An introduction to fractional calculus

Fundamental ideas and numerics

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Nonlocal operators (Andreu-Vaillo et al. 2010)

Let $\Omega \subset \mathbb{R}^n$ denote a **bounded** and **open** domain.
The action of a **nonlocal diffusion** operator $\mathcal{L}$ on $u(\mathbf{x}) : \Omega \to \mathbb{R}$ is defined as

$$\mathcal{L}u(\mathbf{x}) = 2\int_{\mathbb{R}^n} (u(\mathbf{y}) - u(\mathbf{x}))\gamma(\mathbf{x}, \mathbf{y})\, \mathrm{d}\mathbf{y}, \qquad \forall\, \mathbf{x} \in \Omega \subseteq \mathbb{R}^n.$$

- the *volume* Ω is non-zero,
- the *kernel* $\gamma(\mathbf{x}, \mathbf{y}) : \Omega \times \Omega \to \mathbb{R}$ is **nonnegative** and **symmetric**.

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The first **interesting equation** is the *nonlocal steady-state*

$$\begin{cases} -\mathcal{L}u = f, & \text{on } \Omega, \\ u = 0, & \text{on } \Omega_{\mathcal{I}}, \end{cases}$$

the **equality constraint** should be defined in general on an *interaction volume* $\Omega_{\mathcal{I}}$ that is **disjoint** from Ω; typically $\Omega_{\mathcal{I}} = \mathbb{R}^n \setminus \Omega \equiv \Omega^c$.

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The fractional Laplacian is the pseudo-differential operator with Fourier symbol $\mathfrak{F}$ satisfying

$$(-\Delta)^{\alpha}\mathfrak{u}(\xi) = |\xi|^{2\alpha}\hat{u}(\xi), \quad 0 < \alpha \leq 1,$$

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Fractional Laplacian: integral formulation

An equivalent characterization of the fractional Laplacian is given by

$$(-\Delta)^\alpha u = c_{n,\alpha}\int_{\mathbb{R}^n}\frac{u(\mathbf{x})-u(\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^{n+2\alpha}}\,\mathrm{d}\mathbf{y}, \qquad 0<\alpha<1, \;\; c_{n,\alpha} = \alpha 2^{2\alpha}\frac{\Gamma\left(\frac{(n+2)}{2}\right)}{\Gamma(1/2)\Gamma(1-\alpha)}.$$

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$$-\mathcal{L} = (-\Delta)^{\alpha}, \quad 0 < \alpha < 1, \qquad \gamma(\mathbf{x},\mathbf{y}) = \frac{c_{n,\alpha}}{2|\mathbf{y}-\mathbf{x}|^{n+2\alpha}} \, \forall \, \mathbf{x},\mathbf{y} \in \mathbb{R}^n.$$

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We can play around with the definitions...

Fractional Laplacian (10 equivalent definitions)

We denote by $\mathbb{L}^p$ ($p \in [1, \infty)$) the Lebesgue spaces, $\mathcal{C}_0$ the space of continuous functions vanishing at infinity, and with $\mathcal{C}_{bu}$ the space of bounded uniformly continuous functions.

Theorem (Kwaśnicki 2017, Theorem 1.1)

Let $\mathcal{X}$ be any of the spaces $\mathbb{L}^p$, $p \in [1, \infty)$, $\mathcal{C}_0$ or $\mathcal{C}_{bu}$, and let $f \in \mathcal{X}$, $\beta = 2\alpha$. The following definitions of $\mathcal{L}f \in \mathcal{X}$ are equivalent:

(a) Fourier definition:

$$\mathcal{F}(\mathcal{L}f)(\xi) = -|\xi|^\beta \mathcal{F}f(\xi)$$

(if $\mathcal{X} = \mathbb{L}^p$, $p \in [1, 2]$);

(b) distributional definition:

$$\int_{\mathbb{R}^d} \mathcal{L}f(y)\varphi(y)dy = \int_{\mathbb{R}^d} f(x)L\varphi(x)dx$$

for all Schwartz functions φ, with $\mathcal{L}\varphi$ defined, for example, as in (a);

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(c) Bochner's[1] definition:

$$\mathcal{L}f = \frac{1}{|\Gamma(-\frac{\beta}{2})|} \int_0^\infty (e^{t\Delta} f - f) t^{-1-\beta/2} dt,$$

with the Bochner's integral of an $\mathcal{X}$-valued function;

[1] Bochner's integral extends the definition of Lebesgue integral to functions that take values in a Banach space, as the limit of integrals of simple functions.

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(d) Balakrishnan's definition:

$$\mathcal{L}f = \frac{\sin \frac{\beta\pi}{2}}{\pi} \int_0^\infty \Delta(sI - \Delta)^{-1} f \, s^{\beta/2-1} ds,$$

(e) singular integral definition:

$$\mathcal{L}f = \lim_{r \to 0^+} \frac{2^\beta \Gamma(\frac{d+\beta}{2})}{\pi^{d/2} |\Gamma(-\frac{\beta}{2})|} \int_{\mathbb{R}^d \setminus B(x,r)} \frac{f(\cdot + z) - f(\cdot)}{|z|^{d+\beta}} dz,$$

with the limit in $\mathcal{X}$;

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(f) Dynkin's definition:

$$\mathcal{L}f = \lim_{r\to 0^+} \frac{2^\beta \Gamma(\frac{d+\beta}{2})}{\pi^{d/2}|\Gamma(-\frac{\beta}{2})|} \int_{\mathbb{R}^d \setminus \overline{B}(x,r)} \frac{f(\cdot+z)-f(\cdot)}{|z|^d(|z|^2-r^2)^{\beta/2}}\, dz,$$

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(g) quadratic form definition: $\langle \mathcal{L}f, \varphi \rangle = \mathcal{E}(f, \varphi)$ for all φ in the Sobolev space $H^{\beta/2}$, where

$$\mathcal{E}(f,g) = \frac{2^{\beta}\Gamma(\frac{d+\beta}{2})}{2\pi^{d/2}|\Gamma(-\frac{\beta}{2})|} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \frac{(f(y)-f(x))(\overline{g(y)}-\overline{g(x)})}{|x-y|^{d+\beta}}\, dxdy$$

(if $\mathcal{X} = \mathbb{L}^2$);

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(h) semigroup definition:

$$\mathcal{L}f = \lim_{t \to 0^+} \frac{P_t f - f}{t},$$

where $P_t f = f * p_t$ and $\mathcal{F}p_t(\xi) = e^{-t|\xi|^\beta}$;

(i) definition as the inverse of the Riesz potential:

$$\frac{\Gamma(\frac{d-\beta}{2})}{2^\beta \pi^{d/2} \Gamma(\frac{\beta}{2})} \int_{\mathbb{R}^d} \frac{\mathcal{L}f(\cdot + z)}{|z|^{d-\beta}} \, dz = -f(\cdot)$$

(if $\beta < d$ and $\mathcal{X} = \mathbb{L}^p$, $p \in [1, \frac{d}{\beta})$);

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Let $\mathcal{X}$ be any of the spaces $\mathbb{L}^p$, $p \in [1, \infty)$, $\mathcal{C}_0$ or $\mathcal{C}_{bu}$, and let $f \in \mathcal{X}$, $\beta = 2\alpha$. The following definitions of $\mathcal{L}f \in \mathcal{X}$ are equivalent:

(j) definition through harmonic extensions:

$$\begin{cases} \Delta_x u(x,y) + \beta^2 c_\beta^{2/\beta} y^{2-2/\beta} \partial_y^2 u(x,y) = 0 \quad \text{for } y > 0, \\ u(x,0) = f(x), \\ \partial_y u(x,0) = \mathcal{L}f(x), \end{cases}$$

where $c_\beta = 2^{-\beta} |\Gamma(-\frac{\beta}{2})| / \Gamma(\frac{\beta}{2})$ and where $u(\cdot, y)$ is a function of class $\mathcal{X}$ which depends continuously on $y \in [0, \infty)$ and $\|u(\cdot, y)\|_{\mathcal{X}}$ is bounded in $y \in [0, \infty)$.

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Let $\mathcal{X}$ be any of the spaces $\mathbb{L}^p$, $p \in [1, \infty)$, $\mathcal{C}_0$ or $\mathcal{C}_{bu}$, and let $f \in \mathcal{X}$, $\beta = 2\alpha$. The following definitions of $\mathcal{L}f \in \mathcal{X}$ are equivalent.
In addition, in (c), (e), (f), (h) and (j), convergence in the uniform norm can be relaxed to pointwise convergence to a function in $\mathcal{X}$ when $\mathcal{X} = \mathcal{C}_0$ or $\mathcal{X} = \mathcal{C}_{bu}$. Finally, for $\mathcal{X} = \mathbb{L}^p$ with $p \in [1, \infty)$, norm convergence in (e), (f), (h) or (j) implies pointwise convergence for almost all x.

- Convergence properties described here are for the *full-space definitions* of the fractional Laplace operator $\mathcal{L}$.
- We can invent **numerical methods** starting from each of these definitions.

Fractional Laplacian: equations on bounded domains

If Ω is **bounded** we can modify our first definition as follows.

- Take $u : \Omega \to \mathbb{R}$ and extend it to zero outside of Ω:

$$(-\Delta)^{\alpha} \tilde{u} = f \text{ in } \Omega, \qquad \tilde{u} = 0 \text{ in } \Omega^c = \mathbb{R}^n \setminus \Omega.$$

where

$$(-\Delta)^{\alpha} \tilde{u} = c_{n,\alpha} \int_{\mathbb{R}^n} \frac{\tilde{u}(\mathbf{x}) - \tilde{u}(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|^{n+2s}} \, \mathrm{d}\mathbf{y}$$

and thus $\tilde{u}$ is the extension by zero to $\mathbb{R}^n$ of a function $u : \Omega \to \mathbb{R}$ in $\mathbb{L}^2(\Omega)$.

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Stochastic interpretation.

As we have seen when discussing the other derivatives, we can interpret also the Fractional Laplacian in a stochastic way. Indeed, one can prove that it is the infinitesimal generator of a 2α-stable Lévy process. The **boundary conditions** means that the particles are killed upon reaching Ω^c.

Fractional Laplacian: equations on bounded domains

The second definition relies instead on **spectral theory**.

- Recall that $-\Delta : \mathcal{D}(-\Delta) \subset \mathbb{L}^2(\Omega) \to \mathbb{L}^2(\Omega)$ is an unbounded, positive and closed operator with dense domain $\mathcal{D}(-\Delta) = \mathbb{H}^1_0(\Omega) \cap \mathbb{H}^2(\Omega)$ with a compact inverse.

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- There is a *countable* collection of eigenpairs $\{\lambda_k, \varphi_k\}_{k\in\mathbb{N}} \subset \mathbb{R}^+ \times \mathbb{H}_0^1(\Omega)$ such that $\{\varphi_k\}_{k\in\mathbb{N}}$ is an **orthonormal basis** of $\mathbb{L}^2(\Omega)$ (and of $\mathbb{H}_0^1(\Omega)$).

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- The **fractional power of the Dirichlet Laplacian** can thus be defined $\forall\, u \in \mathcal{C}^\infty_0$ as

$$(-\Delta)^\alpha u = \sum_{k=1}^{+\infty} \lambda_k^\alpha u_k \varphi_k, \qquad u_k = \langle w, \varphi_k \rangle_{\mathbb{L}^2(\Omega)} = \int_\Omega w \varphi_k \, \mathrm{d}x, \quad k \in \mathbb{N}$$

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Extension

This definition of $(-\Delta)^\alpha$ can be extended by density to

$$\mathbb{H}^\alpha(\Omega) = \left\{ w = \sum_{k=1}^{+\infty} w_k \varphi_k \,:\, \sum_{k=1}^{+\infty} \lambda_k^s w_k^2 < +\infty \right\}.$$

☹ definitions on bounded domains aren't equivalent!

The **integral definition** of the Fractional Laplacian in

$$(-\Delta)^\alpha \tilde{u} = f \text{ in } \Omega, \qquad \tilde{u} = 0 \text{ in } \Omega^c = \mathbb{R}^n \setminus \Omega,$$

and the **spectral definition**

$$(-\Delta)^\alpha u = \sum_{k=1}^{+\infty} \lambda_k^\alpha u_k \varphi_k, \qquad u_k = \langle w, \varphi_k \rangle_{\mathbb{L}^2(\Omega)} = \int_\Omega w \varphi_k \, \mathrm{d}x, \quad k \in \mathbb{N},$$

are **NOT EQUIVALENT**!

Differences

Their difference is **positive** and **positivity preserving** (Musina and Nazarov 2014, Theorems 1 and 2). Furthermore, if we call $d(x, \partial\Omega)$ the distance for $x \in \Omega$ to the boundary $\partial\Omega$ we find

$$\text{(integral) } u(x) \approx d(x, \partial\Omega)^\alpha + v(x), \; \text{(spectral) } u(x) \approx \begin{cases} d(x, \partial\Omega)^{2\alpha} + v(x), & \alpha \in (0, 1/2), \\ d(x, \partial\Omega) + v(x), & \alpha \in (1/2, 1), \end{cases}$$

for a smooth $v(x)$.

Equations of interest

Selecting the **right definition** for the problem the setting one has in mind (finite domain, infinite domain, . . .) we can formulate several PDE with this new operator.

Diffusion-reaction $\partial_t u + (-\Delta)^\alpha u + c(t,x)u = 0$, Domain $(0,+\infty) \times \mathbb{R}^n$,

Quasi-geostrophic $\partial_t \theta + u \cdot \nabla\theta + \kappa(-\Delta)^\alpha \theta = f$, Domain $[0,T] \times \mathbb{R}^2$,

Cahn-Hilliard $\partial_t u + (-\Delta)^\alpha(-\varepsilon^2 \Delta u + f(u)) = 0$, Domain $(O,T] \times (0,2\pi)^2$,

Porous medium $\partial_t u + (-\Delta)^\alpha(|u|^{m-1}\,\mathrm{sign}(u)) = 0$, Domain $(0,+\infty) \times \mathbb{R}^n$,

Schrödinger $i\hbar\partial_t \psi = D_\alpha(-\hbar^2\Delta)^\alpha \psi + V(r,t)\psi$, Domain $(r,t) \in \mathbb{R}^3 \times (0,+\infty)$,

Ultrasound $c_0^{-2}\partial_t^2 p = \nabla^2 p - \{\tau\partial_t(-\Delta)^\alpha + \eta(-\Delta)^{\alpha+1/2}\}p$, Domain $(-\infty,+\infty) \times \mathbb{R}^n$.

See **the review** (Lischke et al. 2020) for an updated *list of references*.

The Spectral Fractional Laplacian

Let us focus on problem using the **spectral Fractional Laplacian**

$$(-\Delta)^{\alpha} u = \sum_{k=1}^{+\infty} \lambda_k^{\alpha} u_k \varphi_k, \qquad u_k = \langle w, \varphi_k \rangle_{\mathbb{L}^2(\Omega)} = \int_{\Omega} w \varphi_k \, \mathrm{d}x, \quad k \in \mathbb{N}.$$

❓ How can we obtain **reliable numerical methods**?

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The Matrix-Transfer Technique

The idea from (Ilic et al. 2005, 2006) goes as follows, suppose that we have a *discretization scheme* for $-\Delta$ on Ω. That is, we can build $A_n = -\Delta_h \approx -\Delta$ on a discrete Ω_h ($h \to 0$ for $n \to +\infty$), then:

$$(-\Delta)^\alpha \approx (-\Delta_h)^\alpha = A_n^\alpha,$$

i.e., we have to compute a **matrix function** of (sparse) matrix discretizing the ordinary Laplacian on the domain of interest.

The Finite Difference Example

The simplest example we can think of is using **finite differences** on $\Omega = [0,1]$ to solve for

$$\begin{cases} (-\Delta)^\alpha u = f(x), & x \in (0,1), \\ u(0) = u(1) = 0. \end{cases}$$

This can be rewritten as

$$A_n = \frac{1}{h^2} T_{n-2}(2 - 2\cos(\theta)), \; h = \frac{1}{n-1},$$

on the grid $\{x_j = jh\}_{j=0}^{n}$, and solved on the inner nodes

$$\mathbf{u}_n(2:n-1) = A_n^{-\alpha}\mathbf{f}(2:n-1),$$

via *diagonalization*.

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```
n = 100; h = 1/(n-1);
x = linspace(0,1,n).';
e  = ones(n-2,1);
An = spdiags([-e,2*e,-e]/h^2,-1:1,
 ↪  n-2,n-2);
f  = sin(pi*x);
u = [0;An\f(2:n-1);0];
[U,L,V] = eig(full(An));
ualpha = @(alpha)
 ↪  [0;V'\(L.^alpha\(U\f(2:n-1)));0];
```

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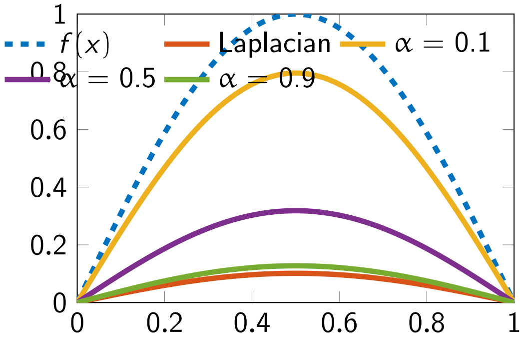

The general case

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- We need to compute $g(z) = z^{-\alpha}$ for $\alpha \in (0, 1)$,
- on a matrix A_n that is either **symmetric and positive definite**, or of a matrix that is *similar* to an SPD matrix,
- A_n has also a condition number that grows (at least quadratically) with its size, i.e., is ill-conditioned.

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What method do we select?

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- on a matrix A_n that is either **symmetric and positive definite**, or of a matrix that is *similar* to an SPD matrix,
- A_n has also a condition number that grows (at least quadratically) with its size, i.e., is ill-conditioned.

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The general case

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- Is this the case?

The Polynomial Krylov Method

If we use a polynomial Krylov subspace

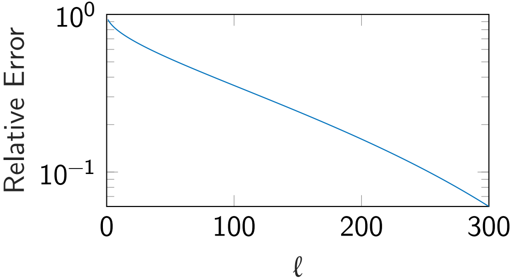
$$\mathcal{K}_\ell(A_n, v) = \mathrm{Span}\{\mathbf{v}, A_n\mathbf{v}, \dots, A_n^{\ell-1}\mathbf{v}\}$$

to solve the problem, then the behavior is controlled by the approximation property

$$\|\mathbf{x} - \mathbf{x}_\ell\| \leq C \cdot \min_{p(z)\in\mathbb{P}_{\ell-1}} \max_{z\in\Lambda(A_n)} |p(z) - z^{-\alpha}|$$

for $\mathbb{P}_{\ell-1}$ the set of polynomial of degree $\leq \ell$, and C a constant *independent* of A and ℓ.

```
ytrue = mpower(full(An),-alpha)*b;
[Q,H] = arnoldi(An,b,l);
for j=1:l
 y = Q(:,1:j)*(mpower(H(1:j,1:j),
 ↪ -alpha)*(Q(:,1:j)'*b));
 err(j) = norm(y-ytrue)./norm(ytrue);
end
```



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A general framework

Given a set of scalars $\{\sigma_1, \ldots, \sigma_{k-1}\} \subset \overline{\mathbb{C}}$ (the extended complex plane), that are not eigenvalues of A, let

$$q_{k-1}(z) = \prod_{j=1}^{k-1} (\sigma_j - z).$$

The rational Krylov subspace of order k associated with A, $\mathbf{v}$ and q_{k-1} is defined by

$$\mathcal{Q}_k(A, \mathbf{v}) = [q_{k-1}(A)]^{-1} \mathcal{K}_k(A, \mathbf{v}), \qquad \mathcal{K}_k(A, \mathbf{v}) = \mathrm{Span}\{\mathbf{v}, A\mathbf{v}, \ldots, A^{k-1}\mathbf{v}\}.$$

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A matrix expression

Given $\{\mu_1, \ldots, \mu_{k-1}\} \subset \overline{\mathbb{C}}$ such that $\sigma_j \neq \mu_j^{-2}$, we define the matrices

$$C_j = (\mu_j \sigma_j A - I)(\sigma_j I - A)^{-1}, \text{ and } \mathcal{Q}_k(A, \mathbf{v}) = \mathrm{Span}\{\mathbf{v}, C_1\mathbf{v}, \ldots, C_{k-1} \cdots C_2 C_1 \mathbf{v}\}.$$

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We are left our usual problem: **how do we select the poles?**

Pole Selection Strategies

Given a function $g(z)$ we find an **explicit (minimal) rational approximation**:

$$g(z) = \frac{P_\ell(z)}{Q_q(z)},\; P_\ell \in \mathbb{P}_\ell[x],\; Q_q \in \mathbb{P}_q[x],$$

and use its poles for the RK-Method.

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Obtain *optimal* rational approximation by solving **best approximation formulations**.

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Direct rational approximations

Sometimes it may be worth our while to use directly $g(A_n)\mathbf{v} = Q_q(A_n)^{-1}P_\ell(A_n)\mathbf{v}$.

Best Uniform Rational Approximation (BURA)

We try to find the poles by solving the min-max problem

$$\max_{t\in[0,1]} |t^{\alpha} - r_{\alpha,k}(t)| = \min_{r_k(t)\in\mathbb{R}_{k,k}} \max_{t\in[0,1]} |t^{\alpha} - r_k(t)|, \qquad \alpha \in (0,1),$$

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- But how do we compute $r_{\alpha,k}(t)$ in practice?
- There is no *explicit solution*, thus we need to use a **numerical method**.

Best Uniform Rational Approximation (BURA)

The *workhorse* for computing BURA is the **Remez algorithm** (Braess 1986, § 6.B)

- Determine the points at which the error of the BURA equioscillates.
- Starting with a *suitable initial guess*, it iteratively determines a rational approximation passing through these points while shifting one or more toward a nearby local maximum.
- Implementation is delicate matter, observe we want both stability and possibly quadratic convergence.

Chose $P^{(0)}/Q^{(0)} \in \mathbb{R}_{m,n}$ and l points $\{x_i^1\}_{i=1}^l$;
$k \leftarrow 1$;
while *not satisfied* **do**
  Determine $P^{(k)}/Q^{(k)} \in \mathbb{R}_{m,n}$ and $\eta_k \in \mathbb{R}$ such that for $i = 1, 2, \ldots, l$

$$f(x_i^k) - P^{(k)}(x_i^k)/Q^{(k)}(x_i^k) = (-1)^i \eta_k$$

  Determine $x_1^{k+1} < x_2^{k+1} < \cdots < x_l^{k+1}$ such that for $i = 1, 2, \ldots, l$

$$s(-1)^i (f - P^{(k)}/Q^{(k)})(x_i^{k+1}) \geq |\eta_k|,$$

  and that for one $i \in \{1, 2, \ldots, l\}$ the left-hand side equals $\|f - P^{(k)}/Q^{(k)}\|$, $s = \pm 1$;
  $k \leftarrow k + 1$;
end

Best Uniform Rational Approximation (BURA)

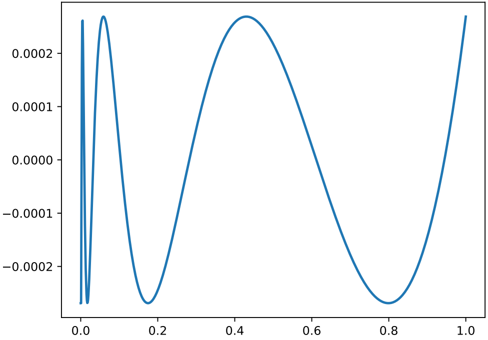
A **recent** and **available implementation** is given in the Python baryrat package, see (Hofreither 2021).

```
import numpy as np
import baryrat

alpha = 0.5
def f(x): return x**alpha
r = baryrat.brasil(f, [0,1], 5)
```

That gives us the `r.poles(0)`:

$$\sigma = \{-3.21294874e+00, -1.62633499e-01, -1.27958136e-02, -6.62129541e-04, -1.22326563e-05\}.$$



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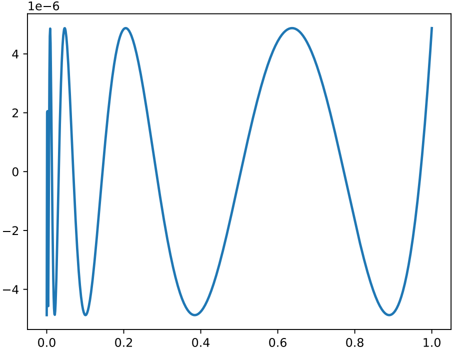

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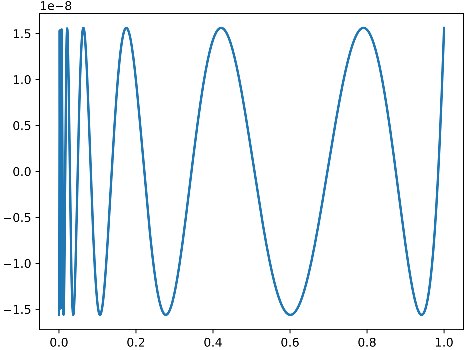

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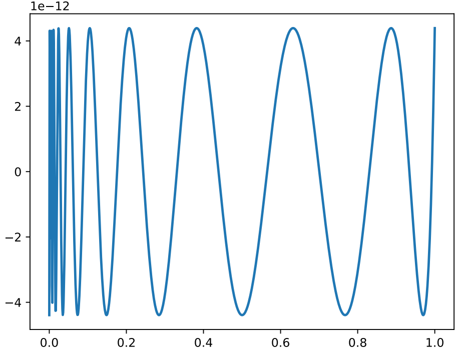

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Best Uniform Rational Approximation (BURA)

One can couple the error analysis with the one coming from the discretization of the Laplacian to get overall results (Harizanov et al. 2020).

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Let $\Omega \subset \mathbb{R}^2$ and suppose that the solution is in $\mathbb{H}^2(\Omega) \cup \mathbb{H}^1_0(\Omega)$ and satisfies $\|(-\Delta)^{-\alpha} f\|_{\mathbb{H}^2(\Omega)} \leq c\|f\|$. Then for $f \in \mathbb{H}^{1+\gamma}(\Omega)$, $\gamma > 0$, the solution $\mathbf{u}_h$ given by

$$\mathbf{u}_h = \lambda_{1,h}^{-\alpha}(\lambda_{1,h} A^{-1})^{\alpha} I_h f, \quad A = M_n^{-1} A_n, \quad I_h \text{ Interpolation},$$

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🔨 Using **lumped FEM**, it is possible to have the error of the **fully discrete scheme** (Harizanov et al. 2020, Corollary 4.3), and then balance the discretization and the BURA error.

🔧 The intend usage of these scheme is *outside* of a Krylov method.

Quadrature-based approaches

Another viable approach is to use a *rational approximation* based on a **quadrature formula**.

- There is more than a *connection* between **quadrature formulas** and **rational approximations**.
- Padé approximants can be viewed as formal Gaussian quadrature methods (Brezinski 1980, Page 34).
- This connection was already know to Gauß

  C. F. Gauss, Methodus nova integralium valores per approximationem inveniendi, Comment. Soc. Reg. Scient. Gotting. Recent., 1814

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The idea is always the same **1.** Find an integral representation of the function of interest. **2.** Find a change of variables that makes a Gauss-type weight appears. **3.** Rational approximation is obtained by the Gauss quadrature formula. **4.** The error analysis relies on the analysis for the formula.

The Gauss-Jacobi approach

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We do **step 1** by looking through a book:

Proposition (Bhatia 1997, example V.1.10, 21, section 5.5.5)

Let $A \in \mathbb{R}^{n \times n}$ be such that $\Lambda(A) \subset \mathbb{C} \setminus (-\infty, 0]$. For $\alpha \in (0,1)$ the following representation holds

$$A^{\alpha} = \frac{\sin(\alpha\pi)}{\alpha\pi} A \int_0^{\infty} \left(\rho^{1/\alpha} I + A\right)^{-1} \, \mathrm{d}\rho.$$

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Now do **step 2**, i.e., a *change of variables*:

$$\rho^{1/\alpha} = \tau \frac{1-t}{1+t}, \qquad \tau > 0.$$

The Gauss-Jacobi approach

By plugging the change of variables in the integral, we find

$$A^{\alpha} = \frac{2\sin(\alpha\pi)\tau^{\alpha}}{\pi} A \int_{-1}^{1} (1-t)^{\alpha-1}(1+t)^{-\alpha} \left(\tau(1-t)I + (1+t)A\right)^{-1} \mathrm{d}t.$$

The Gauss-Jacobi approach

By plugging the change of variables in the integral, we find

$$A^{\alpha} = \frac{2\sin(\alpha\pi)\tau^{\alpha}}{\pi} A \int_{-1}^{1} (1-t)^{\alpha-1}(1+t)^{-\alpha} \left(\tau(1-t)I + (1+t)A\right)^{-1} \mathrm{d}t.$$

We made the **weights of the Gauss-Jacobi quadrature** appear, thus

$$\left(\frac{1}{\tau}A\right)^{\aleph} \approx \frac{1}{\tau}A \sum_{j=1}^{k} \frac{2\sin(\alpha\pi)}{\pi} \frac{\omega_j}{1+\theta_j} \left(\frac{1-\theta_j}{1+\theta_j} + \frac{1}{\tau}A\right)^{-1},$$

- ω_j and θ_j are, respectively, the weights and nodes of the Gauss–Jacobi quadrature formula with weight function $(1-t)^{\alpha-1}(1+t)^{-\alpha}$,
- we should use *error analysis* to fix the τ parameter.
- From (Frommer, Güttel, and Schweitzer 2014, Lemma 4.4) we know that the k-point Gauss-Jacobi quadrature corresponds to the $(k-1, k)$-Padé approximant of $(z/\tau)^{\alpha-1}$ centered at 1.

The Gauss-Jacobi approach

As we have seen from the BURA example, we may be interested in $g(z) = z^{-\alpha}$, $\alpha \in (0,1)$, but it is easy to rewrite the approximation as

$$z^{-\alpha/2} \approx \sum_{j=1}^{k} \frac{2\sin(\alpha\pi)\tau^{1-\alpha/2}}{\pi} \frac{\omega_j}{1+\theta_j} \left(\frac{\tau(1-\theta_j)}{1+\theta_j} + z \right)^{-1} \triangleq R_{k-1,k}(z), \quad \tau > 0$$

- ω_j and θ_j are the weights and nodes of the Gauss–Jacobi quadrature formula with weight $(1-x)^{-\alpha}(1+x)^{\alpha-1}$.
- If we rearrange the expression we then find

$$R_{k-1,k}(z) = \frac{p_{k-1}(z)}{q_k(z)} = \frac{\chi \prod_{r=1}^{k-1}(z+\epsilon_r)}{\prod_{j=1}^{k}(z+\eta_j)}, \quad \chi = \frac{\eta_k}{\tau^\alpha} \frac{\binom{k+\alpha/2-1}{k-1}}{\binom{k-\alpha}{k}} \prod_{j=1}^{k-1} \frac{\eta_j}{\epsilon_j}.$$

for

$$\epsilon_r = \tau \frac{1-\zeta_r}{1+\zeta_r}, \quad r = 1,2,\ldots,k-1, \qquad \eta_j = \frac{\tau(1-\theta_j)}{1+\theta_j}, \quad j = 1,2,\ldots,k.$$

The Gauss-Jacobi approach

To fix the $\tau > 0$ parameter we need the error analysis from (Aceto and Novati 2019) to bound the *truncation error*:

$$E_{k-1,k}(\lambda/\tau) \triangleq (\lambda/\tau)^{-\alpha} - R_{k-1,k}(\lambda/\tau).$$

- When working with these expression, usually one can manipulate and express them in terms of *Gauss-Hypergeometric functions*, then use their asymptotic to produce the bound, *e.g.*, in this case

$$z = 1 - \frac{\lambda}{t}, \quad (1-z)^{-\alpha} = {}_2F_1\left(\begin{array}{c} 1, \alpha \\ 1 \end{array} ; z \right), \quad |\arg(1-z)| < \pi.$$

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Proposition (Aceto and Novati 2019, Proposition 2)

For large values of k, the following representation for the truncation error holds

$$E_{k-1,k}(\lambda/\tau) = 2\sin(\alpha\pi)(\lambda/\tau)^{-\alpha}\left[\frac{\sqrt{\lambda}-\sqrt{\tau}}{\sqrt{\lambda}+\sqrt{\tau}}\right]^{2k}(1 + O(1/k)).$$

The Gauss-Jacobi approach

Theorem (Aceto and Novati 2019, Theorem 2)

If $\mathcal{L}$ is a self-adjoint positive operator on a separable Hilbert space $\mathbb{H}$ with spectrum $\Lambda(\mathcal{L}) \subset [c, +\infty)$, $c > 0$ having a compact inverse, then

$$\left\| \mathcal{L}^{-\alpha} - \tau_k^{-\alpha} R_{k-1,k}\left(\frac{1}{\tau_k}\mathcal{L}\right) \right\|_{\mathbb{H}\to\mathbb{H}} \leq 2\sin(\alpha\pi) c^{-\alpha} \left(\frac{2k\sqrt{e}}{\alpha}\right)^{-4\alpha} \left[2\ln\left(\frac{2k}{\alpha}\right)+1\right]^{2\alpha} \left(1 + O(k^{-2})\right),$$

for

$$\tau_k = c\left(\frac{\alpha}{2ke}\right)^2 \exp\left(2W\left(\frac{4k^2 e}{\alpha^2}\right)\right),$$

where W denotes the Lambert W-function.

It becomes increasingly difficult if the spectrum is close to the branch point of $z^{-\alpha}$.

The Gauss-Jacobi approach (bounded operators)

If $\mathcal{L}_N$ is a **bounded operator**, i.e., $\Lambda(\mathcal{L}_N) \in [c, \lambda_N]$ then the $\min$-$\max$ problem for $|E_{k-1,k}(\lambda/\tau)|$ have two different solutions for *small* and *large* values of k.
We call $\bar{\lambda} = \frac{\tau}{\alpha^2}(k + \sqrt{k^2+1})^2$

$\bar{\lambda} < \lambda_N$ (k smalll) The previous estimate is still good, i.e.,

$$\tau_k = c\left(\frac{\alpha}{2ke}\right)^2 \exp\left(2W\left(\frac{4k^2e}{\alpha^2}\right)\right),$$

$\bar{\lambda} > \lambda_N$ (k large) then

$$\hat{\tau}_k = \left(-\frac{\alpha\sqrt{(}\lambda_N)}{8k}\ln\left(\frac{\lambda_N}{c}\right) + \sqrt{\left(\frac{\alpha\sqrt{\lambda_N}}{8k}\ln\left(\frac{\lambda_N}{c}\right)\right)^2 + \sqrt{c\lambda_N}}\right)^2.$$

The Gauss-Jacobi approach (bounded operators)

Theorem (Aceto and Novati 2019, Theorem 3)

Let $\overline{k}$ be such that for each $k \geq \overline{k}$ we have $\overline{\lambda} = \overline{\lambda}(k) > \lambda_N$. Then for each $k \geq \overline{k}$, taking $\tau = \hat{\tau}_k$, the following bound holds

$$\left\| \mathcal{L}_N^{-\alpha} - \hat{\tau}_k^{-\alpha} R_{k-1,k}\left(\frac{1}{\hat{\tau}_k}\mathcal{L}_N\right) \right\|_2 \leq 2\sin(\alpha\pi)(c\lambda_N)^{-\alpha/2}\exp\left(-4k\left(\frac{c}{\lambda_N}\right)^{1/4}\right)(1+O(k^{-1})).$$

- The bound gets worse when we refine the discretization of the differential operator!
- The choice of τ is better than the asymptotically selected value $\tau_\infty = \sqrt{c\Lambda_N}$.

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- The choice of τ is better than the asymptotically selected value $\tau_\infty = \sqrt{c\Lambda_N}$.

The choice is made as

$$\tau_{k,N} = \begin{cases} \tau_k, & k < \overline{k}, \\ \hat{\tau}_k, & k \geq \overline{k}, \end{cases} \qquad \text{for } \overline{k} = \left\lceil \frac{\alpha}{2\sqrt{2}}\sqrt{\ln\left(\frac{\lambda_N}{c}e^2\right)}\left(\frac{\lambda_N}{c}\right)^{\frac{1}{4}}\right\rceil.$$

A Gauss-Laguerre approach (Aceto and Novati 2022)

We start again from an **integral representation** (Bonito and Pasciak 2015)

$$\mathcal{L}^{-\alpha} = \frac{2\sin(\alpha\pi)}{\pi}\int_0^{+\infty} t^{2\alpha-1}(\mathcal{I} + t^2\mathcal{L})^{-1}\mathrm{d}t, \qquad \alpha \in (0,1).$$

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Then, we go for the **change of variables** $y = \ln t$ we obtain

$$\begin{aligned}\mathcal{L}^{-\alpha} =& \frac{2\sin(\alpha\pi)}{\pi} \int_{-\infty}^{+\infty} e^{2\alpha y}(\mathcal{I} + e^{2y}\mathcal{L})^{-1}\mathrm{d}y, \qquad \alpha \in (0,1).\\ =& \int_{-\infty}^{0} e^{2\alpha y}(\mathcal{I} + e^{2y}\mathcal{L})^{-1}\mathrm{d}y + \int_0^{+\infty} e^{2\alpha y}(\mathcal{I} + e^{2y}\mathcal{L})^{-1}\mathrm{d}y\end{aligned}$$

$$\begin{array}{l} 2\alpha y = -x \\ 2(1-\alpha)y = x \end{array} \quad \to = \frac{1}{2\alpha}\int_0^{+\infty} e^{-x}(\mathcal{I} + e^{-x/\alpha}\mathcal{L})^{-1}\mathrm{d}x + \frac{1}{2(1-\alpha)}\int_0^{+\infty} e^{-x}(e^{-x/(1-\alpha)}\mathcal{I} + \mathcal{L})^{-1}\mathrm{d}x.$$

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Then, we go for the **change of variables** $y = \ln t$ we obtain

$$\mathcal{L}^{-\alpha} = \frac{\sin(\alpha\pi)}{\alpha\pi} I^{(1)}(\mathcal{L}) + \frac{\sin(\alpha\pi)}{(1-\alpha)\pi} I^{(2)}(\mathcal{L}),$$

for

$$I^{(1)}(\lambda) = \int_0^{+\infty} e^{-x}(1+e^{-x/\alpha}\lambda)^{-1}\mathrm{d}x, \qquad I^{(2)}(\lambda) = \int_0^{+\infty} e^{-x}(e^{-x/(1-\alpha)}+\lambda)^{-1}\mathrm{d}x.$$

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The weight $\omega(x) = e^{-x}$, is the weight of **Gauss-Laguerre** formulas.

A Gauss-Laguerre approach (Aceto and Novati 2022)

If we call the weights $w_j^{(n)}$ and nodes $\vartheta_j^{(n)}$ (in ascending order) of the Gauss-Laguerre formula, then we obtain the following $(2n-1, 2n)$ rational approximation:

$$\mathcal{L}^{-\alpha} \approx \frac{\sin(\alpha\pi)}{\alpha\pi} R^{(1)}_{n-1,n}(\mathcal{L}) + \frac{\sin(\alpha\pi)}{(1-\alpha)\pi} R^{(2)}_{n-1,n}(\mathcal{L}) \triangleq R_{2n-1,2n}(\mathcal{L}),$$

where

$$\begin{aligned} R^{(1)}_{n-1,n}(\lambda) &= \sum_{j=1}^{n} w_j^{(n)} \left(1 + e^{-\vartheta_j^{(n)}/\alpha}\lambda\right)^{-1}, \\ R^{(2)}_{n-1,n}(\lambda) &= \sum_{j=1}^{n} w_j^{(n)} \left(e^{-\vartheta_j^{(n)}/(1-\alpha)} + \lambda\right)^{-1}. \end{aligned}$$

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Third step is using **error estimate for Gauss-Laguerre formulas** to get the bound.

A Gauss-Laguerre approach (Aceto and Novati 2022)

The analysis treats separately the two integrals and requires expressing the error as a *contour integral*:

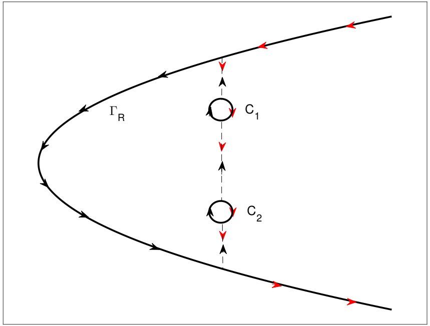
$$E_n(f) = \frac{1}{2\pi i}\int_\Gamma \frac{q_n(z)}{L_n(z)} f(z)\mathrm{d}z,$$

here $L_n(z)$ is the Laguerre polynomial, $q_n(z)$ is the so-called associated function defined by

$$q_n(z) = \int_0^{+\infty} \frac{e^{-x} L_n(x)}{z-x}\mathrm{d}x, \quad z \notin [0,+\infty),$$

and Γ is a contour containing $[0,+\infty)$ with the additional property that **no singularity** of $f(z)$ **lies on or within this contour**; see (Davis and Rabinowitz 1984, §4.6).

A Gauss-Laguerre approach (Aceto and Novati 2022)

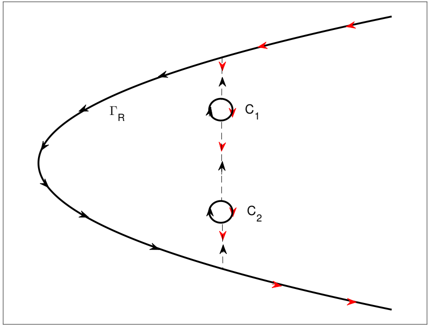


The error can be written as

$$E_n(f) = \frac{1}{2\pi i}\left\{\int_{\Gamma_R} - \int_{C_1} - \int_{C_2}\right\} \frac{q_n(z)}{L_n(z)} f(z)dz.$$

Denote with C_1 and C_2 two arbitrary small circles surrounding the two poles and define $\Gamma = \Gamma_R \cup C_1 \cup C_2$.

A Gauss-Laguerre approach (Aceto and Novati 2022)



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Then using:

$$\frac{q_n(z)}{L_n(z)} = 2\pi e^{-z}\left[\exp\left(\sqrt{-z}\right)\right]^{-2\sqrt{n}} \times$$

$$\times \left(1 + O\left(\frac{1}{n}\right)\right), \quad z \notin [0, +\infty),$$

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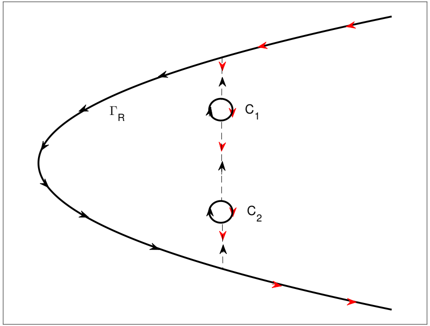

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One arrives at

$$|E_n(f)| \leq 4\pi \left|\mathrm{Res}\left(f(z), z_0\right) e^{-z_0}\right| \times \\ \times \left[\exp\left(\mathrm{Re}\left(\sqrt{-z_0}\right)\right)\right]^{-2\sqrt{n}} \times \\ \times \left(1 + O\left(\frac{1}{n}\right)\right).$$

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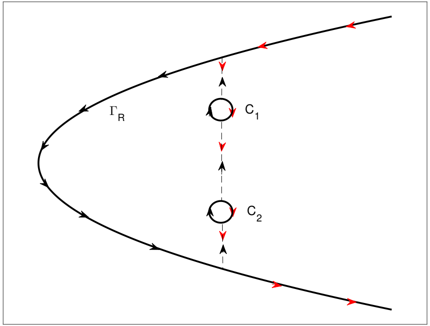

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Procedure

Apply the idea at $f(z) = (1 + e^{-z/\alpha}\lambda)^{-1}$, and $f(z) = (e^{-z/(1-\alpha)} + \lambda)^{-1}$. For the two integrals.

A Gauss-Laguerre approach (Aceto and Novati 2022)

Theorem (Aceto and Novati 2022, Proposition 5.3)

Let $R_{2n-1,2n}(\mathcal{L})$ be the Gauss-Laguerre rational approximation. Then, with respect to the operator norm in $\mathbb{H}$ we have for n large enough

$$\left\|\mathcal{L}^{-\alpha} - R_{2n-1,2n}(\mathcal{L})\right\| \leq 4\sin(\alpha\pi)\exp\left(-3\left(n\alpha^2\pi^2\right)^{1/3}\right)\left(1 + O\left(n^{-1/3}\right)\right).$$

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- The **convergence** is now **independent of the spectral information** of the matrix, we just need to scale A to have spectrum in $[1, +\infty)$.
- Truncation and balancing strategies can be applied to the quadratures observing that nodes and weights decay exponentially, i.e., apply

$$\mathcal{L}^{-\alpha} \approx \frac{\sin(\alpha\pi)}{\alpha\pi} R^{(1)}_{k_{n_1}-1,k_{n_1}}(\mathcal{L}) + \frac{\sin(\alpha\pi)}{(1-\alpha)\pi} R^{(2)}_{k_{n_2}-1,k_{n_2}}(\mathcal{L}).$$

Laplace-Stieltjes and Cauchy-Stieltjes functions

Functions expressed as Stieltjes integrals admit a representation of the form:

$$f(z) = \int_0^\infty g(t,z)\mu(t)\,\mathrm{d}t,$$

where

- $\mu(t)\mathrm{d}t$ is a (non-negative) on $[0,\infty]$, measure,
- $g(t,z)$ is integrable with respect to that measure.

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Cauchy-Stieltjes

Let $f(z)$ be a function defined on $\mathbb{C} \setminus \mathbb{R}_-$. Then, $f(z)$ is a *Cauchy-Stieltjes* function if there is a positive measure $\mu(t)dt$ on $\mathbb{R}_+$ such that

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The function we are interested in is of this class for $\alpha \in (0,1)$:

$$f(z) = z^{-\alpha} = \frac{\sin(\alpha\pi)}{\pi}\int_0^\infty \frac{t^{-\alpha}}{t+z}\,\mathrm{d}t.$$

In (Massei and Robol 2021) is given a general bound for the whole class of functions.

Back to Zolotarev

To **obtain the poles** we consider the approach of minimizing the expression of the error within the Krylov space for the entire class of functions: we **return to Zolotarev**.

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Let us write **compactly**: $\mathcal{W} = \mathcal{K}(A, \mathbf{v}, \Psi)$ for the rational Krylov subspace with poles Ψ. Then we can write the approximation error as:

$$\|\mathbf{x}_{\mathcal{W}} - \mathbf{x}\|_2 \leq 2 \cdot \|\mathbf{v}\|_2 \cdot \min_{r(z) \in \frac{\mathbb{P}_\ell}{\Psi}} \max_{z \in [a,b]} |f(z) - r(z)|.$$

where $\mathbf{x}_{\mathcal{W}} = Uf(U^H AU)U^H \mathbf{v}$ for U an orthonormal basis of $\mathcal{W}$, and $\mathbf{x} = f(A)\mathbf{v}$.

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Now comes the clever observation, the function we want to approximate is of the form

$$f(A)v = \int_0^\infty g(t, A)\mu(t)\, \mathrm{d}t, \qquad g(t, A) \in \{e^{-tA}, (tI + A)^{-1}\}$$

$\Rightarrow$ Since the **projection is linear** we need poles to approximate uniformly well (in t) the matrix exponentials and resolvents.

Cauchy-Stieltjes functions

For Cauchy-Stieltjes function, we just need the result for the resolvent function.

Theorem (Massei and Robol 2021, Theorem 1)

Let A be Hermitian positive definite with spectrum contained in $[a, b]$ and U be an orthonormal basis of $\mathcal{U}_{\mathcal{R}} = \mathcal{K}_\ell(A, v, \Psi)$. Then, $\forall t \in [0, \infty)$, we have the following inequality:

$$\|(tI + A)^{-1}\mathbf{v} - U(tI + A_\ell)^{-1}\mathbf{v}_\ell\|_2 \leq \frac{2}{t+a}\|\mathbf{v}\|_2 \min_{r(z)\in\frac{\mathcal{P}_\ell}{\Psi}} \frac{\max_{z\in[a,b]}|r(z)|}{\min_{z\in(-\infty,0]}|r(z)|}$$

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- We got back to our favorite 4^{th} problem of Zolotarev! Than we do not know how to solve in close form in general...

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For Cauchy-Stieltjes function, we just need the result for the resolvent function.

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Let A be Hermitian positive definite with spectrum contained in $[a, b]$ and U be an orthonormal basis of $\mathcal{U}_{\mathcal{R}} = \mathcal{K}_\ell(A, v, \Psi)$. Then, $\forall t \in [0, \infty)$, we have the following inequality:

$$\|(tI + A)^{-1}\mathbf{v} - U(tI + A_\ell)^{-1}\mathbf{v}_\ell\|_2 \leq \frac{2}{t+a}\|\mathbf{v}\|_2 \min_{r(z)\in\frac{\mathcal{P}_\ell}{\Psi}} \frac{\max_{z\in[a,b]}|r(z)|}{\min_{z\in(-\infty,0]}|r(z)|}$$

where $A_\ell = U^H A U$ and $\mathbf{v}_\ell = U^H v$.

- We got back to our favorite 4^{th} problem of Zolotarev! Than we do not know how to solve in close form in general...
- this is not the general case, this is the case of two intervals $[a, b]$ and $(-\infty, 0]$ ☻

Solving this particular Zolotarev instance

The Zolotarev constant

Let $\Psi = \{\psi_1, \dots, \psi_\ell\} \subset \overline{\mathbb{C}}$ be a finite set, and I_1, I_2 closed subsets of $\overline{\mathbb{C}}$. Then, we define

$$\theta_\ell(I_1, I_2, \Psi) = \min_{r(z) \in \frac{\mathcal{P}_\ell}{\Psi}} \frac{\max_{I_1} |r(z)|}{\min_{I_2} |r(z)|}.$$

Solving this particular Zolotarev instance

Theorem (Zolotarev)

Let $I = [a, b]$, with $0 < a < b$. Then

$$\min_{\Psi \subset \overline{\mathbb{C}},\ |\Psi| = \ell} \theta_\ell(I, -I, \Psi) \leq 4\rho_{[a,b]}^{\ell}, \qquad \rho_{[a,b]} = \exp\left(-\frac{\pi^2}{\log(4\kappa)}\right), \qquad \kappa = \frac{b}{a}.$$

In addition, the optimal rational function $r_\ell^{[a,b]}(z)$ that realizes the minimum has the form

$$r_\ell^{[a,b]}(z) = \frac{p_\ell^{[a,b]}(z)}{p_\ell^{[a,b]}(-z)}, \qquad p_\ell^{[a,b]}(z) = \prod_{j=1}^{\ell}(z + \psi_{j,\ell}^{[a,b]}), \qquad \psi_{j,\ell}^{[a,b]} \in -I.$$

We denote by $\Psi_\ell^{[a,b]} = \{\psi_{1,\ell}^{[a,b]}, \dots, \psi_{\ell,\ell}^{[a,b]}\}$ the set of poles of $r_\ell^{[a,b]}(z)$.

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For any I_1, I_2 be subsets of the complex plane, and $\Psi \subset \overline{\mathbb{C}}$ we have

shift invariance For any $t \in \mathbb{C}$, it holds $\theta_\ell(I_1 + t, I_2 + t, \Psi + t) = \theta(I_1, I_2, \Psi)$.

monotonicity $\theta_\ell(I_1, I_2, \Psi)$ is monotonic with respect to the inclusion on the parameters I_1 and I_2: $I_1 \subseteq I_1', I_2 \subseteq I_2' \implies \theta_\ell(I_1, I_2, \Psi) \leq \theta_\ell(I_1', I_2', \Psi)$.

Möbius invariance If $M(z)$ is a Möbius transform, that is a rational function $M(z) = (\alpha z + \beta)/(\gamma z + \delta)$ with $\alpha\delta \neq \beta\gamma$, then

$$\theta_\ell(I_1, I_2, \Psi) = \theta_\ell(M(I_1), M(I_2), M(\Psi)).$$

⚠ This solution is for $I_1 = [a, b]$ and $I_2 = [-b, -a]$: we had $[a, b]$ and $(-\infty, 0]$!

Solving this particular Zolotarev instance

We just need to build the right Möbius transform to map

$$(-\infty, 0] \cup [a, b] \mapsto -I \cup I, \quad I = [a', b'],\ 0 < a' < b'.$$

Lemma (Massei and Robol 2021, Lemma 4)

The Möbius transformation

$$T_C(z) = \frac{\Delta + z - b}{\Delta - z + b}, \qquad \Delta = \sqrt{b^2 - ab},$$

maps $[-\infty, 0] \cup [a, b]$ into $[-1, -\widehat{a}] \cup [\widehat{a}, 1]$, with $\widehat{a} = \frac{\Delta + a - b}{\Delta - a + b} = \frac{b - \Delta}{\Delta + b}$. The inverse map $T_C(z)^{-1}$ is given by:

$$T_C^{-1}(z) = \frac{(b + \Delta)z + b - \Delta}{1 + z}.$$

Moreover, for any $0 < a < b$ it holds $\widehat{a}^{-1} \leq \frac{4b}{a}$, and therefore $\rho_{[\widehat{a},1]} \leq \rho_{[a,4b]}$.

Cauchy-Stieltjes functions

- We map the interval $[a, b]$ to $[\hat{a}, 1]$,
- solve *explicitly* the Zolotarev problem there,
- read the poles for our problem.

Proposition (Massei and Robol 2021, Corollary 4)

Let $f(z)$ be a Cauchy-Stieltjes function, A be Hermitian positive definite with spectrum contained in $[a, b]$, U be an orthonormal basis of $\mathcal{K}_\ell(A, v, \Psi_{C,\ell}^{[a,b]})$ with $\Psi_{C,\ell}^{[a,b]}$ given by

$$\Psi_{C,\ell}^{[a,b]} = T_C^{-1}(\Psi_\ell^{[\hat{a},1]})$$

and $\mathbf{x}_\ell = Uf(A_\ell)v_\ell$ with $A_\ell = U^H A U$ and $\mathbf{v}_\ell = U^H \mathbf{v}$. Then

$$\|f(A)\mathbf{v} - \mathbf{x}_\ell\|_2 \leq 8f(a)\|\mathbf{v}\|_2 \rho_{[a,4b]}^{\ell} = 8f(a)\exp\left(-\ell\frac{\pi^2}{\log(16b/a)}\right).$$

Nesting the poles

The poles built this way are still **not nested**. In (Massei and Robol 2021) a technique called method of equidistributed sequences (EDS) is proposed to generate them:

1. Select $\zeta \in \mathbb{R}^+ \setminus \mathbb{Q}$ and generate the sequence $\{s_j\}_{j\in\mathbb{N}} = \{0,\ \zeta - \lfloor\zeta\rfloor,\ 2\zeta - \lfloor 2\zeta\rfloor,\ 3\zeta - \lfloor 3\zeta\rfloor,\ \dots\}$, where $\lfloor\cdot\rfloor$ indicates the greatest integer less than or equal to the argument; this sequence has as asymptotic distribution (in the sense of EDS) the Lebesgue measure on $[0,1]$.
2. Compute the sequence $\{t_j\}_{j\in\mathbb{N}}$ such that $g(t_j) = s_j$ where

$$g(t) = \frac{1}{2M}\int_{a^2}^{t} \frac{dy}{\sqrt{(y-a^2)y(1-y)}}, \qquad M = \int_0^1 \frac{dy}{\sqrt{(1-y^2)(1-(1-a^2)y^2)}},$$

3. Define $\widetilde{\sigma}_j = \sqrt{t_j}$.

The EDS associated with $\Psi_\ell^{[a,b]}, \Psi_{C,\ell}^{[a,b]}$ are obtained by applying either a scaling or the Möbius transformation to the EDS for $\Psi_\ell^{[a,1]}$.

Brute force approaches

It is also possible to try and solve numerically rational approximation problems.

RKFIT (Berljafa and Güttel 2017) Is an iterative method for solving rational Least-Square problems, $\{A, F\} \in \mathbb{C}^{n \times n}$ and $\mathbf{b} \in \mathbb{C}^n$ find a ration function r such that

$$\|F\mathbf{b} - r(A)\mathbf{b}\|_2^2 \to \min .$$

AAA (Nakatsukasa, Sète, and Trefethen 2018) Find a representation of the rational approximant in barycentric form with interpolation at certain support points while performing a greedy selection of them to avoid exponential instabilities.

If we have an idea of *where* the approximation should work, these approaches deliver reasonably good results.

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- A *weighted directed graph* (digraph) is a pair $G = (V, E, W)$, where $V = \{v_1, \ldots, v_n\}$ is a **set of nodes** (or vertices), and $E \subseteq V \times V$ is a **set** of **ordered pairs** of nodes called **edges**, and $W \in \mathbb{R}^{n \times n}$ such that $(W)_{i,j} \neq 0$ iff $(v_i, v_j) \in E$.

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- We call *in–degrees* and *out–degrees*

$$d_i^{(\text{in})} = \deg_{\text{in}}(v_i) = \sum_{j\,:\,(v_j,v_i)\in E} w_{j,i},$$

$$d_i^{(\text{out})} = \deg_{\text{out}}(v_i) = \sum_{j\,:\,(v_i,v_j)\in E} w_{i,j},$$

In matrix language

- If all the weights are equal to one, the **adjacency matrix** $A \in \mathbb{R}^{n\times n}$ is

$$(A)_{i,j} = a_{i,j} = \begin{cases} 1, & \text{if } (v_i, v_j) \in E, \\ 0, & \text{otherwise.} \end{cases}$$

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- **Degree** diagonal **matrices**

$$\begin{aligned} D_{\text{in}} &= \operatorname{diag}(\deg_{\text{in}}(v_1), \ldots, \deg_{\text{in}}(v_n)) \\ &= \operatorname{diag}(d_1^{(\text{in})}, \ldots, d_n^{(\text{in})}), \\ D_{\text{out}} &= \operatorname{diag}(\deg_{\text{out}}(v_1), \ldots, \deg_{\text{out}}(v_n)) \\ &= \operatorname{diag}(d_1^{(\text{out})}, \ldots, d_n^{(\text{out})}). \end{aligned}$$

Laplacians on Graphs

Undirected case

Let $G = (V, E)$ be a weighted undirected graph with weight matrix W, weighted degree matrix D and weighted incidence matrix B. Then the **graph Laplacian** L of G is

$$L = D - W.$$

The *normalized random walk* version of the graph Laplacian is

$$D^{-1}L = I - D^{-1}W,$$

where I is the identity matrix. Observe that $D^{-1}W$ is a row–stochastic matrix, i.e. it is nonnegative with row sums equal to 1. The *normalized symmetric* version is

$$D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}.$$

If G is unweighted then $W = A$ in the above definitions. Here we assume that every vertex has nonzero degree.

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Directed case

Let $G = (V, E, W)$ be a weighted directed graph, with degree matrices D_{out} and D_{in} The **nonnormalized directed graph Laplacian** L_{out} and L_{in} of G are

$$L_{\text{out}} = D_{\text{out}} - W, \qquad L_{\text{in}} = D_{\text{in}} - W.$$

⚠ To define the **normalized versions**, we need to invert either the D_{in} or the D_{out} matrices, but the absence of isolated vertices is no longer sufficient to ensure this!

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It is **interesting to look at diffusion on graphs**:

$$\text{find } u : [0, T] \longrightarrow \mathbb{R}^n$$

$$\text{s.t.} \begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} u(t) = -\kappa L_{\cdot/\text{in}/\text{out}} u(t), & t \in (0, T], \\ u(0) = u_0, & \text{prescribed}, \end{cases}$$

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$\Rightarrow$ it *could be* interesting to look at **fractional diffusion** on graphs.

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If G is *undirected*, i.e., $L = L^T$, everything follows by **diagonalization**, see, e.g., (Riascos and Mateos 2014).

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Proposition (Benzi, Bertaccini, et al. 2020)

Given a weighted graph $G = (V, E, W)$ and its Laplacian with respect to the out degree L_{out}, the function $f(x) = x^{\alpha}$ is defined on the spectrum of L_{out} and induces a matrix function for all $\alpha \in (0, 1]$.

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We could also investigate the **the decay of the entries** of the fractional power, but leave the subject aside and refer to (Benzi, Bertaccini, et al. 2020).

Laplacian on Graphs: computation

⚠ For the computation of the products $L_{\text{out}}^{\alpha}\mathbf{v}$ it is necessary to **modify the strategies** we have seen: all the bounds and constructions required that 0 was not in the spectrum.

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In (Benzi and Simunec 2022) different strategies for accommodating this feature of L_{out} are investigated:

- Use a **rank-one** shift, since the right and left eigenvectors $\mathbf{1}$ and $\vec{z}$ of L_{out} can be easily computed, we compute

$$f(L^T)\mathbf{b} = f(L^T + \theta\mathbf{z}\mathbf{1}^T)\mathbf{b} + [f(0) - f(\theta)]\mathbf{z}, \text{ for any } \theta > 0,$$

and in the rational Krylov subspace we solve the linear system at the same cost at which we solve the ones for L^T via Sherman-Morrison:

$$(L^T + \theta\mathbf{z}\mathbf{1}^T - \xi I)^{-1} = (L^T - \xi I)^{-1} + \frac{\theta}{\xi(\theta - \xi)}\mathbf{z}\mathbf{1}^T.$$

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and in the rational Krylov subspace we solve the linear system at the same cost at which we solve the ones for L^T by doing

$$(L^T + \theta\mathbf{z}\mathbf{1}^T - \xi I)^{-1}\mathbf{w} = \boldsymbol{\psi} + \frac{\mathbf{1}^T\mathbf{w}}{\theta - \xi}\mathbf{z} \text{ and } (L^T - \xi I)\boldsymbol{\psi} = \mathbf{w} - (\mathbf{1}^T\mathbf{w})\mathbf{z},$$

to **avoid cancellation** for $\xi \approx 0$.

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- Project L on the $n-1$ dimensional subspace $\mathcal{S} = \mathrm{Span}\{\mathbf{1}\}^{\perp} = \mathrm{Range}(\tilde{Q})$ and compute

$$\begin{aligned} f(L^T)\mathbf{b} &= f(L^T)\mathbf{v} + \beta f(L^T)\mathbf{z} & &\leftarrow 0 \neq \beta = \mathbf{1}^T\mathbf{b} \text{ and } \mathbf{b} = \mathbf{v} + \beta\mathbf{z} \text{ for } \mathbf{v} \perp \mathbf{1} \\ &= Qf(Q^T L^T Q)Q^T\mathbf{v} + \beta f(0)\mathbf{z} & &\leftarrow QQ^T = I - \mathbf{1}\mathbf{1}^T/n,\ Q = [\tilde{Q}, \mathbf{1}/\sqrt{n}]. \end{aligned}$$

  - Q can be built so that $\{Q, Q^T\}\mathbf{v}$ costs $O(n)$.

A gallery of open problems

“*When sorrows come, they come*
not single spies, but in battalions”
Hamlet, Act IV, Scene V.

- Of the many problems we have discussed along the way, one that came back many times was the **selection of optimal poles** for the different matrix-equation/Rational Krylov based solvers (e.g., *all-at-once*, multi-dimensional approaches);

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- Inventing **reduced memory** methods for the integration of fractional partial differential equations in time and space, i.e.,

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- **Error analysis** entangling convergence of the Rational Krylov method and Finite Element (Isogeometric) Discretizations for FPDEs;
- Solving FPDEs on **unlimited spatial domains**.

Fractional Schrödinger equation

As we have discussed at the beginning of the lecture, there are several formulations of the Fractional Laplacian that should be naturally considered on the whole space.

An example is the **Schrödinger equation**

$$i\hbar^{\beta}\, {}^{CA}D^{\beta}\psi = -D_{\alpha}(-\hbar^2\Delta)^{\alpha/2}\psi + V(\mathbf{x}, t)\psi,$$

that is naturally defined on the whole space.

To treat it numerically, the usual procedure is to couple it with **artificial boundary conditions of absorbing type**. It might be of interest to have **numerical methods** that can work with **infinite** or **semi-infinite matrices** that do not need this artificial correction.

Conclusions

- We focused on *few discretization*, there are many other viable approaches (*collocation*, *finite elements*, *IgA*,...). *Most* of the reasoning we did can be **adapted to these other cases**.
- There are **other classical problems** that admits a fractional extension, *e.g.*, optimal control, model order reduction, eigenvalue problems,...

"*The universe (which others call the Library) is composed of an indefinite and perhaps infinite number of hexagonal galleries, with vast air shafts between, surrounded by very low railings. From any of the hexagons one can see, interminably, the upper and lower floors. The distribution of the galleries is invariable.*"

Jorge Luis Borges, The Library of Babel.

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