Mathematical Institute

Peter Julius Waldert, BSc BSc

Wolfson College

General Kernel Spectral Methods for Equilibrium Measures

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Academic Supervisors

Dr. Timon Gutleb[a]

Prof. José A. Carrillo de la Plata MA, FEurASc, FSIAM, MAE, FIMA[a]

[a]Mathematical Institute, University of Oxford

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Chapter 4

Spectral Method

In this chapter we will construct a spectral method in the basis of Jacobi polynomials to explore the solution of equilibrium distributions $\rho(\boldsymbol{x})$. Starting from a many-body system and considering the continuous limit as $N_p \to \infty$, in Chapter 2 we have already established the governing equation of the particle density distribution $\rho(\boldsymbol{x})$ in such a system.

Can we put together a numerical method to solve for the equilibrium distribution (cf. Definition 2.1)? Let us consider the problem from the bottom up and start from the solution: The basic idea behind spectral methods is to assume a solution $\rho(\boldsymbol{x})$ of the form

$$\rho(\boldsymbol{x}) = \sum_{k=0}^{N-1} \rho_k \varphi_k(\boldsymbol{x}) \,, \quad \rho_k \in \mathbb{R}, \varphi_k : \mathbb{R}^d \mapsto \mathbb{R} \,, \quad k = 0, ..., N-1 \,,$$

with N coefficients $\boldsymbol{\rho} := (\rho_0, ..., \rho_{N-1})^T$ multiplying N basis functions φ_k.

4.1 Orthogonal Polynomials forming a Basis

The following section will introduce a few necessary objects and tools to understand the basis of functions we are working with to construct the spectral method, the basis of Jacobi polynomials.

We start with the Pochhammer symbol, another name for the *rising factorial*, an unusual notation for a function but standard in the context of the special functions that will be introduced on top of it.

Definition 4.1: Rising Factorial (Pochhammer Symbol)

The nth rising factorial of $x \in \mathbb{R}$ is given by

$$(x)_n := \prod_{k=0}^{n-1} (x+k) \in \mathbb{R}\,.$$

For example, $(3.141)_5 = 3.141 \cdot 4.141 \cdot 5.141 \cdot 6.141 \cdot 7.141$.

Remark 4.1: When the argument is a nonpositive integer, the rising factorial $(-m)_n = -m \cdot (-m+1) \cdot \ldots \cdot (-m+n-1)$ vanishes when $n \geq m+1$ for $n \in \mathbb{N}$ and $m \in \mathbb{N}_0$ as 0 is among the factors.

As a second prerequisite, we introduce the closely intertwined beta- and gamma-functions.

Definition 4.2: Gamma Function

Aligning with the factorial for integer arguments, $\Gamma : \mathbb{R}^+ \mapsto \mathbb{R}$ is given by

$$\Gamma(x) := \int_0^\infty t^{x-1} \mathrm{e}^{-t} \mathrm{d}t\,.$$

Remark 4.2: When $x \in \mathbb{R}, n \in \mathbb{N}_0$ such that $x, x+n \notin \mathbb{Z}_-$ are not negative integers, there is an important relation to the gamma function (Definition 4.2),

$$(x)_n = \frac{\Gamma(x+n)}{\Gamma(x)}\,.$$

Definition 4.3: Beta Function

$B : \mathbb{R}^+ \times \mathbb{R}^+ \mapsto \mathbb{R}$ is given by

$$B(x_1, x_2) := \int_0^1 t^{x_1-1} (1-t)^{x_2-1} \mathrm{d}t\,.$$

Note that following from this definition, there is a relationship with the gamma-function

$$B(x_1, x_2) = \frac{\Gamma(x_1)\Gamma(x_2)}{\Gamma(x_1+x_2)}\,. \tag{4.1}$$

In order to efficiently construct a spectral method, we need an orthogonal basis.

Definition 4.4: Orthogonal Polynomials

Are univariate polynomials

$$p_n : \mathbb{R} \mapsto \mathbb{R},\ p_n(x) = \sum_{k=0}^{n} c_k x^k \,.$$

that form an orthogonal basis under some inner product $\langle p_n, p_m \rangle_w$ with weight function $w(x)$, given by

$$\langle f, g \rangle_w := \int_{-1}^{1} f(x)g(x)w(x)\,\mathrm{d}x \,.$$

Remark 4.3: The inner product satisfies $\langle x \mapsto xf(x), g \rangle_w = \langle f, x \mapsto xg(x) \rangle_w$.

Theorem 4.1: Three-Term Recurrence Relationship

All orthogonal polynomials $\{p_0, p_1, p_2, ...\}$ (cf. Definition 4.4) have (at least) a three-term recurrence relationship of the form

$$A_n p_{n+1}(x) = B_n p_n(x) + C_n p_{n-1}(x) \,.$$

Proof. Consider "xp_n":$= x \mapsto xp_n(x)$, a polynomial with $\deg(xp_n) \leq n + 1$. By the linear independence of all orthogonal polynomials p_n with respect to the inner product $\langle \cdot, \cdot \rangle_w$, it must be possible to write

$$xp_n(x) = \sum_{k=0}^{n+1} \hat{a}_k p_k(x) \,, \quad \text{for some } \hat{a}_k \in \mathbb{R}, k = 0, ..., n+1 \,.$$

Now, for all $n \geq 0$ and $m \leq n + 1$ we have

$$\langle xp_n, p_m \rangle_w = \sum_{k=0}^{n+1} \hat{a}_k \langle p_k, p_m \rangle_w = \sum_{k=0}^{n+1} \hat{a}_k \delta_{i,k} = \hat{a}_m \langle p_m, p_m \rangle_w \,,$$

due to the orthogonality relationship (Theorem 4.2). Therefore,

$$\hat{a}_m = \frac{\langle xp_n, p_m \rangle_w}{\langle p_m, p_m \rangle_w} \quad \text{for all } m \leq n + 1 \,. \tag{4.2}$$

But when $\underline{m < n - 1}$, we have $\deg(xp_m) < n$ so $xp_m(x) = \sum_{k=0}^{n-1} \hat{b}_k p_k(x)$ for some (potentially 0) $\hat{b}_k \in \mathbb{R}$, and therefore $\langle p_n, xp_m \rangle_w = \sum_{k=0}^{n-1} \hat{b}_k \langle p_n, p_k \rangle_w = 0$, which, by the symmetry of the inner product (Remark 4.3), also implies $\langle xp_n, p_m \rangle_w = 0$ which, by Equation (4.2), allows us to conclude that the earlier coefficients $\hat{a}_m = 0$.

We recall that $xp_n(x) = \sum_{k=0}^{n+1} \hat{a}_k p_k(x)$, which in combination with our insights on the $\hat{a}_m$ above means that

$$xp_n(x) = \hat{a}_{n-1} p_{n-1}(x) + \hat{a}_n p_n(x) + \hat{a}_{n+1} p_{n+1}(x) \,,$$

concluding the proof. □

For example, for the Chebyshev polynomials (cf. Definition 4.8) we have

$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x) \,.$$

Using the Pochhammer symbol introduced in Definition 4.1, we can now define the generalised hypergeometric series ${}_pF_q$ (cf. Definition 4.5) and a special case of it, the Gaussian hypergeometric function (cf. Lemma 4.1).

Definition 4.5: Generalised Hypergeometric Series

The generalised hypergeometric series ${}_pF_q : \mathbb{R}^p \times \mathbb{R}^q \times \mathbb{C} \mapsto \mathbb{C}$ with $p, q \in \mathbb{N}$ is defined by

$${}_2F_1 \left(\begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} ; z \right) := \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_p)_k}{(b_1)_k \cdots (b_q)_k} \frac{z^k}{k!} \,,$$

where $(\cdot)_k$ denotes the rising factorial (cf. Definition 4.1).

Note that any permutation of the first (“top”) arguments $a_1, \dots, a_p$ leaves the function unchanged due to commutativity of multiplication on $\mathbb{C}$. The same holds for the second (“bottom”) arguments $b_1, \dots, b_q$.

Lemma 4.1: Gaussian Hypergeometric Function

The $p = 2$, $q = 1$ special case of the generalised hypergeometric series, commonly referred to as the Gaussian hypergeometric function, can also be evaluated by

$${}_2F_1 \left(\begin{matrix} a_1, -n \\ b_1 \end{matrix} ; z \right) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{(a_1)_k}{(b_1)_k} z^k \,,$$

when the second argument $a_2 = -n$ is a nonpositive integer, so $n \in \mathbb{N}_0$.

Proof. Starting from the definition of the generalised hypergeometric series ${}_pF_q$ with $p = 2$ and $q = 1$ (Definition 4.5),

$$ {}_2F_1\left(\begin{matrix} a_1, -n \\ b_1 \end{matrix}; z\right) = \sum_{k=0}^{\infty} \frac{(a_1)_k(-n)_k}{(b_1)_k} \frac{z^k}{k!} = \sum_{k=0}^{n} \frac{(a_1)_k(-n)_k}{(b_1)_k} \frac{z^k}{k!}\,, $$

which can be terminated at $k = n$ due to Remark 4.1, we can express

$$ \frac{(-n)_k}{k!} = \binom{-n+k-1}{k} = (-1)^k \binom{1+n-k+k-1}{k} = (-1)^k \binom{n}{k} $$

using a well-known relation between the Pochhammer symbol and the binomial coefficient which immediately leads us to

$$ {}_2F_1\left(\begin{matrix} a_1, -n \\ b_1 \end{matrix}; z\right) = \sum_{k=0}^{n} \binom{n}{k} \frac{(a_1)_k}{(b_1)_k} (-z)^k\,, $$

concluding the proof. □

Note that these functions are generally tricky to evaluate efficiently, recent advancements have enabled their usage in a broader range of applications (Michel and Stoitsov 2008; Pearson, S. Olver and Porter 2017; Slevinsky 2023). Implementations are available in the HypergeometricFunctions.jl package in Julia.

More details on the Gaussian hypergeometric series, sometimes simply referred to as the hypergeometric function, its defining differential equation origin, modular interpretations and symmetries may be found in the 1997 book *Hypergeometric Functions, My Love* (Yoshida 1997).

The Jacobi polynomials are then defined from ${}_2F_1$ as follows:

Definition 4.6: Jacobi Polynomials

Let $P^{(a,b)} : \mathbb{C} \mapsto \mathbb{C}$ with $a, b \in \mathbb{R}$ be given by

$$ P_n^{(a,b)}(x) := \frac{(a+1)_n}{n!}\, {}_2F_1\left(\begin{matrix} 1+a+b+n, -n \\ a+1 \end{matrix}; \frac{1-x}{2}\right), $$

using the Gaussian hypergeometric function (Lemma 4.1) and the Pochhammer symbol (Definition 4.1).

Following from this definition,

$$ \begin{aligned} P_0^{(a,b)}(x) &= 1 \\ P_1^{(a,b)}(x) &= (a+1) + (a+b+2)\frac{x-1}{2} \end{aligned} $$

and so on. Also note that $\deg\left(P_k^{(a,b)}\right) = k$.

Lemma 4.2: Jacobi Polynomial Series

Definition 4.6 of $P_n^{(a,b)}$ is equivalent to

$$P_n^{(a,b)}(x) = \frac{\Gamma(a+n+1)}{n!\,\Gamma(a+b+n+1)} \sum_{k=0}^{n} \binom{n}{k} \frac{\Gamma(a+b+n+k+1)}{\Gamma(a+k+1)} \left(\frac{x-1}{2}\right)^k ,$$

where $\Gamma(x)$ is the gamma function (cf. Definition 4.2).

Proof. Inserting into Lemma 4.1, we have

$$\begin{aligned} P_n^{(a,b)}(x) &= \frac{(a+1)_n}{n!} \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{(1+a+b+n)_k}{(a+1)_k} \left(\frac{1-x}{2}\right)^k \\ &= \frac{\Gamma(a+1+n)}{n!\cancel{\Gamma(a+1)}} \sum_{k=0}^{n} \binom{n}{k} \frac{\cancel{\Gamma(a+1)}\Gamma(1+a+b+n+k)}{\Gamma(a+1+k)\Gamma(1+a+b+n)} \left(\frac{x-1}{2}\right)^k \\ &= \frac{\Gamma(a+1+n)}{n!\Gamma(1+a+b+n)} \sum_{k=0}^{n} \binom{n}{k} \frac{\Gamma(1+a+b+n+k)}{\Gamma(a+1+k)} \left(\frac{x-1}{2}\right)^k \end{aligned}$$

using Remark 4.2. □

Special Cases: The Gegenbauer polynomials (cf. Definition 4.7) are a special case, namely when $a = b$. And Chebyshev Polynomials (cf. Definition 4.8) are a special case of them. In the special case when $a = b = 0$, they reduce to the Legendre polynomials $P_n(x) = P_n^{(0,0)}(x)$ F. Olver et al. 2018.

Dot-product notation. Note that in this manuscript we will use the dot-product notation

$$f(x) = \sum_{k=0}^{N-1} f_k P_k^{(a,b)}(x) \quad \Leftrightarrow \quad f(x) = \boldsymbol{f} \cdot \boldsymbol{P}^{(a,b)}(x)\,,$$

to express that a function f is a linear combination of basis polynomials with coefficients $\boldsymbol{f} = (f_0, \ldots, f_{N-1})^T \in \mathbb{R}^N$. So $\boldsymbol{P}^{(a,b)}(x) \in \mathbb{R}^N$ is the vector of Jacobi polynomials $P_0^{(a,b)}(x)$, $P_1^{(a,b)}(x)$, ..., $P_{N-1}^{(a,b)}(x)$.

Theorem 4.2: Jacobi Polynomial Orthogonality

Jacobi polynomials $P_n^{(a,b)}(x)$ are orthogonal on $[-1,1]$ with respect to 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 $P_n^{(a,b)}(x)$.

Proof. See, for example, Arora and Bajpai 1995. □

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

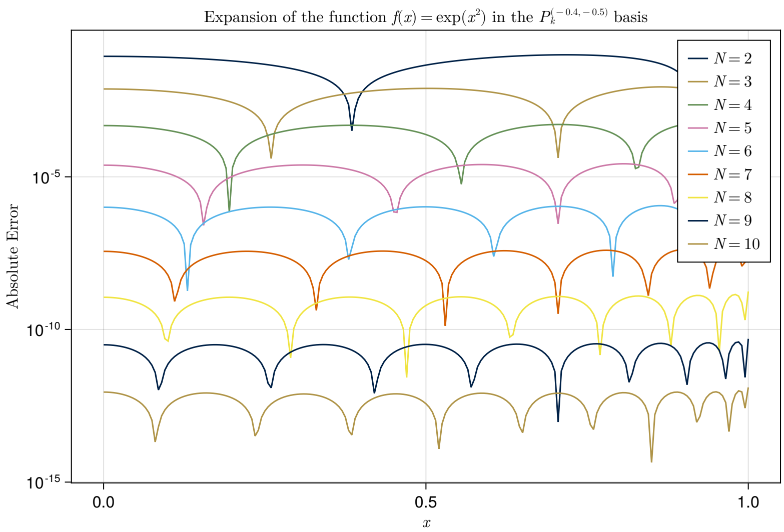

Figure 4.1: Convergence of the Jacobi polynomial expansion $f_N(x) = \sum_{k=0}^{N-1} P_k^{(a,b)}(x)$ of an example function $f(x) = \mathrm{e}^{x^2}$ with $a = -\frac{3}{4}$ and $b = -\frac{1}{2}$. Each added term improves the absolute error between the function and its expansion by a factor, so we have exponential convergence. The number of "arches" of each solution error function, occuring from the roots of $f(x) - f_N(x)$, approximately equals the order N.

Definition 4.7: Gegenbauer (Ultraspherical) Polynomials

$$C_n^{(\lambda)}(z) := \frac{(2\lambda)_n}{n!} \, {}_2F_1\left(-n, 2\lambda + n; \lambda + \frac{1}{2}; \frac{1-z}{2}\right) = \frac{(2\lambda)_n}{(\lambda + \frac{1}{2})_n} P_n^{(\lambda-1/2,\lambda-1/2)}(x)\,.$$

They satisfy a three-term recurrence relation (as all orthogonal polynomials do!)

$$\begin{aligned} C_0^{(\lambda)}(x) &= 1 \\ C_1^{(\lambda)}(x) &= 2\lambda x \\ (n+1)C_{n+1}^{(\lambda)}(x) &= 2(n+\lambda)xC_n^{(\lambda)}(x) - (n+2\lambda-1)C_{n-1}^{(\lambda)}(x). \end{aligned} \quad .$$

F. Olver et al. 2018, p. 18.9.1:

$$xC_n^{(\lambda)}(x) = \tfrac{(n+2\lambda-1)}{2(n+\lambda)}C_{n-1}^{(\lambda)}(x) + \tfrac{n+1}{2(n+\lambda)}C_{n+1}^{(\lambda)}(x). \tag{4.3}$$

From Wikipedia: In spectral methods for solving differential equations, if a function is expanded in the basis of Chebyshev polynomials and its derivative is represented in a Gegenbauer/ultraspherical basis, then the derivative operator becomes a diagonal matrix, leading to fast banded matrix methods for large problems (S. Olver and Townsend 2013).

Are a special case of the Jacobi Polynomials (cf. Definition 4.6) and form an Orthonormal Basis under the weight given by

$$w(x) = (1 + x)^\alpha$$

Definition 4.8: Chebyshev Polynomials

Of the first kind:

$$T_k(x)$$

Of the second kind:

$$U_k(x)$$

Also have a Three-Term Recurrence Relationship, as given below Theorem 4.1.

In order to obtain a recurrence relationship between the coefficients later, we make use of the Jacobi matrix (cf. Definition 4.9).

Definition 4.9: Jacobi Matrix

The Jacobi operator is the matrix $X \in \mathbb{R}^{N\times N}$ satisfying

$$x \cdot P(x) = P(x) \cdot X^T .$$

Finally, now that we have established the basis functions, we can write down an ansatz $\rho : B_1(\mathbf{0}) \mapsto \mathbb{R}$ for the solution of the problem, of the form

$$\rho(\boldsymbol{x}) := \left(1 - \|\boldsymbol{x}\|_2^2\right)^{m-\frac{\alpha+d}{2}} \sum_{k=0}^{N-1} \rho_k P_k^{\left(m-\frac{\alpha+d}{2},\frac{d-2}{2}\right)}(2\,\|\boldsymbol{x}\|_2^2 - 1)\,. \tag{4.4}$$

with $P_k^{(a,b)}$ the Jacobi polynomials and $\{\rho_k\}_{k=0,\ldots,N-1}$ the coefficients.

The spectral method can then be written as a linear system involving a matrix (operator).

Definition 4.10: Operator

Either the attractive or the repulsive operator can be sparse.
Obtained using Theorem 4.3.

$(-\Delta)^{-s}$ denotes the inverse fractional Laplacian $\Delta := \nabla^2$ with power $s \in (0,1)$.

The fractional Laplacian $(-\Delta)^{-s}$ is given by the Riesz potential Kwaśnicki 2017.

Definition 4.11: Riesz Potential

For a given function $u : \mathbb{R}^d \mapsto \mathbb{R}$ and $\gamma \in \mathbb{R}$, its *Riesz potential* $I_\gamma[u]$ is given by

$$I_\gamma[u](\boldsymbol{x}) := \frac{2^{-\gamma}\Gamma(\frac{d-\gamma}{2})}{\pi^{d/2}\Gamma(\gamma/2)} \int_{\mathbb{R}^d} \frac{u(\boldsymbol{z})}{\|\boldsymbol{x}-\boldsymbol{z}\|_2^{d-\gamma}} \mathrm{d}\boldsymbol{z}\,.$$

Theorem 4.3: Power-law Potential of the nth Jacobi Polynomial

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

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

reduces to a Gaussian hypergeometric function as follows:

$$\int_{B_1(\mathbf{0})} \|\boldsymbol{x}-\boldsymbol{y}\|_2^\beta \left(1-\|\boldsymbol{y}\|_2^2\right)^{m-\frac{\alpha+d}{2}} P_n^{\left(m-\frac{\alpha+d}{2}, \frac{d-2}{2}\right)} \left(2\|\boldsymbol{y}\|_2^2-1\right) \mathrm{d}\boldsymbol{y}$$
$$= \frac{\pi^{d/2}\Gamma\left(1+\frac{\beta}{2}\right)\Gamma\left(\frac{\beta+d}{2}\right)\Gamma\left(m+n-\frac{\alpha+d}{2}+1\right)}{\Gamma\left(\frac{d}{2}\right)\Gamma(n+1)\Gamma\left(\frac{\beta}{2}-n+1\right)\Gamma\left(\frac{\beta-\alpha}{2}+m+n+1\right)} {}_2F_1\left(\begin{matrix} n-\frac{\beta}{2}, -m-n+\frac{\alpha-\beta}{2} \\ \frac{d}{2} \end{matrix}; \|\boldsymbol{x}\|_2^2\right).$$

Proof (adapted from Gutleb, Carrillo and S. Olver 2022). We begin by applying Lemma 4.2 to the inside of the integrand.

$$\begin{aligned} I &:= \int_{B_1(\mathbf{0})} \|\boldsymbol{x}-\boldsymbol{y}\|_2^\beta \left(1-\|\boldsymbol{y}\|_2^2\right)^a P_n^{(a,b)} \left(2\|\boldsymbol{y}\|_2^2-1\right) \mathrm{d}\boldsymbol{y} \\ &= C_{a,b,n} \sum_{k=0}^n \binom{n}{k} C_{a,b,n,k} \int_{B_1(\mathbf{0})} \|\boldsymbol{x}-\boldsymbol{y}\|_2^\beta \left(1-\|\boldsymbol{y}\|_2^2\right)^a \left(\|\boldsymbol{y}\|_2^2-1\right)^k \mathrm{d}\boldsymbol{y} \\ &= C_{a,b,n} \sum_{k=0}^n \binom{n}{k} C_{a,b,n,k} (-1)^k \int_{B_1(\mathbf{0})} \|\boldsymbol{x}-\boldsymbol{y}\|_2^\beta \left(1-\|\boldsymbol{y}\|_2^2\right)^{a+k} \mathrm{d}\boldsymbol{y} \end{aligned}$$

where $a := m - \frac{\alpha+d}{2}$ and $b := \frac{d-2}{2}$. Note that from the first to the second line, we used $\frac{z-1}{2} = \frac{2\|\boldsymbol{y}\|_2^2-1-1}{2} = \|\boldsymbol{y}\|_2^2 - 1$.

The constants are

$$\begin{aligned} C_{a,b,n} &:= \frac{\Gamma(a+1+n)}{n!\Gamma(1+a+b+n)} \\ C_{a,b,n,k} &:= \frac{\Gamma(1+a+b+n+k)}{\Gamma(a+1+k)}. \end{aligned}$$

We identify the remaining integral as the Riesz potential $I_{\beta+d}[u](\boldsymbol{x})$ of the function $u(\boldsymbol{y}) := \left(1-\|\boldsymbol{y}\|_2^2\right)^{a+k}$, which we can evaluate using Lemma 2.4 from Biler, Imbert and Karch 2011:

$$\begin{aligned}\int_{B_1(\mathbf{0})} \|\boldsymbol{x}-\boldsymbol{y}\|_2^\beta \left(1-\|\boldsymbol{y}\|_2^2\right)^{a+k} \mathrm{d}\boldsymbol{y} &= c_{\beta+d} I_{\beta+d}\left[\boldsymbol{y}\mapsto \left(1-\|\boldsymbol{y}\|_2^2\right)^{a+k}\right](\boldsymbol{x}) \\ &= c_{\beta+d} C_{a+k,\beta,d}\cdot {}_2F_1\left(\begin{matrix}\frac{d-(\beta+d)}{2}, -a-k-\frac{\beta+d}{2} \\ d/2\end{matrix}; \|\boldsymbol{x}\|_2^2\right) \\ &= c_{\beta+d} C_{a+k,\beta,d}\cdot {}_2F_1\left(\begin{matrix}-\beta/2, -m-k+\frac{\alpha-\beta}{2} \\ d/2\end{matrix}; \|\boldsymbol{x}\|_2^2\right),\end{aligned}$$

as $-a-k-\frac{\beta+d}{2} = -m+\frac{\alpha+d}{2}-k-\frac{\beta+d}{2} = -m-k+\frac{\alpha-\beta}{2}$ with constants

$$\begin{aligned} c_{\beta+d} &:= \frac{2^{\beta+d}\pi^{d/2}\Gamma\left(\frac{\beta+d}{2}\right)}{\Gamma(-\beta/2)} && \text{from aforementioned definition of the Riesz potential} \\ C_{a+k,\beta,d} &:= \frac{\Gamma(a+k+1)\Gamma(-\beta/2)}{2^{\beta+d}\Gamma(d/2)\Gamma\left(a+k+\frac{\beta+d}{2}+1\right)} && \text{from Lemma 2.4}, \end{aligned}$$

and therefore

$$c_{\beta+d}C_{a+k,\beta,d} = \frac{\cancel{2^{\beta+d}}\pi^{d/2}\Gamma\left(\frac{\beta+d}{2}\right)\Gamma(a+k+1)\cancel{\Gamma(-\beta/2)}}{\cancel{\Gamma(-\beta/2)}\cancel{2^{\beta+d}}\Gamma(d/2)\Gamma\left(a+k+\frac{\beta+d}{2}+1\right)} = \frac{\pi^{d/2}B\left(\frac{\beta+d}{2}, a+k+1\right)}{\Gamma(d/2)},$$

using Equation (4.1). So that finally,

$$\begin{aligned}&\int_{B_1(\mathbf{0})} \|\boldsymbol{x}-\boldsymbol{y}\|_2^\beta \left(1-\|\boldsymbol{y}\|_2^2\right)^{a+k} \mathrm{d}\boldsymbol{y} \\ &\quad = \frac{\pi^{d/2}}{\Gamma(d/2)} B\left(\tfrac{\beta+d}{2}, m-\tfrac{\alpha+d}{2}+k+1\right)\cdot {}_2F_1\left(\begin{matrix}-\beta/2, -m-k+\frac{\alpha-\beta}{2} \\ d/2\end{matrix}; \|\boldsymbol{x}\|_2^2\right).\end{aligned}$$

Plugging this back into the original form above, carrying along the same parameters,

$$I = C_{a,b,n}\sum_{k=0}^{n}\binom{n}{k} C_{a,b,n,k}(-1)^k \frac{\pi^{d/2}}{\Gamma(d/2)} B(\cdot,\cdot)\,{}_2F_1\left(\dots;\|\boldsymbol{x}\|_2^2\right)$$

we can apply Equation (2.1) in Gutleb, Carrillo and S. Olver 2022 after some algebra, the special case of an identity given in Prudnikov et al. 1986 to obtain a ${}_3F_2$ (three terms in the numerator, two in the denominator) function

$$I \propto {}_3F_2\left(\begin{matrix}-\beta/2, n-\beta/2, -m-n+\frac{\alpha-\beta}{2} \\ d/2, -\beta/2\end{matrix}; \|\boldsymbol{x}\|_2^2\right),$$

which we expand into its definition Definition 4.5 to see that two terms cancel:

$$I \propto \sum_{k=0}^{\infty} \frac{\cancel{(-\beta/2)_k}, (n-\beta/2)_k, \left(-m-n+\frac{\alpha-\beta}{2}\right)_k}{(d/2)_k\cancel{(-\beta/2)_k}} \frac{\|\boldsymbol{x}\|_2^{2k}}{k!},$$

which results back in a ${}_2F_1$ function (two terms in the numerator, one in the denominator), the so-called Gaussian hypergeometric function, cf. Lemma 4.1, and after combining $C_{a,b,n}$, $C_{a,b,n,k}$, $\frac{\pi^{d/2}}{\Gamma(d/2)}$ with the gamma-function expansion of $B\left(\frac{\beta+d}{2}, m-\frac{\alpha+d}{2}+k+1\right)$ according to Equation (4.1), and cancelling terms, one finally obtains

$$I = \frac{\pi^{d/2}\Gamma\left(1+\frac{\beta}{2}\right)\Gamma\left(\frac{\beta+d}{2}\right)\Gamma\left(m+n-\frac{\alpha+d}{2}+1\right)}{\Gamma\left(\frac{d}{2}\right)\Gamma(n+1)\Gamma\left(\frac{\beta}{2}-n+1\right)\Gamma\left(\frac{\beta-\alpha}{2}+m+n+1\right)}\,{}_2F_1\left(\begin{matrix} n-\frac{\beta}{2}, -m-n+\frac{\alpha-\beta}{2} \\ \frac{d}{2}\end{matrix}; \|\boldsymbol{x}\|_2^2\right),$$

concluding the proof. □

Lemma 2.4 from Biler, Imbert and Karch 2011; Magnus et al. 1967 is based on the *Weber-Schafheitlin* integral of two Bessel functions given in Milne-Thomson 1945. The Weber-Schafheitlin integrals are related to the fractional Laplacians of aforementioned functions because the Fourier transform of ${}_2F_1$ is a Bessel function. For a more generalised version of Lemma 2.4, see Huang 2014.

Theorem 4.3 gives an explicit expression for the main integral $\hat{Q}^\beta : L \mapsto L$, an operator from the function space L to the function space L, we are interested in:

$$\hat{Q}^\beta[\rho](x) = \sum_{k=0}^{N-1} \rho_k \int_{B_1} |x-y|^\beta (1-|y|^2)^{m-\frac{\alpha+d}{2}} P_n^{(m-\frac{\alpha+d}{2}, \frac{d-2}{2})}(2|y|^2-1)\mathrm{d}y$$

which is used to construct the spectral method operator Q^β (cf. Definition 4.10), acting on the coefficients $\boldsymbol{\rho}$.

The operator $\hat{Q}^\beta$ acting on an equilibrium measure $\rho(\boldsymbol{x})$ returns the energy $\tilde{E}(\boldsymbol{x}) = \hat{Q}^\beta[\rho](\boldsymbol{x})$ at a point $\boldsymbol{x} \in B_1(\mathbf{0})$ in our domain.

Lemma 4.3: Mass of the Solution

For a given solution $\rho : B_1(\mathbf{0}) \mapsto \mathbb{R}$, its *mass* $M \in \mathbb{R}$ is given by Equation (2.6). Provided the appropriate ansatz given in Equation (4.4), an expansion of weighted radial Jacobi polynomials with coefficients ρ_k, its *mass* is given by

$$M := \int_{\mathrm{supp}(\rho)} \rho(y)\,\mathrm{d}y = \frac{\pi^{d/2}\Gamma(a+1)}{\Gamma(a+d/2+1)}\rho_0\,,$$

so solely depending on the first coefficient ρ_0.

Proof (adapted from Gutleb, Carrillo and S. Olver 2022). To shorten notation, let $b := \frac{d-2}{2}$. The domain and radial symmetry of our problem suggests the use of hyperspherical coordinates:

$$
\begin{aligned}
M = \int_{B_1(\mathbf{0})} \rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} &= \sum_{k=0}^{N-1} \rho_k \int_{B_1(\mathbf{0})} \left(1 - \|\boldsymbol{x}\|_2^2\right)^a P_k^{(a,b)}(2\,\|\boldsymbol{x}\|_2^2 - 1)\,\mathrm{d}\boldsymbol{x} \\
&= \sum_{k=0}^{N-1} \rho_k \int_{\partial B_1(\mathbf{0})} \mathrm{d}\Omega \int_{r=0}^{1} (1-r^2)^a P_k^{(a,b)}(2r^2-1) r^{d-1}\,\mathrm{d}r \\
&= \Omega_d \sum_{k=0}^{N-1} \rho_k \int_{r=0}^{1} (1-r^2)^a P_k^{(a,b)}(2r^2-1) r^{d-1}\,\mathrm{d}r\,,
\end{aligned}
$$

where $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface area of the d-dimensional hypersphere (cf. Lemma 4.4) with radius $R = 1$. Substituting $u := 2r^2 - 1$, therefore $r^2 = \frac{1+u}{2}$ and $(1-r^2)^a = \left(\frac{1-u}{2}\right)^a = 2^{-a}(1-u)^a$ as well as $\mathrm{d}r = \frac{\mathrm{d}u}{4r}$,

$$
\begin{aligned}
M &= 2^{-a}\Omega_d \sum_{k=0}^{N-1} \rho_k \int_{u=-1}^{1} (1-u)^a P_k^{(a,b)}(u) r^{d-1} \frac{\mathrm{d}u}{4r} \\
&= 2^{-2}2^{-a}\Omega_d \sum_{k=0}^{N-1} \rho_k \int_{-1}^{1} (1-u)^a P_k^{(a,b)}(u) r^{d-2}\,\mathrm{d}u\,,
\end{aligned}
$$

we notice that $r^{d-2} = \left(\frac{1+u}{2}\right)^{\frac{d-2}{2}} = 2^{-b}(1+u)^b$ and so we have

$$
\begin{aligned}
M &= 2^{-2}2^{-a}2^{-b}\Omega_d \sum_{k=0}^{N-1} \rho_k \int_{-1}^{1} (1-u)^a (1+u)^b P_k^{(a,b)}(u)\,\mathrm{d}u \\
&= 2^{-(2+a+b)}\Omega_d \sum_{k=0}^{N-1} \rho_k \int_{-1}^{1} (1-u)^a (1+u)^b P_k^{(a,b)}(u) P_0^{(a,b)}(u)\,\mathrm{d}u \\
&= 2^{1-(2+a+b)} \frac{\pi^{d/2}}{\Gamma(d/2)} \sum_{k=0}^{N-1} \rho_k \frac{2^{a+b+1}\Gamma(a+1)\Gamma(b+1)}{0!(a+b+1)\Gamma(a+b+1)} \delta_{0,k} \\
&= \frac{\pi^{d/2}\Gamma(a+1)}{\Gamma\left(a + d/2 + 1\right)}\,\rho_0\,,
\end{aligned}
$$

which relies on the classical orthogonality condition of the Jacobi polynomials given in Theorem 4.2 with the 0th polynomial $P_0(u) = 1$. □

Lemma 4.4: Surface area of the hypersphere

The surface area of the d-dimensional hypersphere $\partial B_R(\mathbf{0})$ is given by

$$
\Omega_d(R) = \frac{\mathrm{d}}{\mathrm{d}R} V_d(R) = \frac{\mathrm{d}}{\mathrm{d}R}\left(\frac{2\pi^{d/2}}{d\Gamma(d/2)} R^d\right) = \frac{2\pi^{d/2}}{\Gamma(d/2)} R^{d-1}\,.
$$

Proof. We find Ω_d by evaluation of the d-dimensional Gaussian integral

$$I_d := \int_{\mathbb{R}^d} \mathrm{e}^{-\|\boldsymbol{x}\|_2^2} \,\mathrm{d}\boldsymbol{x} = \int_{\mathbb{R}} \mathrm{d}x_1 ... \int_{\mathbb{R}} \mathrm{d}x_d \, \mathrm{e}^{-x_1^2 - ... - x_d^2} = \left(\int_{\mathbb{R}} \mathrm{e}^{-x_1^2} \,\mathrm{d}x_1 \right)^d = (I_1)^d \,,$$

using Fubini's theorem ($I_d < \infty$). Considering the case $d = 2$, we have

$$I_2 = \int_{\mathbb{R}^2} \mathrm{e}^{-\|\boldsymbol{x}\|_2^2} \,\mathrm{d}\boldsymbol{x} = \int_0^{2\pi} \mathrm{d}\theta \int_0^{\infty} r\mathrm{e}^{-r^2} \,\mathrm{d}r = -2\pi \int_0^{-\infty} \mathrm{e}^u \frac{\mathrm{d}u}{2} = \pi \int_{-\infty}^0 \mathrm{e}^u \,\mathrm{d}u = \pi \,,$$

taking the classical approach of transitioning to polar coordinates r, θ (with Jacobi determinant r^{d-1} in the d-dimensional case) immediately leading us to $I_1 = \sqrt{\pi}$. Generalising this to higher dimensions d with hyperspherical coordinates,

$$I_d = \int_{\mathbb{R}^d} \mathrm{e}^{-\|\boldsymbol{x}\|_2^2} \,\mathrm{d}\boldsymbol{x} = \Omega_d \int_0^{\infty} r^{d-1} \mathrm{e}^{-r^2} \,\mathrm{d}r = \Omega_d \int_0^{\infty} s^{d/2-1} \mathrm{e}^{-s} \frac{\mathrm{d}s}{2} = \frac{\Omega_d}{2} \Gamma(d/2) \,,$$

where once again $r := \|\boldsymbol{x}\|_2$ and using a substitution $s := r^2$, we must find equality with the above result $I_d = \pi^{d/2}$,

$$I_d = \pi^{d/2} \overset{!}{=} \frac{1}{2} \Omega_d \Gamma(d/2) \quad \Leftrightarrow \quad \Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)} \,.$$

Now integrating over the R-ball $B_R(\mathbf{0})$, we obtain $V_d(R) := |B_R(\mathbf{0})| = \Omega_d \int_0^R r^{d-1} \,\mathrm{d}r = \frac{\mathbb{R}^d \Omega_d}{d}$ and therefore $\Omega_d(R) = \frac{\mathrm{d}V_d(R)}{\mathrm{d}R} = \frac{2\pi^{d/2}}{\Gamma(d/2)} R^{d-1}$. □

4.2 Derivation of Operator

Based on the Three-Term Recurrence Relationship (cf. Theorem 4.1).

One can even determine an explicit relationship between the coefficients in the Jacobi expansion by considering the Jacobi Matrix (cf. Definition 4.9).

Considering the operator $\hat{Q}^\beta[\rho]$ as in Theorem 4.3, from the ansatz $\rho(\boldsymbol{x})$ (cf. Equation (4.4)) we have

$$\hat{Q}^\beta(x) = \sum_{k=0}^{N-1} \rho_k \int_{B_1(\mathbf{0})} \|\boldsymbol{x} - \boldsymbol{y}\|_2^\beta \left(1 - \|\boldsymbol{y}\|_2^2\right)^a P_k^{(a,b)} \left(2 \|\boldsymbol{y}\|_2^2 - 1\right) \mathrm{d}\boldsymbol{y} \,. \tag{4.5}$$

We are now interested in a numerical representation of the operator $\hat{Q}^\beta$ acting on the function $\rho \in L^2$, so an equivalent (linear) operator $Q^\beta : \mathbb{R}^N \mapsto \mathbb{R}^N$ acting on the coefficients $\rho_k \in \mathbb{R}$, $k = 1, ..., N$. As every finite-dimensional linear operator must have a matrix representation, we are looking for a $Q^\beta \in \mathbb{R}^{N \times N}$ such that

$$\hat{Q}^\beta[\rho](\boldsymbol{x}) = \boldsymbol{P}_k^{(a,b)} \left(2 \|\boldsymbol{x}\|_2^2 - 1\right) \cdot Q^\beta \boldsymbol{\rho} \,,$$

where $\boldsymbol{P}_k^{(a,b)}\left(2\left\|\boldsymbol{x}\right\|_2^2-1\right) \in \mathbb{R}^N$ is the vector of Jacobi polynomials $P_0^{(a,b)}(x)$, $P_1^{(a,b)}(x)$, ..., $P_{N-1}^{(a,b)}(x)$ evaluated at $2\left\|\boldsymbol{x}\right\|_2^2-1$ as introduced in and after Definition 4.6.

Therefore, starting from Equation (4.5), we obtain

$$\begin{aligned}\hat{Q}^\beta[\rho](\boldsymbol{x}) &= \sum_{k=0}^{N-1} \rho_k \hat{Q}^\beta[wP_k](\boldsymbol{x}) = \sum_{k=0}^{N-1} \rho_k \sum_{j=0}^{N-1} q_{kj} P_k^{(a,b)}\left(2\left\|\boldsymbol{x}\right\|_2^2-1\right) \\ &= \sum_{j=0}^{N-1}\sum_{k=0}^{N-1} \rho_k q_{kj} P_k^{(a,b)}\left(2\left\|\boldsymbol{x}\right\|_2^2-1\right),\end{aligned}$$

which we will rewrite in matrix-form,

$$\begin{aligned}\hat{Q}^\beta[\rho](\boldsymbol{x}) = \boldsymbol{P}(\boldsymbol{x}) \cdot \begin{pmatrix} \sum_{k=0}^{N-1} \rho_k q_{k,1} \\ \vdots \\ \sum_{k=0}^{N-1} \rho_k q_{k,N} \end{pmatrix} &= \boldsymbol{P}(\boldsymbol{x}) \cdot \underbrace{\begin{pmatrix} q_{11} & \dots & q_{1N} \\ \vdots & \ddots & \vdots \\ q_{N1} & \dots & q_{NN} \end{pmatrix}}_{=:Q^\beta} \begin{pmatrix} \rho_0 \\ \vdots \\ \rho_{N-1} \end{pmatrix} \\ &= \boldsymbol{P}_k^{(a,b)}\left(2\left\|\boldsymbol{x}\right\|_2^2-1\right) \cdot Q^\beta \boldsymbol{\rho}\end{aligned}$$

where we used $\boldsymbol{P}(\boldsymbol{x}) = \boldsymbol{P}_k^{(a,b)}\left(2\left\|\boldsymbol{x}\right\|_2^2-1\right)$ as a shorthand giving us the form of the operator matrix. Each value q_{kj} in it is therefore chosen to satisfy ...

To be done / included.

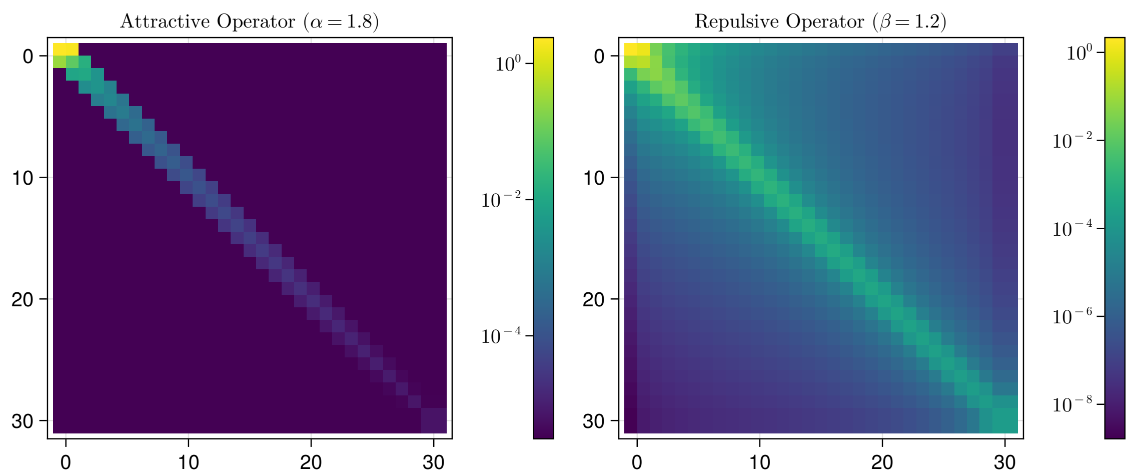

Figure 4.2: The attractive and repulsive operators (matrices) as given in Definition 4.10, the matrix values are shown in a $\log_{10}$ color scale. Due to the choice of basis, the attractive operator is exactly banded. The repulsive parameter is only approximately banded, which the spy plots effectively demonstrate.

The bandedness of the attractive operator is due to the three-term recurrence relationship of the Jacobi polynomial basis.

For the attractive-repulsive interaction potential, the full operator is given by

$$Q_{\alpha,\beta} := \frac{R^\alpha}{\alpha} Q^\alpha - \frac{R^\beta}{\beta} Q^\beta \tag{4.6}$$

for some interval radius $R \in \mathbb{R}^+$, usually chosen as the smallest possible R such that $\mathrm{supp}(\rho) \subseteq [-R, R]$.

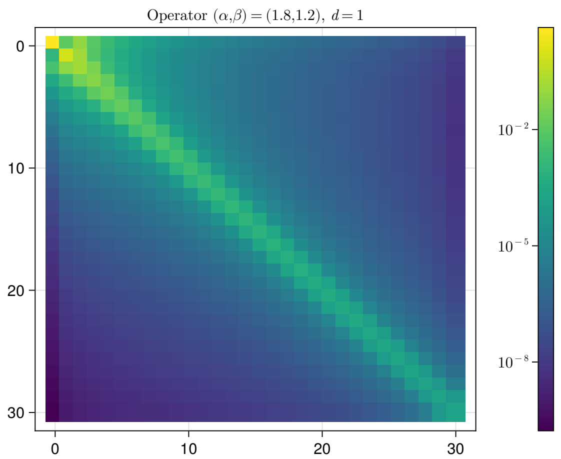

Figure 4.3: Spy plot of $Q_{\alpha,\beta}$, the combination of the attractive-repulsive operators. Inverting this operator and applying it to $(1, 0, ..., 0)^T \in \mathbb{R}^N$ will yield the unnormalised coefficients ρ_k of the solution expansion given in Equation (4.4).

4.3 Results

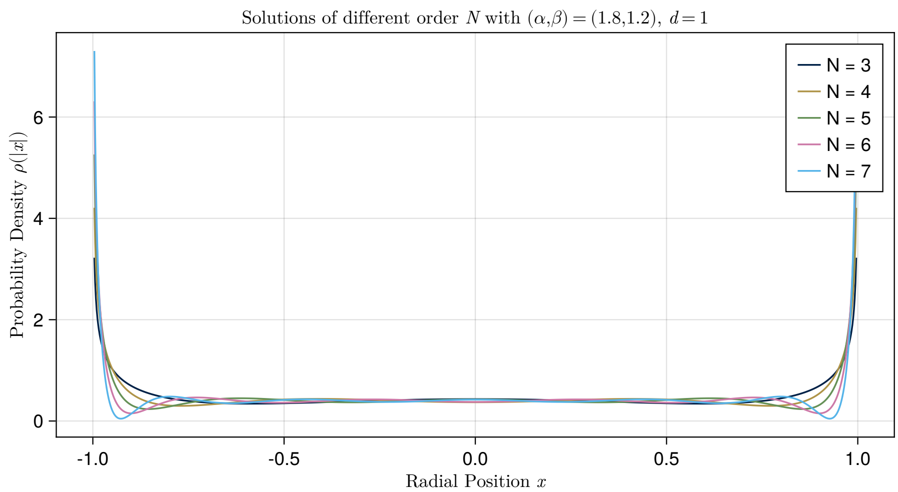

Figure 4.4: Particle density distribution function solutions ρ of increasing order N to the attractive-repulsive problem with interaction potential $K_{alpha,\beta}(r)$, $\alpha = 2.5$ and $\beta = 1.2$. Reflected along the y-axis for better visibility of the domain.

4.4 Outer Optimisation Routine

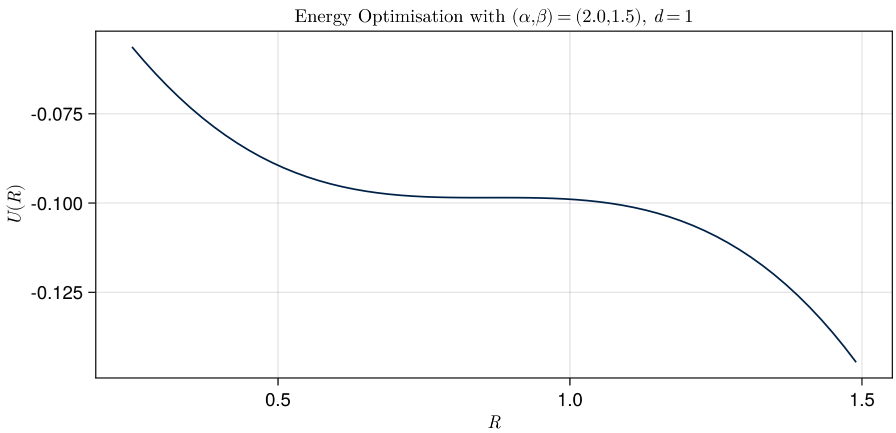

Figure 4.5: The total potential U as a function of the support radius R. This is the goal function minimised by the outer optimisation routine.

Note that using this setup, the operators themselves do not need to be recomputed upon a change in R (cf. Equation (4.6)). The provided implementation uses Least Recently Used (LRU) caching to automatically store operators for a given parameter set and order N.

4.5 Comparison with Analytic Solutions

As introduced in Section 2.7, there are some analytical solutions available which allow us to perform some further analysis of the numerical method in these special cases.

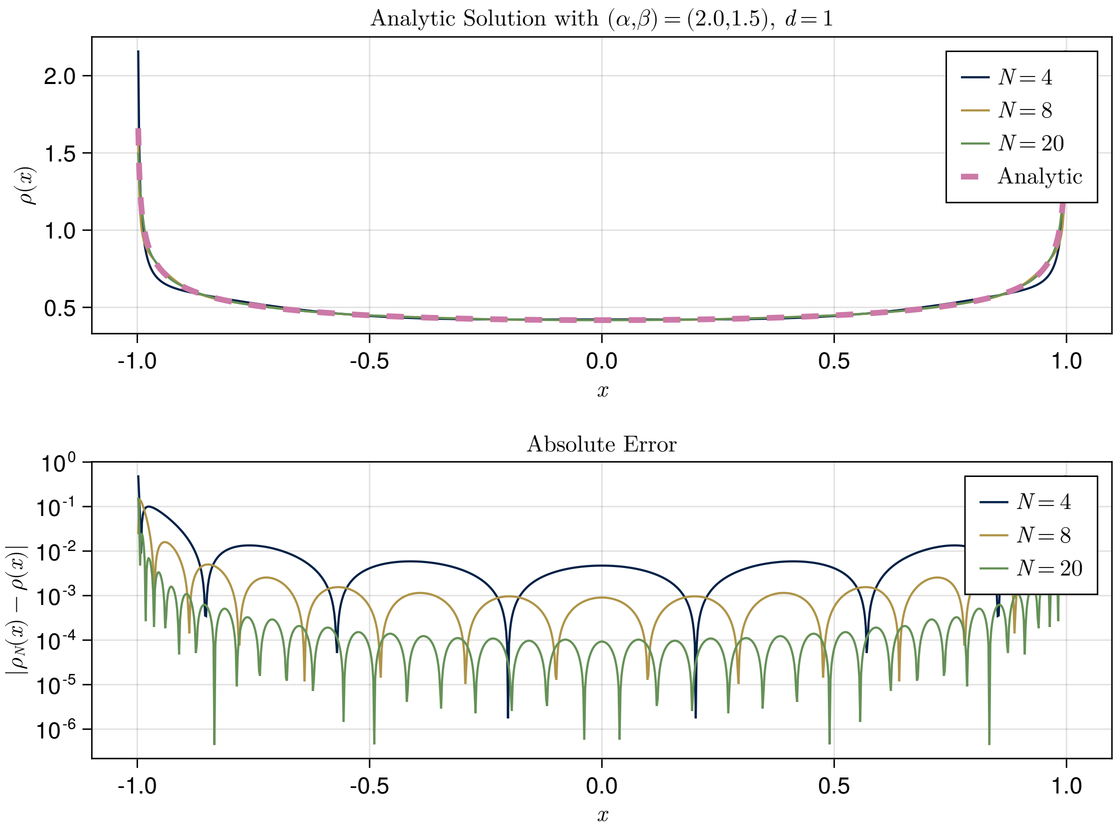

Figure 4.6: The analytic solution $\rho(x)$ given in Equation (2.7) compared to the (spectral method) solutions of different order N. The “arches” occur as a result of the roots of $\rho(x) - \rho_N(x)$, their number approximately equals the order N (a polynomial of degree N has N roots).

There are more analytic solutions available for other parameter ranges, we will not analyse them here.

Definition 4.12: Spectral Convergence

Definition 3.6 (Convergence at spectral speed) An N -point approximation φ_N of a function f converges to f at spectral speed if $|\varphi_N - f|$ decays pointwise in $[-1, 1]$ faster than $O(N^{-p})$ for any $p = 1, 2, ...$ so $p \in \mathbb{N}$.

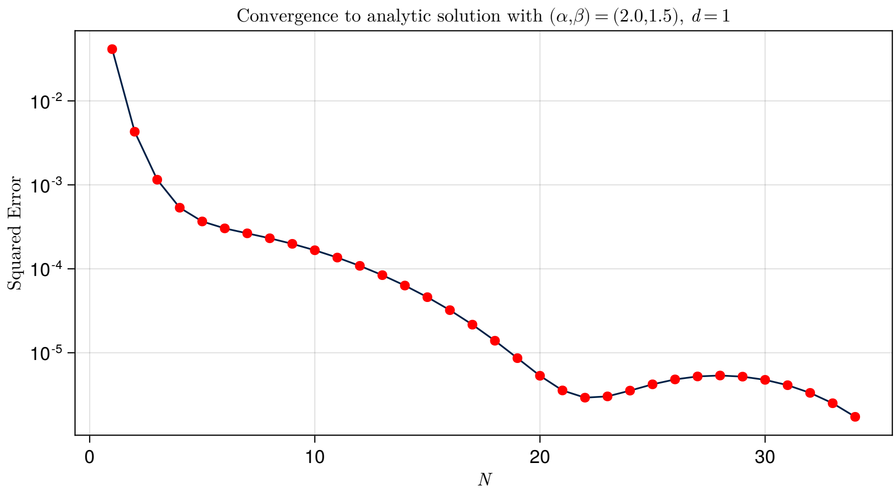

Figure 4.7: Convergence of the numerical solution to the known analytic solution (cf. Equation (2.7)) in a special case where it is known, squared error plotted as a function of the highest order in the expansion N.

4.6 Discussion

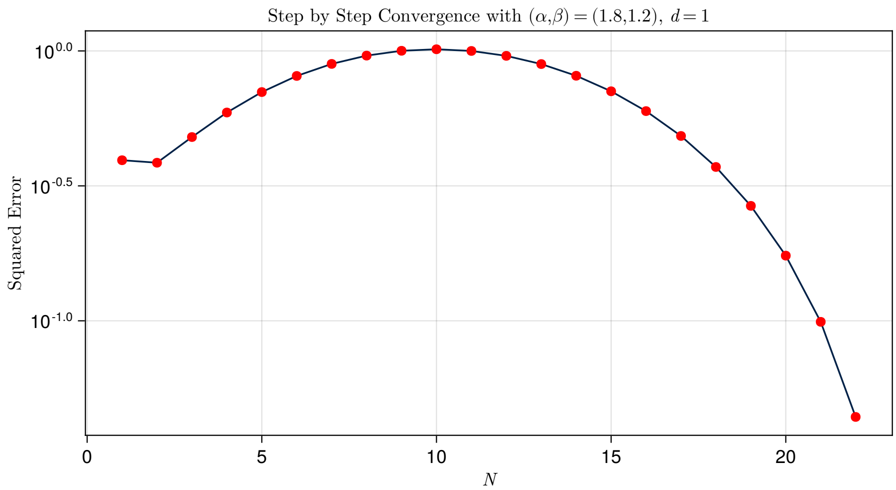

Figure 4.8: Step-by-step convergence of numerical solutions $\rho_N(x)$ as compared to $\rho_{24}(x)$, visualised using the squared error of the pointwise evaluation of both functions in 200 points.

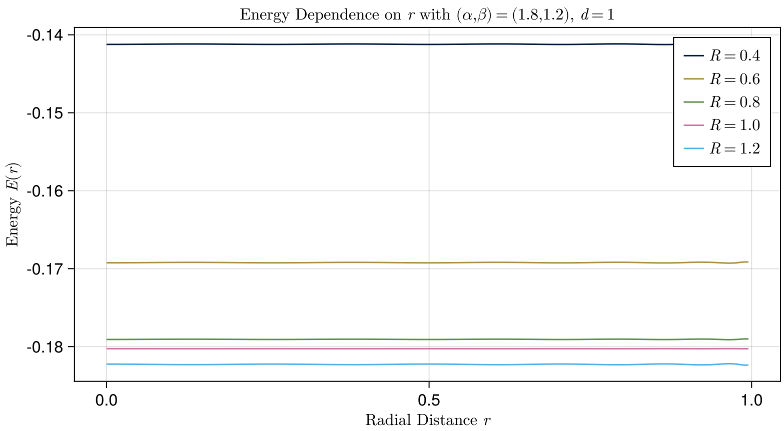

Figure 4.9: Plot of the spatial energy dependence on r, for different values of the domain support radius R. As one can see, $E(\boldsymbol{x}) = \boldsymbol{P}_k^{(a,b)}\left(2\left\|\boldsymbol{x}\right\|_2^2 - 1\right) Q_{\alpha,\beta}\boldsymbol{\rho}$ constant and this figure is only present as visual proof to increase our confidence in the construction of the spectral method.

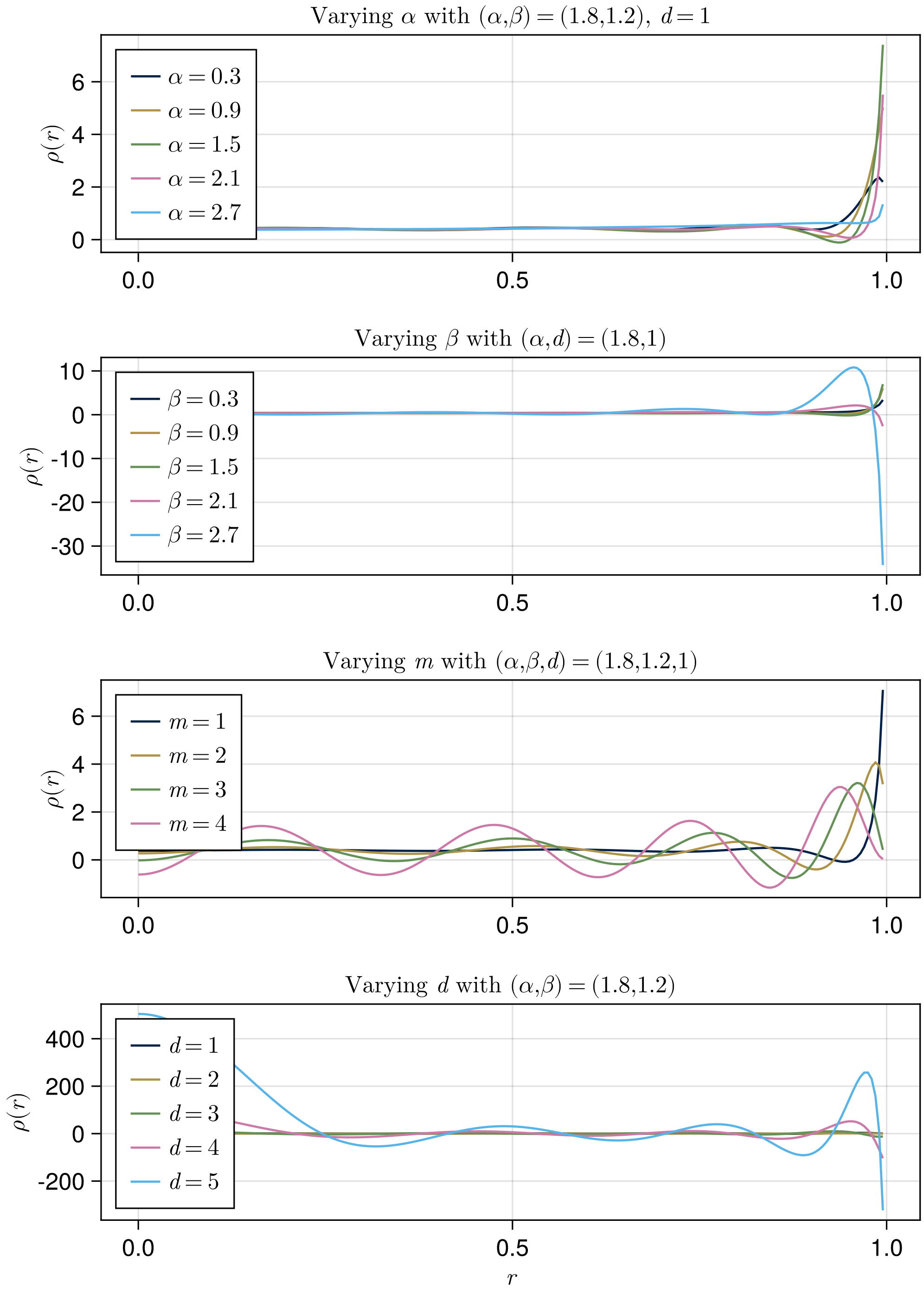

Figure 4.10: Varying different parameters in the solver to demonstrate their effect. See also, Chapter 5.

Acronyms, Definitions and Theorems

Definitions

Theorems

Lemmata

Remarks

Bibliography

Arora, Manmohan S. and S. D. Bajpai (Jan. 1995). 'A new proof of the orthogonality of Jacobi polynomials'. In: *Demonstratio Math.* 28.1, pp. 177–180. ISSN: 2391-4661. DOI: 10.1515/dema-1995-0122.

Biler, Piotr, Cyril Imbert and Grzegorz Karch (June 2011). 'Barenblatt profiles for a nonlocal porous medium equation'. In: *C. R. Math.* 349.11, pp. 641–645. ISSN: 1631-073X. DOI: 10.1016/j.crma.2011.06.003.

Gutleb, Timon S., José A. Carrillo and Sheehan Olver (Dec. 2022). 'Computation of Power Law Equilibrium Measures on Balls of Arbitrary Dimension'. In: *Constr. Approx.*, pp. 1–46. ISSN: 1432-0940. DOI: 10.1007/s00365-022-09606-0.

Huang, Yanghong (Aug. 2014). 'Explicit Barenblatt profiles for fractional porous medium equations'. In: *Bull. London Math. Soc.* 46.4, pp. 857–869. ISSN: 0024-6093. DOI: 10.1112/blms/bdu045.

Kwaśnicki, Mateusz (Feb. 2017). 'Ten Equivalent Definitions of the Fractional Laplace Operator'. In: *FCAA* 20.1, pp. 7–51. ISSN: 1314-2224. DOI: 10.1515/fca-2017-0002.

Magnus, Wilhelm, Fritz Oberhettinger, R. P. Soni and Eugene P. Wigner (Dec. 1967). 'Formulas and Theorems for the Special Functions of Mathematical Physics'. In: *Phys. Today* 20.12, pp. 81–83. ISSN: 0031-9228. DOI: 10.1063/1.3034082.

Michel, N. and M. V. Stoitsov (Apr. 2008). 'Fast computation of the Gauss hypergeometric function with all its parameters complex with application to the Pöschl–Teller–Ginocchio potential wave functions'. In: *Comput. Phys. Commun.* 178.7, pp. 535–551. ISSN: 0010-4655. DOI: 10.1016/j.cpc.2007.11.007.

Milne-Thomson, L. M. (Aug. 1945). *A Treatise on the Theory of Bessel Functions*. Vol. 156. 3955. Nature Publishing Group. DOI: 10.1038/156190a0.

Olver, F.W.J., A.B.O. Daalhuis, D.W. Lozier, B.I. Schneider, R.F. Boisvert, C.W. Clark, B.R. Miller and B. V. Saunders (eds.) (Dec. 2018). *NIST Digital Library* *of Mathematical Functions*. http://dlmf.nist.gov. DOI: 10.1023/A:1022915830921. (Visited on 18/08/2023).

Olver, Sheehan and Alex Townsend (Aug. 2013). 'A Fast and Well-Conditioned Spectral Method'. In: *SIAM Review*. DOI: 10.1137/120865458.

Pearson, John W., Sheehan Olver and Mason A. Porter (Mar. 2017). 'Numerical methods for the computation of the confluent and Gauss hypergeometric functions'. In: *Numer. Algorithms* 74.3, pp. 821–866. ISSN: 1572-9265. DOI: 10.1007/s11075-016-0173-0.

Prudnikov, A.P., Y.A. Brychkov, I.U.A. Brychkov and O.I. Marichev (1986). *Integrals and Series: More special functions*. Integrals and Series. Gordon and Breach Science Publishers. ISBN: 9782881246821.

Slevinsky, Richard Mikael (July 2023). 'Fast and stable rational approximation of generalized hypergeometric functions'. In: *arXiv*. Preprint. DOI: 10.48550/arXiv.2307.06221.

Yoshida, Masaaki (1997). *Hypergeometric Functions, My Love*. Wiesbaden, Germany: Vieweg+Teubner Verlag. ISBN: 978-3-322-90166-8. DOI: 10.1007/978-3-322-90166-8.

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