITION 1.2 (Fractional Laplace operator). *We define the negative fractional Laplace operator* $(-\Delta)^{\frac{\gamma}{2}}$ *for* $\gamma \in (0,2)$ *via the following singular integral*

$$(-\Delta)^{\frac{\gamma}{2}} f(x) = \frac{2^{\gamma}|\Gamma(\frac{d+\gamma}{2})|}{\pi^{\frac{d}{2}}\Gamma(-\frac{\gamma}{2})} \lim_{\epsilon \to 0^+} \int_{\mathbb{R}^d \setminus B_\epsilon} \frac{f(x)-f(y)}{|x-y|^{d+\gamma}} dy,$$

where $B_\epsilon = B(0,\epsilon)$ *denotes a ball of radius* ϵ *around the origin. Equivalently with range of validity* $\gamma \in (0,d)$ *we can write the fractional Laplacian as the inverse of the Riesz potential, thus denoted* $(-\Delta)^{-\frac{\gamma}{2}}$*:*

$$(-\Delta)^{-\frac{\gamma}{2}} f(x) = \frac{\Gamma(\frac{d-\gamma}{2})}{\pi^{\frac{d}{2}} 2^{\gamma}\Gamma(\frac{\gamma}{2})} \int_{\mathbb{R}^d} \frac{f(x-y)}{|y|^{d-\gamma}} \mathrm{d}y = \frac{\Gamma(\frac{d-\gamma}{2})}{\pi^{\frac{d}{2}} 2^{\gamma}\Gamma(\frac{\gamma}{2})} \int_{\mathbb{R}^d} \frac{f(y)}{|x-y|^{d-\gamma}} \mathrm{d}y.$$

Motivating the use of spectral methods

$$\text{If} \quad f(x) := V(x) G_{pq}^{mn}\left(\begin{matrix}\mathbf{a}\\ \mathbf{b}\end{matrix}\middle|\, |x|^2\right), \quad \text{then}$$

$$(-\Delta)^{\frac{\gamma}{2}} f(x) = 2^{\gamma} V(x) G_{p+2,q+2}^{m+1,n+1}\left(\begin{matrix}1-\frac{d+2l+\gamma}{2}, & \mathbf{a}-\frac{\gamma}{2}, & -\frac{\gamma}{2}\\ 0, & \mathbf{b}-\frac{\gamma}{2}, & 1-\frac{d+2l}{2}\end{matrix}\middle|\, |x|^2\right),$$

Dyda, B., Kuznetsov, A. & Kwaśnicki, M. Fractional *Laplace Operator and Meijer G-function*. Constr. Approx. 45, 427–448 (2017).

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$$(-\Delta)^{\frac{\gamma}{2}} f(x) = 2^\gamma V(x) G_{p+2,q+2}^{m+1,n+1}\left(\begin{matrix}1-\frac{d+2l+\gamma}{2}, & \mathbf{a}-\frac{\gamma}{2}, & -\frac{\gamma}{2}\\ 0, & \mathbf{b}-\frac{\gamma}{2}, & 1-\frac{d+2l}{2}\end{matrix}\middle| |x|^2\right),$$

If $\quad f(x) = (1-|x|^2)^{\frac{\gamma}{2}} V(x) P_n^{(\frac{\gamma}{2},\frac{d}{2}+l-1)}(2|x|^2-1), \quad$ then

$$(-\Delta)^{\frac{\gamma}{2}} f(x) = \frac{2^\gamma \Gamma(1+\frac{\gamma}{2}+n)\Gamma(\frac{d+2l+\gamma}{2}+n)}{n!\,\Gamma(\frac{d+2l}{2}+n)} V(x) P_n^{(\frac{\gamma}{2},\frac{d}{2}+l-1)}(2|x|^2-1),$$

Dyda, B., Kuznetsov, A. & Kwaśnicki, M. *Fractional Laplace Operator and Meijer G-function*. Constr. Approx. 45, 427–448 (2017).

Riesz potentials and Jacobi polynomials (I)

THEOREM 2.16. *On the d-dimensional unit ball B_1 the power law potential, with power $\alpha \in (-d, 2+2m-d)$, $m \in \mathbb{N}_0$ and $\beta > -d$, of the n-th weighted radial Jacobi polynomial*

$$(1-|y|^2)^{m-\frac{\alpha+d}{2}} P_n^{(m-\frac{\alpha+d}{2}, \frac{d-2}{2})}(2|y|^2-1)$$

reduces to a Gaussian hypergeometric function as follows:

$$\int_{B_1} |x-y|^\beta (1-|y|^2)^{m-\frac{\alpha+d}{2}} P_n^{(m-\frac{\alpha+d}{2}, \frac{d-2}{2})}(2|y|^2-1)\mathrm{d}y$$

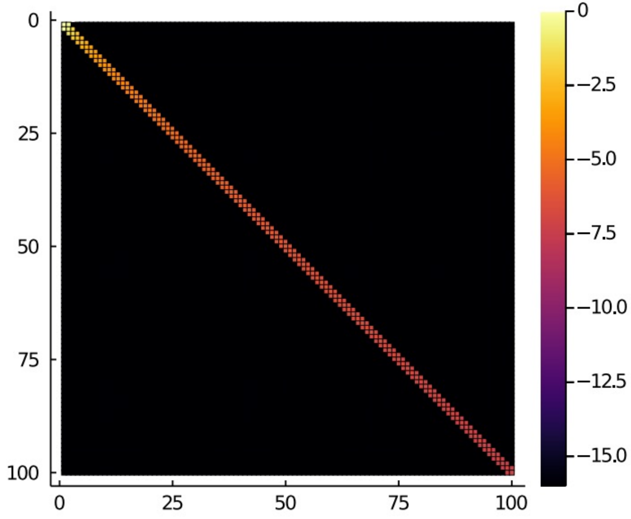
$$= \frac{\pi^{d/2}\Gamma(1+\frac{\beta}{2})\Gamma(\frac{\beta+d}{2})\Gamma(m+n-\frac{\alpha+d}{2}+1)}{\Gamma(\frac{d}{2})\Gamma(n+1)\Gamma(\frac{\beta}{2}-n+1)\Gamma(\frac{\beta-\alpha}{2}+m+n+1)} {}_2F_1\left(n-\frac{\beta}{2}, -m-n+\frac{\alpha-\beta}{2}, \frac{d}{2}, |x|^2\right).$$

Riesz potentials and Jacobi polynomials (II)

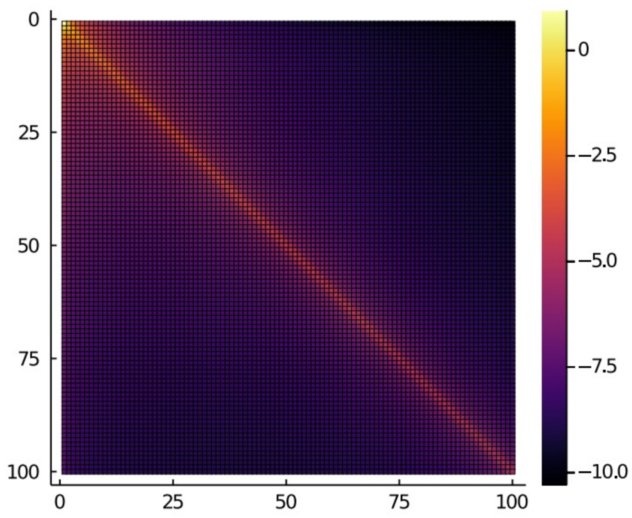
COROLLARY 2.19. *On the unit ball B_1, the power law integral of the Jacobi polynomials $P_n^{(m-\frac{\alpha+d}{2},\frac{d-2}{2})}(2|y|^2-1)$ with weight $(1-|y|^2)^{m-\frac{\alpha+d}{2}}$, $\alpha \in (-d, 2+2m-d)$ and $\beta > -d$ satisfies the following three term recurrence relationship:*

$$\int_{B_1} |x-y|^\beta (1-|y|^2)^{m-\frac{\alpha+d}{2}} P_{n+1}^{(m-\frac{\alpha+d}{2},\frac{d-2}{2})}(2|y|^2-1)\mathrm{d}y$$
$$= (\mathfrak{c}_a|x|^2+\mathfrak{c}_b)\int_{B_1} |x-y|^\beta (1-|y|^2)^{m-\frac{\alpha+d}{2}} P_{n}^{(m-\frac{\alpha+d}{2},\frac{d-2}{2})}(2|y|^2-1)\mathrm{d}y$$
$$+ \mathfrak{c}_c\int_{B_1} |x-y|^\beta (1-|y|^2)^{m-\frac{\alpha+d}{2}} P_{n-1}^{(m-\frac{\alpha+d}{2},\frac{d-2}{2})}(2|y|^2-1)\mathrm{d}y,$$

Banded and approximately banded Riesz potentials

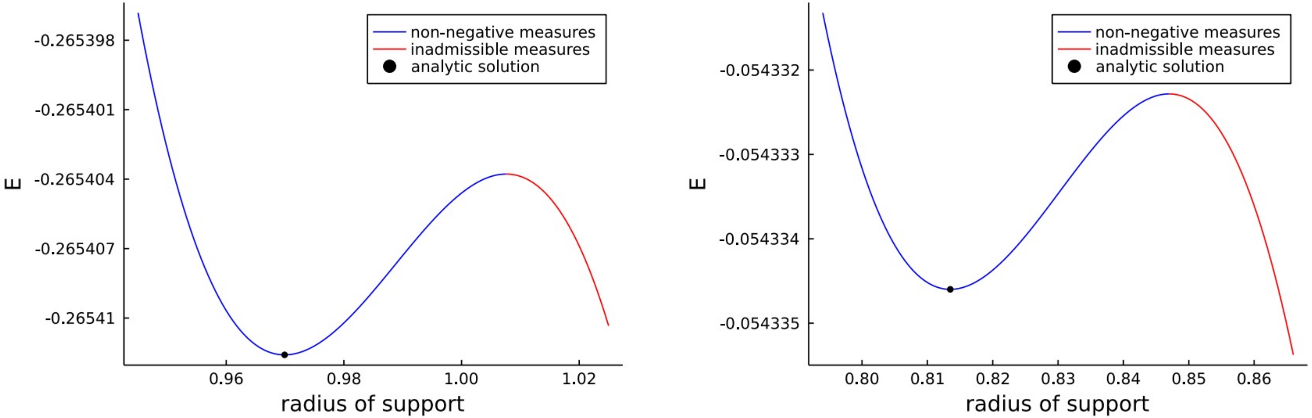


(a) α operator



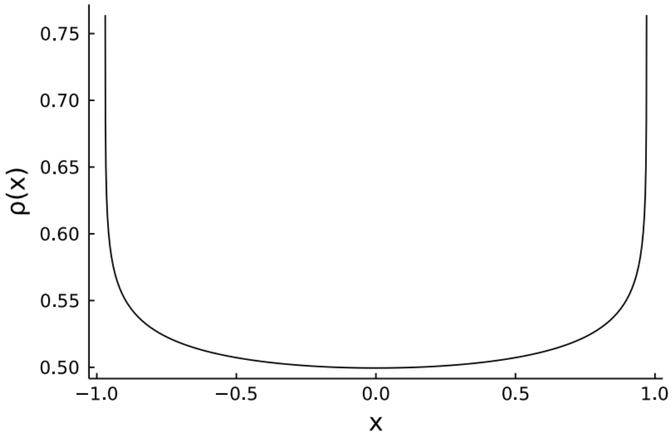
(b) β operator

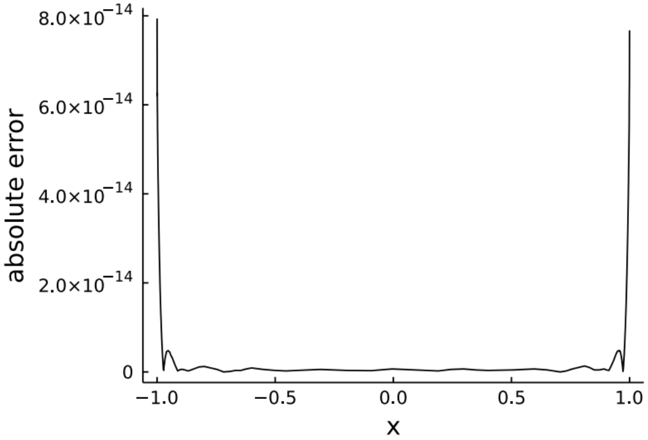
Numerical experiments (I): Verification



(a) $\beta = 1.1$ (b) $\beta = 1.68$

Numerical experiments (I): Verification





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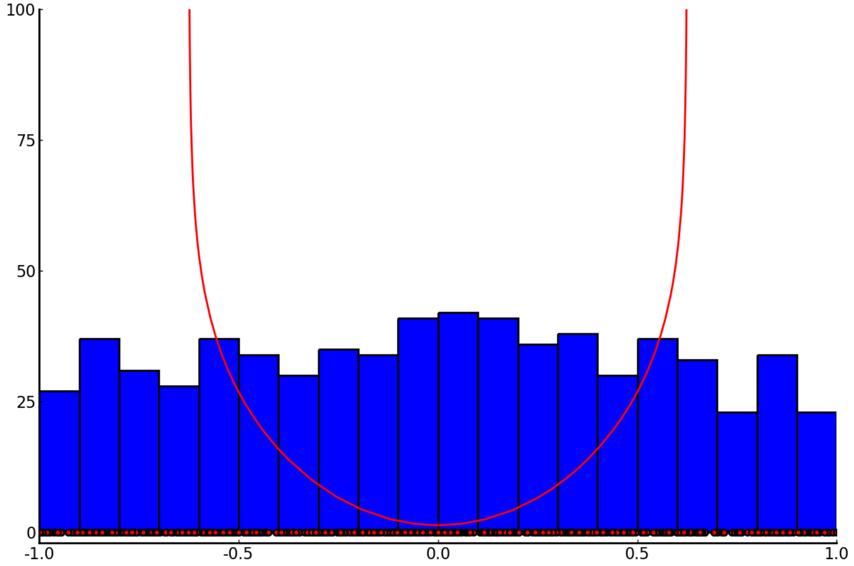

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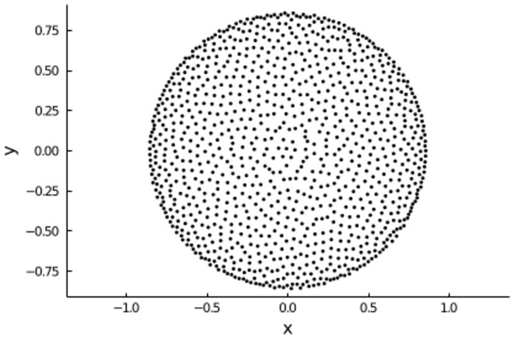
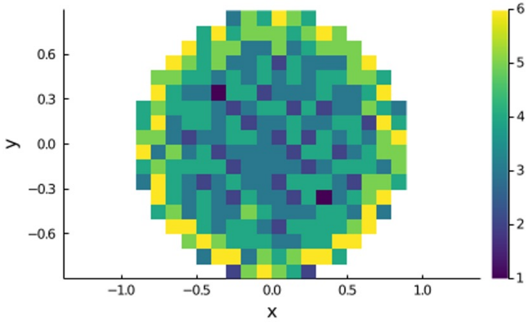
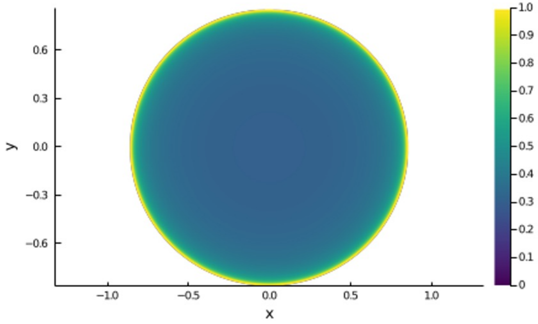


(a) $(\alpha, \beta, d) = (1.3, 1.1, 2)$

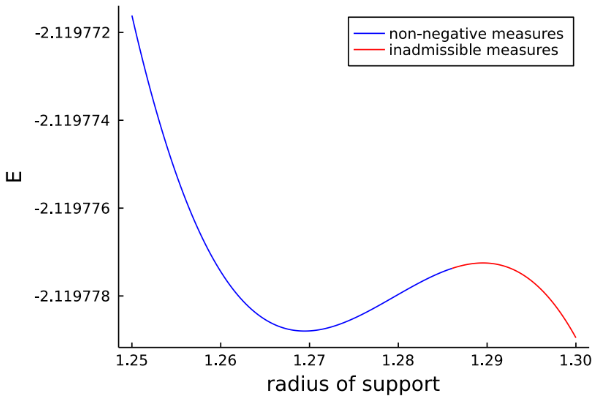


(b) 2D histogram based on (a)

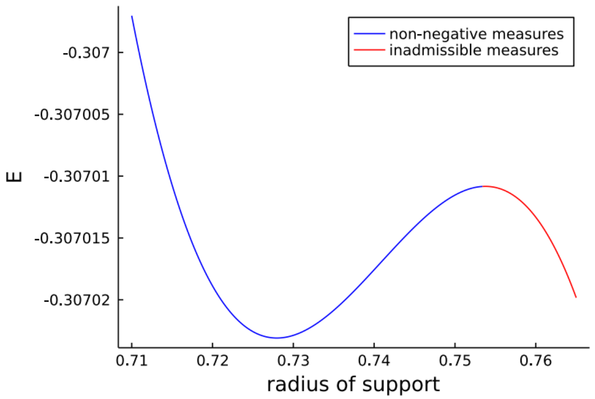


(c) computed measure

Numerical experiments (II): Uniqueness

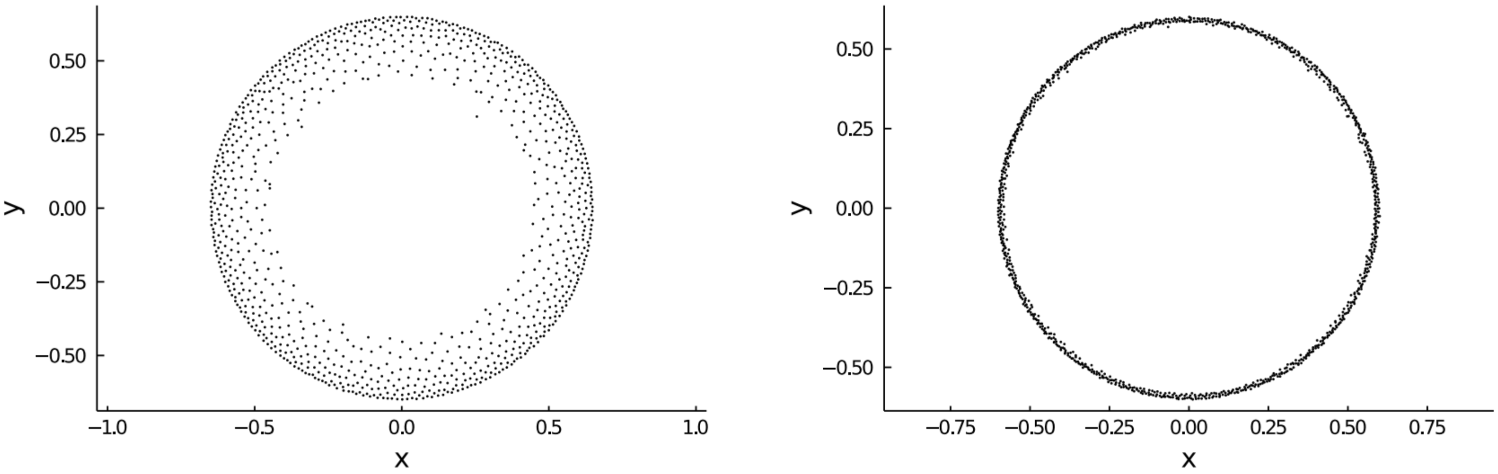


(a) $\alpha = 1.87, \beta = 0.33$



(b) $\alpha = 3.6, \beta = 1.2$

Numerical experiments (III): Gap formation boundary



(a) $\alpha = 4.18, \beta = 0.86$

(b) $\alpha = 3.88, \beta = 1.23$

Numerical experiments (III): Gap formation boundary