A Unified View of Some Numerical Methods for Fractional Diffusion

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Outline

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Model problem

With $\Omega \subset \mathbb{R}^d$ a domain, $s \in (0,1)$:

$$\begin{aligned} \mathcal{L}^s u &= f \qquad \text{in } \Omega, \\ u &= 0 \qquad \text{on } \partial\Omega, \end{aligned}$$

where $\mathcal{L}u = -\operatorname{div}(A\nabla u)$ s.p.d. diffusion operator.

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where $\mathcal{L}u = -\operatorname{div}(A \nabla u)$ s.p.d. diffusion operator.

Use spectral definition: for $u \in H_0^1(\Omega)$:

$$\mathcal{L}^s u = \sum_k \lambda_k^s (u, \varphi_k) \varphi_k$$

Nonlocal problem!

The discrete eigenfunction method (DEM)

M. Matsuki and T. Ushijima. “A note on the fractional powers of operators approximating a positive definite selfadjoint operator.” J. Fac. Sci. Univ. Tokyo Sect. IA Math., 1993

- Galerkin discretization on $V_h \subset H_0^1(\Omega)$
- discrete eigensystem: $\mathcal{L}_h u_j^h = \lambda_j^h u_j^h, \ j = 1, \ldots, n$

$$\mathcal{L}^s u \approx \sum_{j=1}^{n} (\lambda_j^h)^s (u, u_j^h) u_j^h$$

$$u_{\mathrm{DEM}} := \sum_{j=1}^{n} (\lambda_j^h)^{-s} (f, u_j^h) u_j^h$$

DEM in linear algebra terms

With stiffness/mass matrix $K, M \in \mathbb{R}^{n\times n}$: solve eigenproblem

$$Ku_j = \lambda_j^h M u_j, \quad j = 1, \dots, n,$$

where

- $\Lambda = \operatorname{diag}(\lambda_j^h)_{j=1}^n$ matrix of eigenvalues,
- $U \in \mathbb{R}^{n\times n}$ matrix of eigenvectors.

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Let $\mathbf{f} \in \mathbb{R}^n$ coefficient vector of $Q_h f \in V_h$.

$$\mathbf{u}_{\mathrm{DEM}} = U\Lambda^{-s}U^T M\mathbf{f} = (M^{-1}K)^{-s}\mathbf{f}.$$

DEM has quasi-optimal error

A. Bonito, J. Pasciak. "Numerical approximation of fractional powers of elliptic operators." Math Comp. 2015

Using P1 FEM on a quasi-uniform mesh and under standard elliptic regularity assumptions, we have

$$\|u_{\text{exact}} - u_{\text{DEM}}\|_{L_2(\Omega)} \leq C \log(h^{-1}) h^{2s+2\delta} \|f\|_{\dot{H}^{2\delta}}$$

for $f \in \dot{H}^{2\delta}$, $\delta \leq 1 - s$.

DEM is **slow**: $\mathcal{O}(n^3)$ operations for eigendecomposition.

Outline

Rational approximation methods

Assume we have a rational function $r(z)$ such that

$$r(z) \approx z^{-s}$$

We define

$$\mathbf{u}_r = r(M^{-1}K)\mathbf{f}.$$

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Theorem

Let $u_r \in V_h$ from rational approximation. Then

$$\|u_{DEM} - u_r\|_{L_2(\Omega)} \leq \max_{z \in [\lambda_{\min}, \lambda_{\max}]} |z^{-s} - r(z)| \, \|f\|_{L_2(\Omega)}.$$

(cf. [Harizanov et al., 2018] for a similar result)

Realizing a rational approximation method

If r is given in **partial fraction decomposition** form

$$r(z) = c_0 + \sum_{j=1}^{k} \frac{c_j}{z - d_j}, \qquad c_j, d_j \in \mathbb{R},$$

we obtain

$$\mathbf{u}_r = r(M^{-1}K)\mathbf{f} = c_0 + \sum_{j=1}^{k} c_j (M^{-1}K - d_j I_n)^{-1}\mathbf{f}.$$

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With the solutions $\mathbf{w}_j$ of

$$(K - d_j M)\mathbf{w}_j = M\mathbf{f}, \qquad j = 1, \dots, k$$

(shifted diffusion problems), we can write

$$\mathbf{u}_r = c_0 + \sum_{j=1}^{k} c_j \mathbf{w}_j.$$

If $d_j \leq 0$, then usually $K \cong K - d_j M$. **Nonpositive poles!**
$\to$ **parallel realization**

Outline

The BURA method

S. Harizanov, R. Lazarov, S. Margenov, P. Marinov, Y. Vutov. "Optimal solvers for linear systems with fractional powers of sparse SPD matrices." Numer Linear Algebra Appl. 2018

Idea:

- compute BURA $r(z)$ to z^{1-s} in $[0,1]$ with degrees (p,p)
- use $\frac{r(z)}{z} \approx z^{-s}$ in $[0,1]$
- rescale original matrix such that $\lambda_{\max} \leq 1$
- $\frac{r(z)}{z}$ has degrees $(p, p+1)$, PFD:

$$\frac{r(z)}{z} = \sum_{j=1}^{p+1} \frac{c_j}{z - d_j}.$$

Remarks on the BURA method

- $|r(z) - z^{1-s}|$ equioscillates, but

$$|r(z)/z - z^{-s}| = \frac{1}{z}|r(z) - z^{1-s}|$$

  is large for small z
- using estimates from [Harizanov et al., 2018]:

$$\|u_{\text{DEM}} - u_{\text{BURA}}\|_{L_2(\Omega)} \lesssim \kappa^{1-s} E_{s,p} \|f\|_{L_2(\Omega)}$$

  where $E_{s,p} \sim \exp(-\sqrt{(1-s)p})$
- improved approach: κ eliminated
- computing BURAs is difficult
  - modified Remez algorithm
    - hard to implement
    - numerically unstable
  - even with quadruple precision, only $p \lesssim 11$ feasible

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Rational approximations based on quadrature

A. Bonito, J. Pasciak. "Numerical approximation of fractional powers of elliptic operators." Math Comp. 2015

Based on

$$z^{-s} = \frac{2\sin(\pi s)}{\pi} \int_{-\infty}^{\infty} \frac{e^{2sy}}{1 + e^{2y}z} dy,$$

three classes of quadrature rules are proposed.
Third one:

$$r_{\mathrm{BP3}}(z) := \frac{2q\sin(\pi s)}{\pi} \sum_{\ell=-M}^{N} \frac{e^{2sy_\ell}}{1 + e^{2y_\ell}z}.$$

With proper parameter choices, they show:

$$\max_z |z^{-s} - r_{\mathrm{BP3}}(z)| \lesssim \exp(-\sqrt{p})$$

where p is the degree of $r_{\mathrm{BP3}}(z)$.

Outline

Fractional Laplace as a Dirichlet-to-Neumann map

Idea

$(-\Delta)^s u$ in Ω is the Neumann data of a **local** elliptic problem in $\Omega \times (0, \infty)$ with Dirichlet data u.

- Caffarelli, Silvestre 2007
- Stinga, Torrea 2010
- Capella, Dávila, Dupaigne, Sire 2011
- Brändle, Colorado, de Pablo, Sánchez 2013
- Nochetto, Otárola, Salgado 2015

The dimension-extended problem

R.H. Nochetto, E. Otárola, A.J. Salgado. "A PDE approach to fractional diffusion in general domains: A priori error analysis." Found Comp Math. 2015

Let $\alpha = 1 - 2s \in (-1, 1)$.
Find $\mathcal{U}(x, y)$, $x \in \Omega$, $y \in (0, \infty)$ such that

$$\begin{aligned} -\operatorname{div}(y^\alpha \nabla \mathcal{U}) &= 0 && \text{in } \Omega \times (0, \infty), \\ \lim_{y \to \infty} \mathcal{U}(x, y) &= 0 && \forall x \in \Omega, \\ \mathcal{U}(x, y) &= 0 && \forall x \in \partial\Omega, y \in (0, \infty), \\ -(\lim_{y \to 0} y^\alpha \partial_y \mathcal{U}(x, y)) &= d_s f(x) && \forall x \in \Omega. \end{aligned}$$

Then the solution is the Dirichlet trace

$$u(x) = (\mathcal{L}^{-s} f)(x) = \mathcal{U}(x, 0).$$

Numerical approach

R.H. Nochetto, E. Otárola, A.J. Salgado. “A PDE approach to fractional diffusion in general domains: A priori error analysis.” Found Comp Math. 2015

- variational formulation in weighted Sobolev spaces
- can truncate extended direction (exponential convergence)
- discretization using tensor product spaces
- error analysis using P1-functions in y direction

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Higher-order discretizations in y direction:

- Ainsworth, Glusa 2018
- Meidner, Pfefferer, Schürholz, Vexler 2018
- Banjai, Melenk, Nochetto, Otárola, Salgado, Schwab 2018

Discretization

Discretize using tensor product space built from

- $V_h \subset H_0^1(\Omega)$ dim $V_h = n$
- W_h FE space over $(0, Y)$, $w_h(Y) = 0$ dim $W_h = m$

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Can write stiffness matrix as

$$\mathcal{A}^{(\alpha)} = M_y^{(\alpha)} \otimes K + K_y^{(\alpha)} \otimes M,$$

where

- $K, M \in \mathbb{R}^{n\times n}$ standard stiffness/mass matrices in V_h
- $K_y^{(\alpha)}, M_y^{(\alpha)} \in \mathbb{R}^{m\times m}$ weighted stiffness/mass matrices in W_h:

$$[M_y^{(\alpha)}]_{ij} = \int_0^Y y^\alpha \psi_j(y)\psi_i(y)\,dy$$

$$[K_y^{(\alpha)}]_{ij} = \int_0^Y y^\alpha \psi_j'(y)\psi_i'(y)\,dy$$

Closed formula for the solution

Theorem (H. 2019)

The solution of the discrete extended problem has the coefficient vector

$$\mathbf{u}_{EXM} = UEU^T M\mathbf{f}$$

with

$$E = (\mathbf{e}_1^T V \otimes I_n) D^{-1} (V^T \mathbf{e}_1 \otimes I_n) \in \mathbb{R}^{n \times n}$$

Proof: based on a diagonalization argument and linear algebra.

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Recall the Discrete Eigenfunction Method:

$$\mathbf{u}_{\mathrm{DEM}} = U\Lambda^{-s} U^T M\mathbf{f}.$$

$$E \sim \Lambda^{-s}?$$

Interpretation of the matrix E

Doing some linear algebra, we find that E is diagonal and

$$E = r(\Lambda), \qquad r(z) = \sum_{k=1}^{m} \frac{v_k^h(0)^2}{\mu_k^h + z}.$$

where

- μ_k^h, $k = 1, \dots, m$ are discrete eigenvalues of the y problem (**1D**),
- $v_k^h(y)$, $k = 1, \dots, m$ are discrete eigenfunctions of the y problem (**1D**).

Connection to rational approximation

$$\mathbf{u}_{\mathrm{DEM}} = U\Lambda^{-s}U^T M\mathbf{f} = (M^{-1}K)^{-s}\mathbf{f}$$
$$\mathbf{u}_{\mathrm{EXM}} = Ur(\Lambda)U^T M\mathbf{f} = r(M^{-1}K)\mathbf{f}$$

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Extension method can be interpreted (realized, analyzed) as a rational approximation method!

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$$r(z) \overset{?}{\approx} z^{-s}$$

Relation to 1D Neumann-to-Dirichlet map

For $z > 0$, the discrete Galerkin solution $v \in W_h$ of the ODE

$$\begin{aligned} -(y^\alpha v'(y))' + zy^\alpha v(y) &= 0 \quad \forall y \in (0, Y), \\ -\lim_{y \to 0^+} (y^\alpha v'(y)) &= 1, \\ v(Y) &= 0. \end{aligned}$$

satisfies

$$r(z) = v(0).$$

Abstract error estimate for extension method

By studying the exact solution of the ODE and a duality-based error estimate, we can prove:

Theorem (H. 2019)

We have

$$\|u_{DEM} - u_{EXM}\|_{L_2(\Omega)} \leq E_{EXM} \|f\|_{L_2(\Omega)}$$

with

$$E_{EXM} = C_s \left(\frac{\exp(-2\sqrt{\lambda_{\min}^h} Y)}{\sqrt{\lambda_{\min}^h} Y} + \sup_{z \in [\lambda_{\min}^h, \lambda_{\max}^h]} \inf_{w_h \in W_h} \|v_z - w_h\|_b^2 \right).$$

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Ex: for $s = 1/2$ and using maximally smooth splines of degree p in y-direction, we obtain the rate $\mathcal{O}(m^{-2p})$.

Outline

Time stepping method of Vabishchevich

P.N. Vabishchevich. "Numerically solving an equation for fractional powers of elliptic operators." J Comp Phys. 2015

Choose $\delta > 0$ such that $\mathcal{L} \geq \delta I$.
Find $w(t), t \in (0,1)$ from the parabolic equation

$$(t(\mathcal{L}-\delta I)+\delta I)\frac{dw}{dt}+s(\mathcal{L}-\delta I)w = 0 \quad \forall t \in (0,1), \qquad w(0) = \delta^{-s}f.$$

Then the solution of the fractional diffusion problem is

$$w(1).$$

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Scalar equivalent:

$$(t(z-\delta)+\delta)w'(t) + s(z-\delta)w(t) = 0$$

with the solution

$$w(t) = ((1-t)\delta + tz)^{-s},$$
$$w(0) = \delta^{-s}, \qquad w(1) = z^{-s}.$$

Discretization

Semidiscretization in space, $D := K - \delta M$:

$$(tD + \delta M)\mathbf{w}' + sD\mathbf{w} = 0 \quad \forall t \in (0,1), \qquad \mathbf{w}(0) = \delta^{-s}\mathbf{f},$$

where $\mathbf{w} : [0,1] \to \mathbb{R}^n$.

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Time stepping: Choose $\theta \in (0,1]$. For $k \in \{0,\ldots,m\}$, denote

$$t^k = \tau k, \qquad \tau = \frac{1}{m},$$
$$t^{\theta(k)} := \theta t^{k+1} + (1-\theta)t^k,$$
$$\mathbf{w}^{\theta(k)} := \theta \mathbf{w}^{k+1} + (1-\theta)\mathbf{w}^k$$

and introduce the implicit scheme

$$(t^{\theta(k)}D + \delta M)\frac{\mathbf{w}^{k+1} - \mathbf{w}^k}{\tau} + sD\mathbf{w}^{\theta(k)} = 0 \qquad \forall k = 0,\ldots,m-1.$$

Relation to rational approximation

Theorem (H. 2019)

The solution obtained by time stepping is given by

$$\mathbf{u} = U r(\Lambda) U^{-1} \mathbf{f} = r(M^{-1}K)\mathbf{f}$$

with the rational function

$$r(z) = \delta^{-s} \prod_{k=0}^{m-1} \omega_k(z),$$

$$\omega_k(z) = \frac{\left(\frac{t^{\theta(k)}}{\tau} - s(1-\theta)\right)(z-\delta) + \frac{\delta}{\tau}}{\left(\frac{t^{\theta(k)}}{\tau} + s\theta\right)(z-\delta) + \frac{\delta}{\tau}}, \qquad k = 0, \dots, m-1,$$

with degrees (m, m)*.* $r(\cdot)$ *has* ***nonpositive roots*** *if* $\theta = 0.5$*.*

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with degrees (m, m). $r(\cdot)$ *has* ***nonpositive roots*** *if* $\theta = 0.5$.

This time stepping scheme can be interpreted as a rational approximation method – parallel realization!

Outline

Example

$$-\left(\frac{d^2}{dx^2}\right)^s u(x) = 1 \quad \forall x \in (-1,1),$$
$$u(-1) = u(1) = 0$$

Linear FEM with 1024 elements.
eigenvalues of $M^{-1}K$: $\lambda^h_{\min} \approx 9.87$, $\lambda^h_{\max} \approx 1.26 \cdot 10^7$.

All methods realized as rational approximation methods.
Note: convergence theorem is dimension independent.

We consider the spectral error

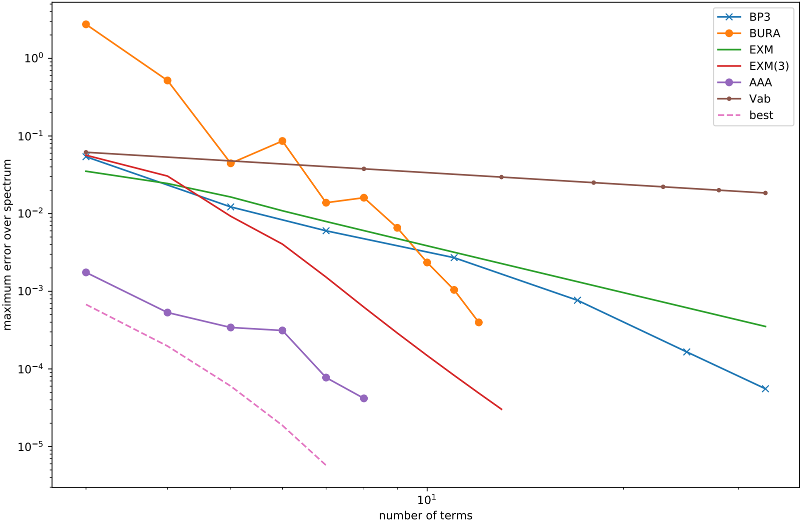
$$\max_{z \in [\lambda_{\min}, \lambda_{\max}]} |z^{-s} - r(z)|$$

and the L_2-error

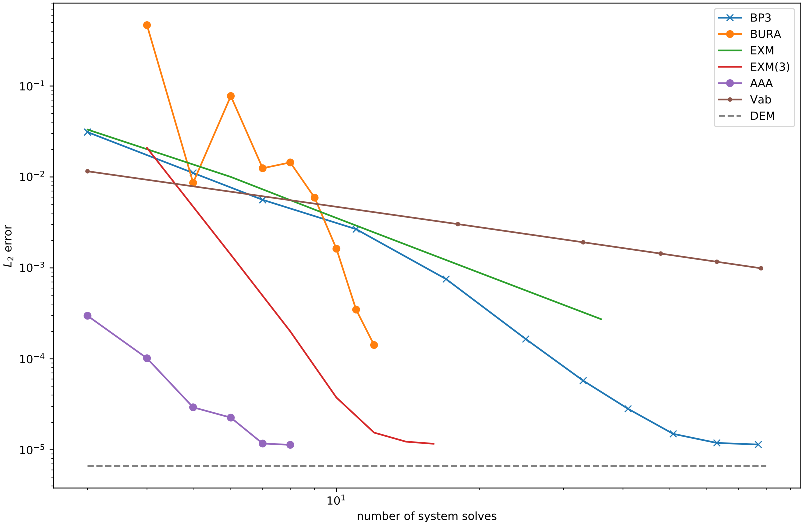
$$\|u_{\text{exact}} - u_r\|_{L_2(\Omega)}$$

in dependence of the degree of the rational function r.

Spectral error – $s = 0.5$

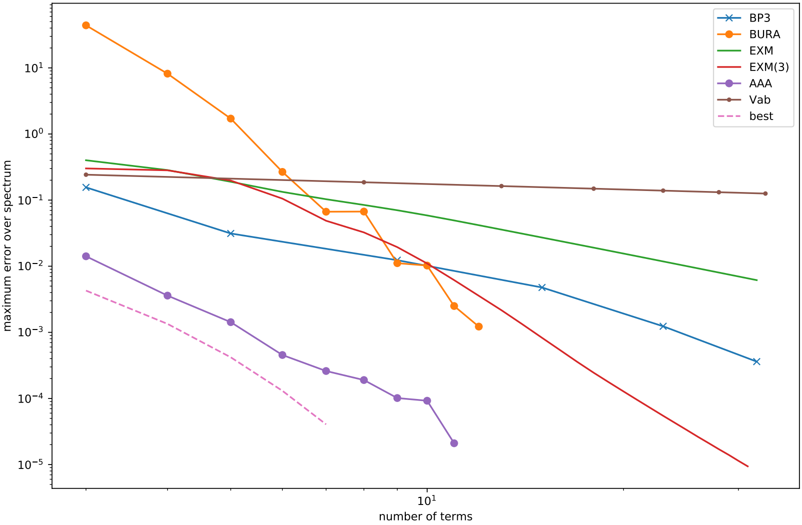


L_2 error – $s = 0.5$

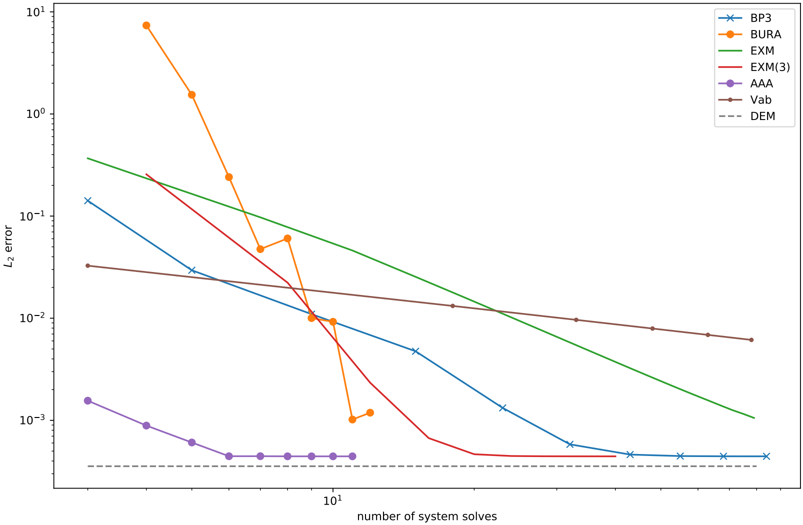


BP3
BURA
EXM
EXM(3)
AAA
Vab
DEM
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
L_2 error
10^{1}
number of system solves

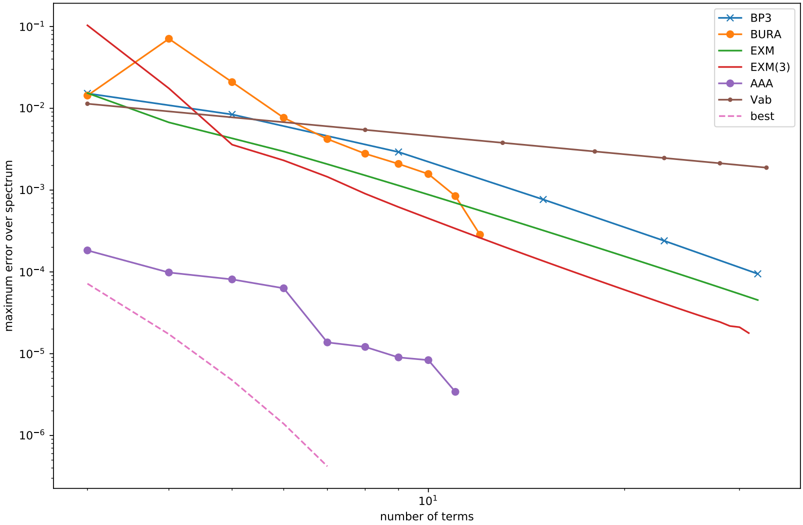
Spectral error – $s = 0.25$



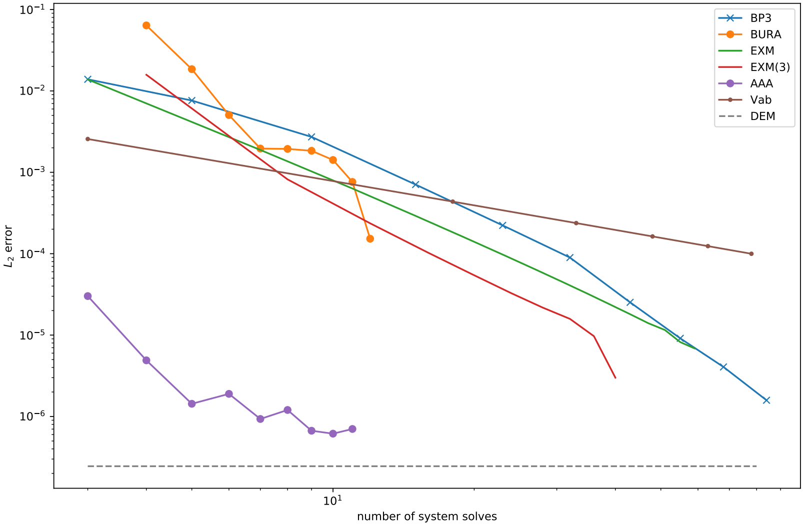
L_2 error – $s = 0.25$



Spectral error – $s = 0.75$



L_2 error – $s = 0.75$



The AAA method

Apply a black-box rational approximation method to

$$z^{-s}, \quad z \in [\lambda_{\min}, \lambda_{\max}].$$

Here:

Y. Nakatsukasa, O. Sète, L.N. Trefethen. "The AAA algorithm for rational approximation." SIAM J Sci Comput. 2018

Use the resulting rational function $r(z)$ for a rational approximation method.

Conclusion

- all presented methods can be interpreted and realized as rational approximation methods
- the max-error of the rational approximation predicts the actual error in the L_2 norm well
- the realization as a rational approximation method is **inherently parallel**
- better ways to get best rational approximations to z^{-s}?
  - analytically – Zolotarev theory?
  - numerically – continuation methods?

Code:

`https://people.ricam.oeaw.ac.at/c.hofreither/`