Efficient Numerical Methods for Fractional Laplacian and time fractional PDEs

Jie Shen

Purdue University

Collaborators: Sheng Chen and Changtao Sheng

ICERM Workshop on Fractional PDEs, June 18-22, 2018

Two main difficulties with fractional PDEs:

- fractional derivatives are non-local operators which are much more difficult and expensive to deal with than local operators.
- fractional PDEs have weakly singularities at $t = 0$ and/or boundaries.

The following two situations will be considered:

- Part I. Solving the fractional Laplacian using the Caffarelli-Silverstre extension
- Part II. Space-time Petrov-Galerkin method for time-fractional diffusion equations

Part I: Fractional Laplacian equations in bounded domains

We consider the fractional Laplacian equation in a bounded domain Ω:

$$\begin{cases} (-\Delta)^s u(\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} = (x_1, x_2, \ldots, x_d) \in \Omega, \\ u|_{\partial\Omega} = 0, \end{cases}$$

where $0 < s < 1$, and the fractional Laplacian operator is defined through the spectral decomposition of Laplace operator.

Two review papers:
What is the fractional Laplacian? by Liscke et al.
Numerical methods for fractional diffusion, by Bonito et al.

Three approaches:

- Using the discrete eigenfunctions of the Laplacian
- Using the Dunford-Taylor formula

$$u = (-\Delta)^{-s} f = \frac{\sin s\pi}{\pi} \int_0^\infty \mu^{-s} (\mu I - \Delta)^{-1} f \, d\mu$$

- Using the Caffarelli-Silvestre extension (cf. Stinga & Torrea '10)

Caffarelli-Silvestre extension

To overcome the difficulty associated with non-local operators, Caffarelli-Silvestre '07 (see Stinga & Torrea '10 for the bounded case) introduced an extension problem in $d+1$ dimension with local differential operators:

$$\begin{cases} \nabla \cdot \left(y^{\alpha} \nabla U(\mathbf{x}, y)\right) = 0, & \text{in } \mathcal{D} = \Omega \times (0, \infty), \\ U(\mathbf{x}, y) = 0, & \text{on } \partial_L \mathcal{D} = \partial\Omega \times [0, \infty), \\ \lim\limits_{y \to 0} y^{\alpha} U_y(\mathbf{x}, y) = -d_s f(\mathbf{x}), & \lim\limits_{y \to \infty} U(\mathbf{x}, y) = 0 \end{cases}$$

where $\alpha = 1 - 2s$ and $d_s = 2^{1-2s}\Gamma(1-s)/\Gamma(s)$. Then, the solution of the fractional Laplacian equation can be expressed as

$$u(x) = U(x, 0).$$

Hence, one only needs to solve the above $d+1$ dimensional problems with local differential operators.

Results by using finite elements

Nochetto, Otarola & Salgado (2016) made a systematical study of the finite element approximation to the extension problem.

Fig. 2 Computational rate of convergence $\#(\mathscr{T}_{\mathcal{Y}})^{-s/(n+1)}$ for quasi-uniform meshes $\mathscr{T}_{\mathcal{Y}}$, with $s = 0.2$ and $n = 1$

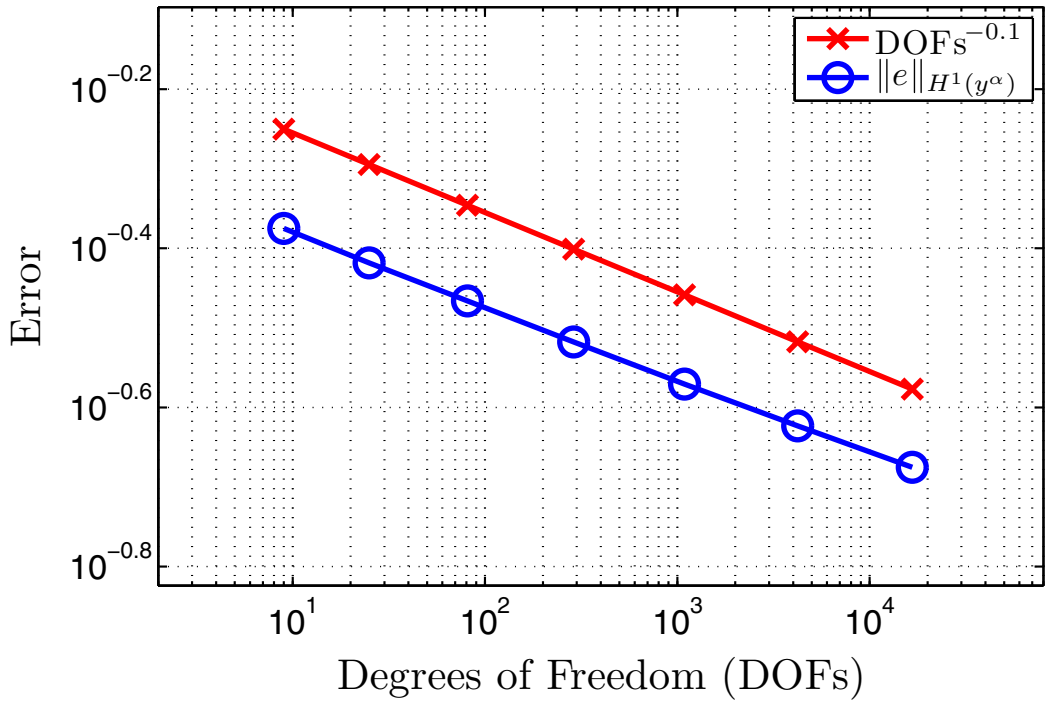

Figure: Q_1 FEM convergence rate of the quasi-uniform mesh (in y), Nochetto et al 2016.

Improved convergence rate with a graded mesh (in y)

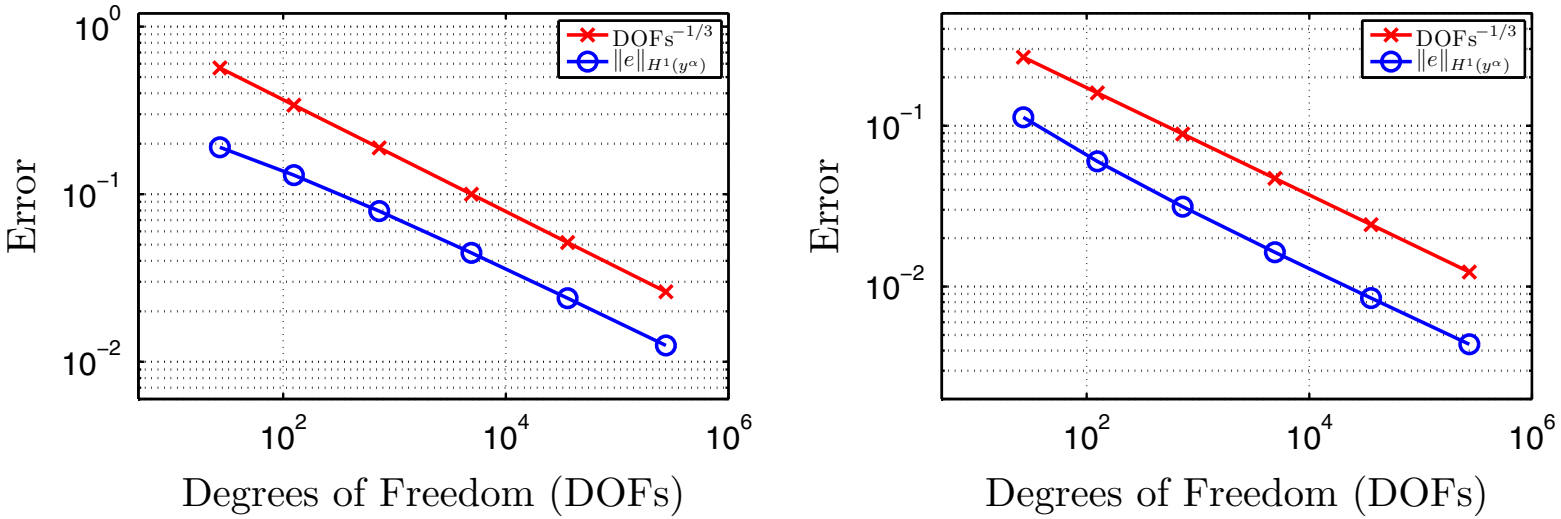

Fig. 3 Computational rate of convergence for approximate solution of the fractional Laplacian over a square with graded meshes on the extended dimension. *Left panel*: rate for $s = 0.2$; *right panel*: rate for $s = 0.8$. In both cases, the rate is $\approx (\#\mathscr{T}_{\mathscr{Y}_k})^{-1/3}$, in agreement with Theorem 5.4 and Remark 5.5

Q. Can we further improve the convergence rate in the extended direction?

Galerkin approximation with Laguerre spectral method in y

The particular weight function y^α in the extension problem calls for the use of generalized Laguerre polynomials $\{\mathcal{L}_k^\alpha(y)\}$ which are mutually orthogonal w.r.t. the weight $y^\alpha e^{-y/2}$.
Let us denote

$$Y_N^\alpha = \text{span}\{\hat{\mathcal{L}}_k^\alpha(y) := \mathcal{L}_k^\alpha(y)e^{-y/2},\ k = 0, 1, \cdots, N\},$$

For the **x**-directions, one can use your favorite approximation space X_K, e.g., FEM or spectral method.
The Galerkin approximation for the extension problem is to find $u_{NK} \in X_{N,K} = Y_N^\alpha \times X_K$ such that

$$(y^\alpha \nabla u_{NK}, \nabla v)_D = d_s(f, v(x, 0))_\Omega, \forall v \in X_{N,K}.$$

Fast solvers

- Let $\{\psi_j(x)\}_{1\le j\le K}$ be a set of basis functions in X_K, we write $u_{NK} = \sum_{k=1}^{N}\sum_{j=1}^{K} \tilde{u}_{kj}\phi_k(y)\psi_j(x)$ and $U = (\tilde{u}_{kj})$.
- Let us denote

$$S^y_{kj} = (y^\alpha \phi_j'(y), \phi_k'(y))_{(0,\infty)}, \quad M^y_{kj} = (y^\alpha \phi_j(y), \phi_k(y))_{(0,\infty)},$$
$$S^x_{kj} = (\nabla_x \psi_j(x), \nabla_x \psi_k(x))_\Omega, \quad M^x_{kj} = (\psi_j(x), \psi_k(x))_\Omega.$$

Then, the linear system for the Galerkin approximation is

$$S^y U M^x + M^y U S^x = F.$$

- Choice of basis functions for Y_N^α:
Let $\mathcal{L}^\alpha_{-1}(y) = 0$, we set $\phi_k(y) := \hat{\mathcal{L}}^\alpha_{k-1}y) - \hat{\mathcal{L}}^\alpha_k(y)$. Then $Y_N^\alpha = \text{span}\{\phi_k(y) : \ k = 0, 1, \cdots, N\}$. and we have

$$\partial_y \phi_k(y) = \frac{1}{2}(\hat{\mathcal{L}}^\alpha_{k-1}y) + \hat{\mathcal{L}}^\alpha_k(y)).$$

Thanks to the orthogonality of generalized Laguerre functions, M^y and S^y are both symmetric penta-diagonal.

Fast solvers: continued

The above linear system can be solved efficiently by using the matrix-diagonalization method.

Let $S^y E = M^y E \Lambda$ where (E, Λ) consists of eigenvectors and eigenvalues of $S^y \bar{x} = \lambda M^y \bar{x}$.

Setting the change of variable $U = EV$, we can reduce the matrix system to a sequence of N problems in x-direction:

$$(\lambda_j M^x + S^x)\bar{v}_j = (E^t (M^y)^{-1} F)_j, \quad j = 1, 2, \cdots, N.$$

Since usually $N \ll K$, this procedure is very efficient, and is not intrusive as your favorite elliptic solver can be used.

Error estimates for the Laguerre spectral methods

- Error estimates with generalized Laguerre functions:

$$\min_{v_N \in Y_N^\alpha} \|\hat{\partial}_y^l (u - v_N)\|_{y^{\alpha+l}} \lesssim N^{(l-m)/2} \|\hat{\partial}_y^m u\|_{y^{\alpha+m}}, \ 0 \le l \le m$$

  where $\hat{\partial}_y = (\partial_y + 1/2)$.

- Then for the problem

$$-\partial_y (y^\alpha \partial_y u) = f, \quad u(0) = 0, \lim_{y \to \infty} u(y) = 0,$$

  the generalized Laguerre-Galerkin method in Y_N^α leads to:

$$\|(u - u_N)_y\|_{y^\alpha} \lesssim N^{(1-m)/2} \|\hat{\partial}_y^m u\|_{y^{\alpha+m-1}}.$$

Error estimates for the extension problem

- The error estimate for Galerkin approximation of the extension problem in $X_{N,K}$ is:

$$\|U - U_{NK}\|_{1,y^\alpha} \lesssim N^{(1-m)/2} \|\hat{\partial}_y^m U\|_{y^{\alpha+m-1}} + \min_{v_K \in X_K} \|\nabla_x (U(x,0) - v_K)\|$$

  The first part is a typical result for spectral approximation.

- Unfortunately, the solution is singular at $y = 0$ so that $\|\hat{\partial}_y^m u\|_{y^{\alpha+m-1}}$ is only bounded for $m = [2s] + 1$. So the Laguerre spectral method converges very slowly in the y-direction.

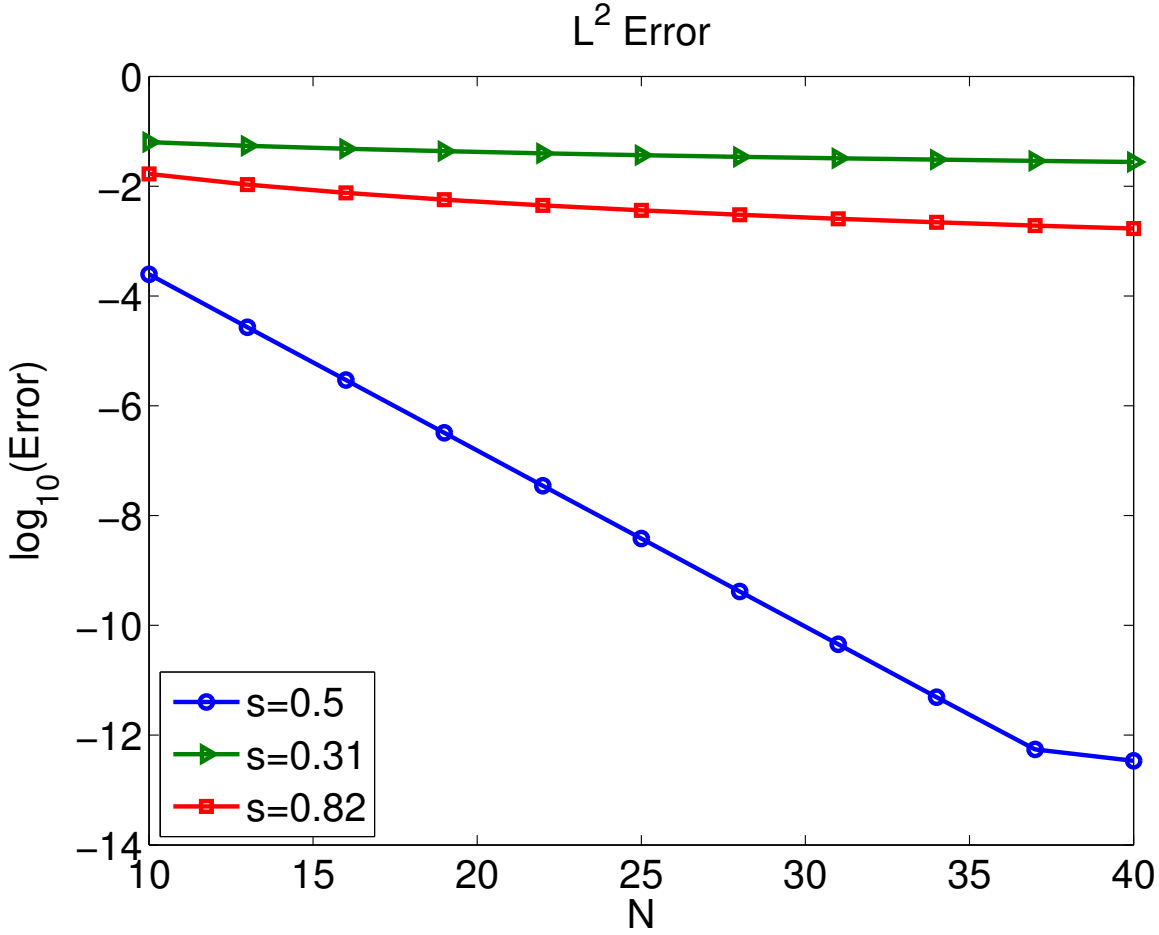

Figure: $\lambda = 2,\ s = 0.5, 0.31, 0.82.$

Form of singularities at $t = 0$

A careful look at the extension problem reveals that the singularity can be explicitly identified so it is possible to use special basic functions to well represent the singular behavior at $y = 0$.

By using a separation of variables approach, one finds that the solution to the extension problem can be expressed as

$$U(\mathbf{x}, y) = \sum_{n=1}^{\infty} \widetilde{U}_n \, \varphi_n(\mathbf{x}) \psi_n(y)$$

where $\psi_n(y)$ is the solution of (Stinga & Torrea '10)

$$\begin{cases} -\psi_n''(y) - \dfrac{1-2s}{y}\psi_n'(y) + \lambda_n \, \psi_n(y) = 0, \quad y \in \Lambda = (0, \infty), \\ \psi_n(0) = 1, \quad \lim\limits_{y \to \infty} \psi_n(y) = 0, \end{cases}$$

which can be expressed by Bessel function of the 2nd kind $K_s(z)$:

$$\psi_n(y) = c_s (\sqrt{\lambda_n} y)^s K_s(\sqrt{\lambda_n} y), \quad c_s = 2^{1-s}/\Gamma(s).$$

Form of singularities at $t = 0$: continued

We have

$$K_s(z) := \frac{s}{2}\frac{I_{-s}(z) - I_s(z)}{\sin(s\pi)}, \quad I_s(z) := \sum_{j=0}^{\infty} \frac{1}{j!\Gamma(j+1+\alpha)}\left(\frac{z}{2}\right)^{2j+s}.$$

So we can derive

$$\begin{aligned}
\psi_n(y) &= c_s(\sqrt{\lambda_n}y)^s K_s(\sqrt{\lambda_n}y) \\
&= \frac{sc_s}{2\sin(s\pi)}\left\{(\sqrt{\lambda_n}y)^s I_{-s}(\sqrt{\lambda_n}y) - (\sqrt{\lambda_n}y)^s I_s(\sqrt{\lambda_n}y)\right\} \\
&= \frac{sc_s}{2\sin(s\pi)} \sum_{j=0}^{\infty} \frac{(\sqrt{\lambda_n}y)^{2j} - (\sqrt{\lambda_n}y)^{2j+2s}}{2^{2j+s}j!\Gamma(j+2-2s)} \\
&= g_{1,n}(y) + y^{2s} g_{2,n}(y),
\end{aligned}$$

where $g_{1,n}(y)$, $g_{2,n}(y)$ are smooth functions.

Enriched spectral method

It is natural to add some some singular parts to the approximation space in the y-direction:

$$Y_N^{\alpha,k} = Y_N^{\alpha} \oplus \{y^{2s}\hat{\mathcal{L}}_j^{\alpha}(y) : \ j = 0, 1, \cdots, k\},$$

and the new approximation space for the extension problem is:

$$X_{N,K}^k = Y_N^{\alpha,k} \times X_K.$$

We have the following error estimate with the new approximation space:

$$\|u - U_{NK}^k(x,0)\|_{H^s(\Omega)} \lesssim N^{-\frac{[2s]}{2}-k} + \min_{v_K \in X_K} \|\nabla(u - v_K)\|.$$

Solution of the linear system

One can apply the same matrix diagonalization process as before, but (S^y, M^y) are usually severely ill conditioned since the added singular functions are "similar at $y = 0$" and have no orthogonal relation with the Laguerre functions. This approach can only be used for small k (which is usually enough).

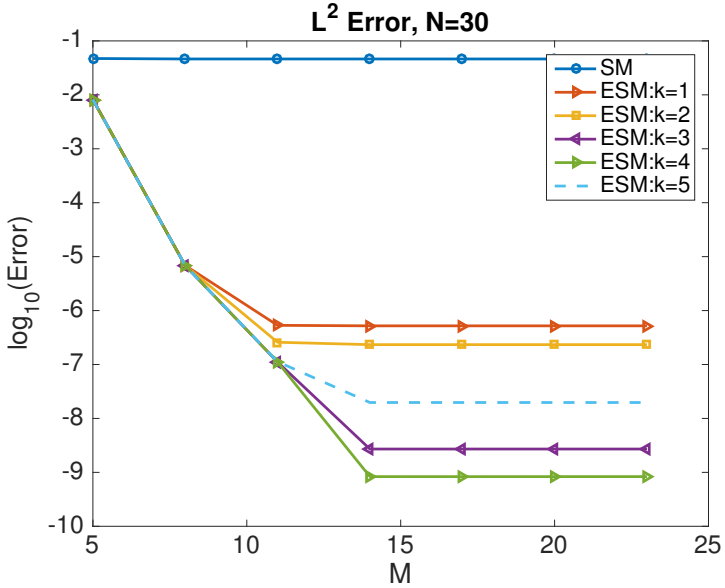

Figure: Error behaviors with the enriched spectral method (1-D): s=0.2

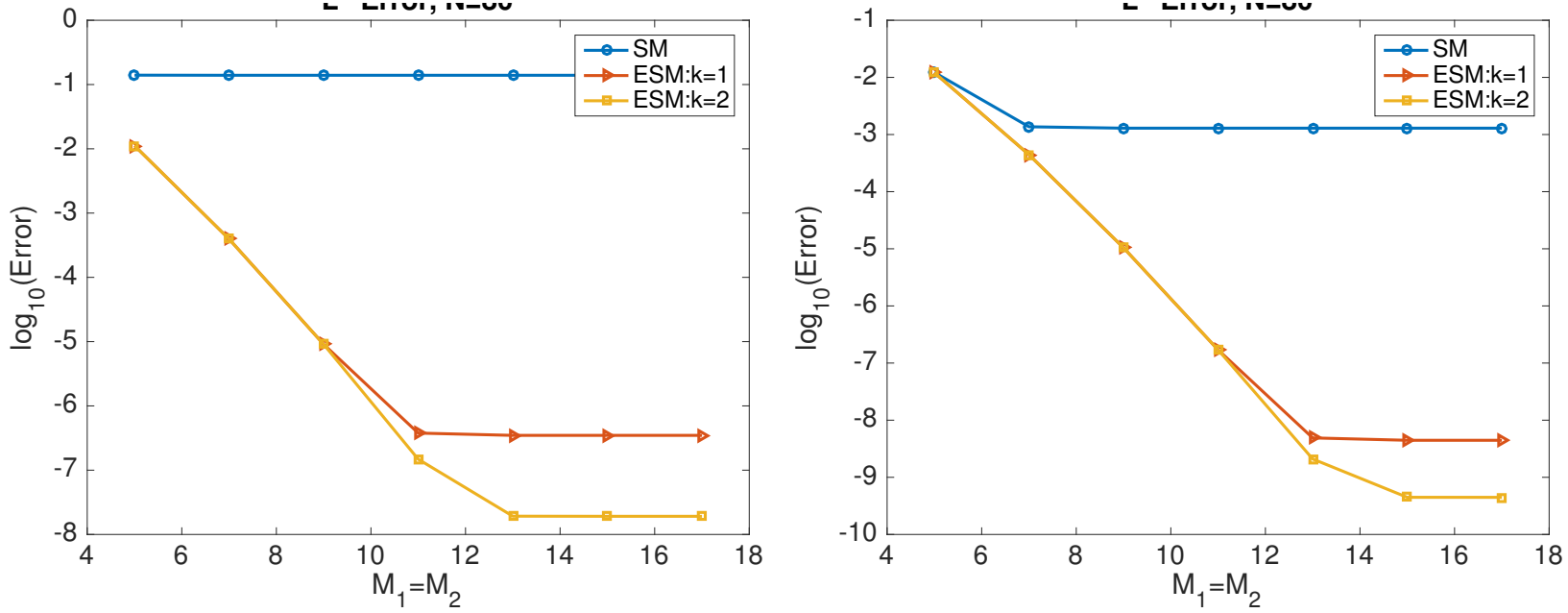

Figure: Smooth solution with a spectral method in $\Omega = (-1, 1)^2$: Left: $s = 0.2$, Right: $s = 0.8$.

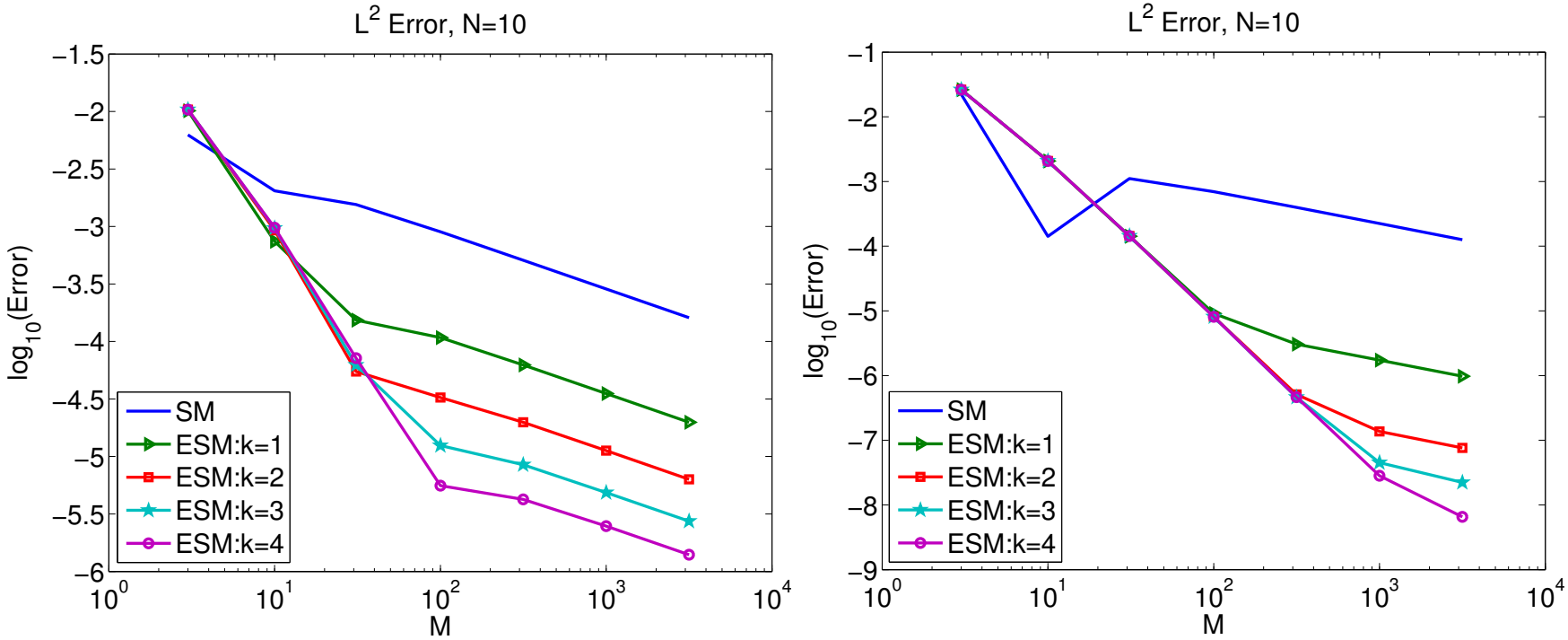

Figure: Non-smooth solution with a finite element method in $\Omega = (-1, 1)$: Left: $f(x) = 1,\ s = 0.2,$ Right: $f(x) = (1 - x^2),\ s = 0.7.$

We consider the following class of fractional PDEs ($0 < \alpha < 1$):

$$ {}_0^C D_t^\alpha v(x,t) + \mathcal{L}v(x,t) + \mathcal{N}(v(x,t)) = 0, \quad \forall (x,t) \in \mathbb{D} := \Omega \times (0,T], $$

with suitable boundary conditions and initial condition, where $\mathcal{L}$ is a linear elliptic operator, $\mathcal{N}$ is a lower-order nonlinear operator, and ${}_0^C D_t^\alpha$ $(0 < \alpha < 1)$ is the left-sided Caputo fractional derivative of order α.

We can reformulate the above problem using the Riemann-Liouville derivative with homogeneous initial condition:

$$ {}_0 D_t^\alpha u(x,t) + \mathcal{L}u(x,t) + \mathcal{N}(u(x,t)) = g(x,t), \quad v(x,0) = 0. $$

Two main difficulties in dealing with time-fractional PDEs:

- Solution at the next time step depends on solutions at all previous time steps.
- The solution is weakly singular at $t = 0$ so a usual approach will not lead to high accuracy.

Some existing approaches:

- Finite-difference methods with graded meshes at $t = 0$.
- Convolution integrals (Lubich '86, ...).
- Spectral-element method with geometric mesh leads exponential convergence (Mao & S. '17), but it is expensive and complicated.
- Space-time spectral methods:
  - using usual polynomials (Li & Xu '10) and Müntz polynomials (Hou & Xu '17);
  - using poly-fractonomials or generalized Jacobi functions (Karniadakis & Zayernouri '15, Chen, S. & Wang, '16, Mao & S. '16).

Petrov-Galerkin formulation for fractional (in time) PDEs

We first consider the linear equations with $\mathcal{N} = 0$:

$$ {}_0D_t^\alpha u(x,t) + \mathcal{L}u(x,t) = g(x,t); \qquad u(x,0) = 0. $$

Petrov-Galerkin formulation: Find $u \in H_0^\alpha(I) \otimes H_{\mathcal{L}}(\Omega)$ s.t.

$$ \mathcal{A}(u,v) := ({}_0D_t^\alpha u, v)_{\mathbb{D}} + (\mathcal{L}^{\frac{1}{2}} u, \mathcal{L}^{\frac{1}{2}} v)_{\mathbb{D}} = (g,v)_{\mathbb{D}}, \quad \forall v \in L^2(I) \otimes H_{\mathcal{L}}(\Omega), $$

where $H_{\mathcal{L}}(\Omega) = \{u \in L^2(\Omega) : (\mathcal{L}^{\frac{1}{2}} u, \mathcal{L}^{\frac{1}{2}} u) < \infty\}$.

The Petrov-Galerkin formulation is well-posed since

$$ \begin{aligned} \mathcal{A}(u, {}_0D_t^\alpha u) &= \|{}_0D_t^\alpha u\|^2_{L^2(\mathbb{D})} + (\mathcal{L}^{\frac{1}{2}} u, {}_0D_t^\alpha \mathcal{L}^{\frac{1}{2}} u)_{\mathbb{D}} \\ &\geq \|{}_0D_t^\alpha u\|^2_{L^2(\mathbb{D})} + C_2 (D_t^{\frac{\alpha}{2}} \mathcal{L}^{\frac{1}{2}} u, {}_tD_T^{\frac{\alpha}{2}} \mathcal{L}^{\frac{1}{2}} u)_{\mathbb{D}} \\ &= \|{}_0D_t^\alpha u\|^2_{L^2(\mathbb{D})} + C_2 \cos(\frac{\pi\alpha}{2}) \|{}_0D_t^{\frac{\alpha}{2}} u\|^2_{L^2(I, H_{\mathcal{L}}(\Omega))} \\ &\geq C_3 (\|{}_0D_t^\alpha u\|^2_{L^2(\mathbb{D})} + \|{}_0D_t^\alpha u\|^2_{L^2(I, H_{\mathcal{L}}(\Omega))}) := C_3 \|u\|^2_{B^\alpha(\mathbb{D})}. \end{aligned} $$

Basis functions in time: using generalized Jacobi functions

We define shifted generalized Jacobi functions (or poly-fractonomials, Karniadakis & Zayernouri '13)

$$J_n^{(\alpha,\eta)}(t) = t^\eta \widetilde{P}_n^{(\alpha,\eta)}(t), \quad t \in I, \quad n \geq 0,$$

where $\widetilde{P}_n^{(\alpha,\eta)}(t) = P_n^{(\alpha,\eta)}(\frac{2t-T}{T})$ is the shifted Jacobi polynomial.

It satisfies the following remarkable property:

$${}_0D_t^\alpha J_n^{(-\alpha,\alpha)}(t) = \frac{\Gamma(n+\alpha+1)}{n!}\widetilde{P}_n^{(0,0)}(t).$$

So we define our approximation space in time by

$$\begin{aligned}\mathcal{F}_N^{(\alpha)} &:= \{t^\alpha \psi(t) : \psi(t) \in \mathcal{P}_N\} \\ &= \text{span}\{J_n^{(-\alpha,\alpha)}(t) = t^\alpha \widetilde{P}_n^{(-\alpha,\alpha)}(t) : 0 \leq n \leq N\},\end{aligned}$$

which incorporates the homogeneous boundary conditions at $t = 0$.

Space-time Petrov-Galerkin method

Let V_h be a finite-dimensional approximation space of $V = H_{\mathcal{L}}(\Omega)$:

$$V_h = \text{span}\{\phi_1, \phi_2, \cdots, \phi_M\}$$

Then, our Petrov-Galerkin method is: Find $u_L \in V_h \otimes \mathcal{F}_N^{(\alpha)}$, such that

$$\mathcal{A}(u_L, v_L) = (g, v_L)_{\mathbb{D}}, \quad \forall v_L \in V_h \otimes \mathcal{P}_N.$$

Q. The above linear system is of size $L = MN$. How to solve it efficiently?

A. Since the domain $\mathbb{D}$ is a (separable) tensor product domain, we can employ a discrete separation of variables.

Fast direct solver

We write $u_L(x,t) = \sum_{m=1}^{M} \sum_{n=0}^{N} \widetilde{u}_{mn} \phi_m(x) J_n^{(-\alpha,\alpha)}(t)$, and denote

$$f_{mn} = (f, \phi_m(x) L_n^{(\alpha)}(t))_\Omega, \quad F = (f_{mn}), \quad U = (\widetilde{u}_{mn}^h),$$

$$s_{pq}^t = \int_I {}_0D_t^\alpha J_q^{(-\alpha,\alpha)}(t) L_p(t) dt, \quad m_{pq}^t = \int_I J_q^{(-\alpha,\alpha)}(t) L_p(t) dt,$$

$$s_{pq}^h = \int_\Omega \mathcal{L}^{\frac{1}{2}} \phi_q \mathcal{L}^{\frac{1}{2}} \phi_p \, dx, \quad m_{pq}^h = \int_\Omega \phi_q \phi_p \, dx,$$

$$S^t = (s_{pq}^t), \quad M^t = (m_{pq}^t), \quad S^h = (s_{pq}^h), \quad M^h = (m_{pq}^h).$$

Then, we have

$$M^h \, U (S^t)^T + S^h \, U (M^t)^T = F.$$

Note that $S^t = \mathbf{I}$, but M^t is full and non-symmetric.

Usual approach: diagonalization with eigen-decomposition

Let $E := (\bar{e}_0, \cdots, \bar{e}_N)$ be the matrix formed by the orthonormal eigenvectors of the generalized eigenvalue problem $M^t \bar{e}_j = \lambda_j S^t \bar{e}_j$ and $\Lambda = \mathrm{diag}(\lambda_0, \cdots, \lambda_N)$, i.e.,

$$M^t E = S^t E \Lambda.$$

Setting $U = VE^T$, we arrive at

$$M^h V + S^h V \Lambda = G := F(S^t E)^{-T}.$$

Hence, the n-th column of the above matrix equation becomes:

$$(\lambda_n S^h + M^h)\mathbf{v}_n = \mathbf{g}_n, \qquad 0 \le n \le N.$$

- Very efficient: only requires solving N elliptic equations in Ω.
- However, since M^t is non-symmetric, this approach suffers from large roundoff errors.

Error comparison with eigen and QZ decompositions

Table: A comparison of decomposition errors between Eigen and QZ decompositions.

M	$\alpha = 0.7$		$\alpha = 0.7$ with enriched basis	
	Eigen	QZ	Eigen	QZ
4	5.91e-15	3.55e-16	3.86e-15	5.97e-16
8	2.56e-13	5.66e-16	2.53e-13	5.72e-16
12	4.05e-11	8.09e-16	6.11e-11	7.79e-16
16	3.27e-09	7.44e-16	7.49e-09	1.00e-15
20	5.85e-07	1.15e-15	9.68e-07	7.24e-16
24	8.23e-05	1.09e-15	2.85e-04	7.85e-16
28	4.54e-03	1.09e-15	2.80e-02	8.00e-16
32	1.88e-03	9.34e-16	9.08e-03	1.14e-15
100	3.16e-02	2.20e-15	1.05e-02	2.20e-15

New approach: QZ-decomposition

We consider the following QZ decomposition:

$$Q\,(S^t)^T Z = A, \quad Q\,(M^t)^T Z = B,$$

where Q, Z are unitary matrices, and A, B are upper triangular matrices.
Setting $U = VQ$, we arrive at

$$M^h\,V\,A + S^h\,V\,B = G := FZ.$$

We can solve the column vectors of V recursively,

$$(a_{n,n}M^h + b_{n,n}S^h)\,\mathbf{v}_n = g_n - h_{n-1}, \quad 0 \le n \le N.$$

where $h_{n-1} = \sum_{k=0}^{n-1} \left(a_{k,n}M^h + b_{k,n}S^h\right)\,\mathbf{v}_k$. with the total cost $= O(N^2M) + NT(M)$ ($T(M)$ the cost of solving one elliptic equation).

Error comparison with eigen and QZ decompositions

Table: A comparison of decomposition errors between Eigen and QZ decompositions.

M	$\alpha = 0.7$		$\alpha = 0.7$ with enriched basis	
	Eigen	QZ	Eigen	QZ
4	5.91e-15	3.55e-16	3.86e-15	5.97e-16
8	2.56e-13	5.66e-16	2.53e-13	5.72e-16
12	4.05e-11	8.09e-16	6.11e-11	7.79e-16
16	3.27e-09	7.44e-16	7.49e-09	1.00e-15
20	5.85e-07	1.15e-15	9.68e-07	7.24e-16
24	8.23e-05	1.09e-15	2.85e-04	7.85e-16
28	4.54e-03	1.09e-15	2.80e-02	8.00e-16
32	1.88e-03	9.34e-16	9.08e-03	1.14e-15
100	3.16e-02	2.20e-15	1.05e-02	2.20e-15

Error estimates

Lemma (Chen, S. & Wang '16). Let $\alpha \in (0,1)$. Then, for any $v \in \mathcal{B}^s_{-\alpha,\alpha}(I)$,

$$\|\pi_N^{(-\alpha,\alpha)} v - v\|_{\omega^{(-\alpha,\alpha)}} \lesssim N^{-(\alpha+s)} \|{}_0D_t^{\alpha+s} v\|_{\omega^{(s,s)}}.$$

and

$$\|{}_0D_t^{\alpha}(\pi_N^{(-\alpha,\alpha)} v - v)\|_I \lesssim N^{-s} \|{}_0D_t^{\alpha+s} v\|_{\omega^{(s,s)}}.$$

Theorem. If $u \in B^\alpha(\mathbb{D}) := H^s(I; L^2(\Omega)) \cap L^2(I; H_{\mathcal{L}}(\Omega))$ and ${}_0D_t^{\alpha+s} u \in L^2(\mathbb{D})$, we have

$$\|u - u_L\|_{B^\alpha(\mathbb{D})} \lesssim N^{-s} \|{}_0D_t^{\alpha+s} u\|_{L^2_{\omega^{(s,s)}}(\mathbb{D})} + \inf_{v_L(t,\cdot) \in V_h} \|u - v_L\|_{H^\alpha(I, H_{\mathcal{L}}(\Omega))}.$$

Unfortunately, u has weak singularity at $t = 0$. The approximation space in time only includes the strongest singular term t^α, so the achievable convergence rate in N is limited.

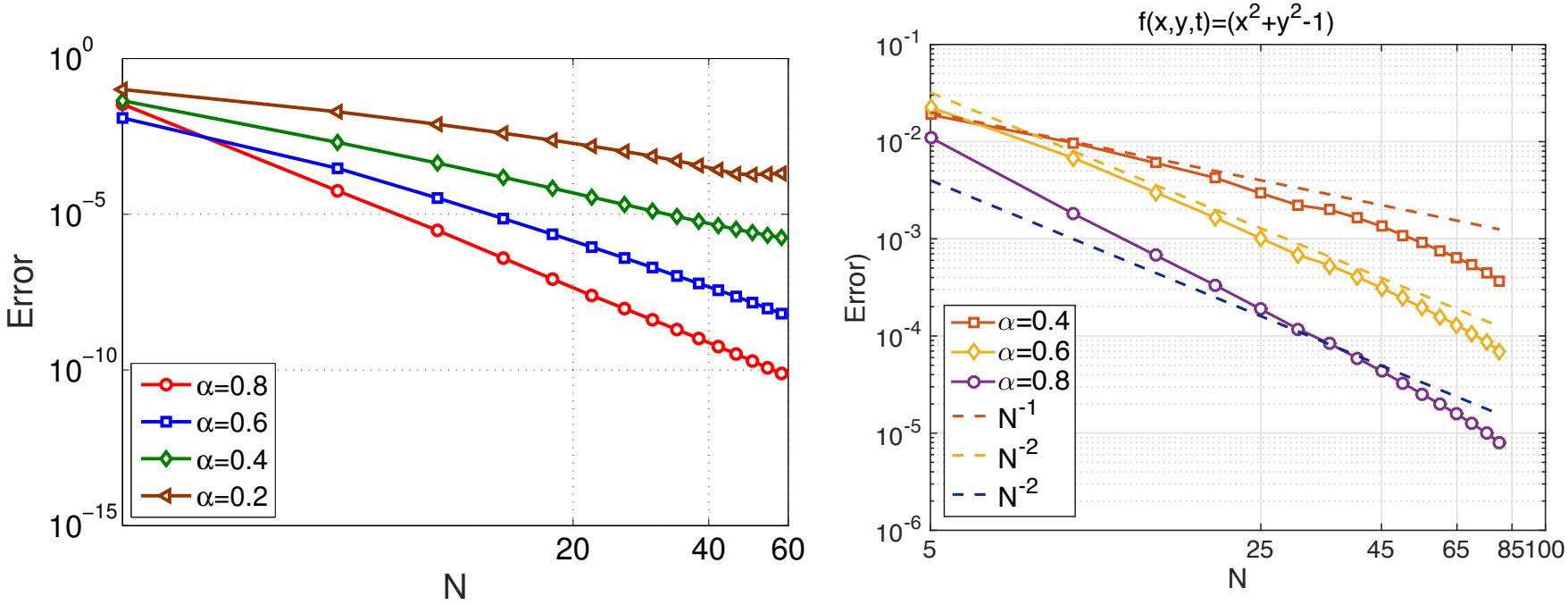

Figure: Error in B^α against various N. Left: with the exact solution $u(x, y, t) = \sin(\pi x)\sin(\pi y) \cdot \sin(\pi t^\alpha)$ in $(-1, 1)^2$; Right: with $f(x, y, t) = (x^2 + y^2 - 1)$ in a disk.

Enriched spectral method

We know from the Mittag-Leffler formula that the solution of fractional ODEs takes the form:

$$u = \sum_{i,j}^{\infty} \gamma_{ij}^{\alpha} t^{i+j\alpha}.$$

The GJFs only include the singular terms $t^{i+\alpha}$. In order to improve the convergence, we need to enrich the approximation space in time by other leading singular functions in the form of $\{t^{i+j\alpha}\}$:

$$\mathcal{F}_N^{(k,\alpha)}(I) = \mathcal{F}_N^{(\alpha)}(I) \oplus \{\text{first k terms of } t^{i+j\alpha} \text{ not in } \mathcal{F}_N^{(\alpha)}(I)\}.$$

Then, the enriched Petrov-Galerkin method is: Find $u_L^k \in V_h \otimes \mathcal{F}_N^{(k,\alpha)}$, such that

$$\mathcal{A}(u_L^k, v_L) = (g, v_L)_{\mathbb{D}}, \quad \forall v_L \in V_h \otimes \mathcal{P}_{N+k}.$$

- Using a modified Gram-Schmidt process, one can construct an orthogonal set of k enriched basis functions.
- The linear system can still be efficiently solved by using the QZ decomposition.
- The convergence rate can be increased to arbitrary order as we increase k.

Improved error estimates for the enriched spectral method

Theorem. Let $\bar{k}+\nu$ $(0<\nu<1)$ be the first $i+j\alpha$ not included in the enriched space.

- For $\max\{0,\alpha-\frac{1}{2}\}<\nu<\alpha$,

$$\|u-u_L^k\|_{B^\alpha(\mathbb{D})} \lesssim N^{-\bar{k}} + \inf_{v_L(t,\cdot)\in V_h} \|u-v_L\|_{H^\alpha(I,H_{\mathcal{L}}(\Omega))}.$$

- For $\alpha<\nu<\min\{1,\alpha+\frac{1}{2}\}$,

$$\|u-u_L^k\|_{B^\alpha(\mathbb{D})} \lesssim N^{-1-\bar{k}} + \inf_{v_L(t,\cdot)\in V_h} \|u-v_L\|_{H^\alpha(I,H_{\mathcal{L}}(\Omega))}.$$

- For $\alpha+\frac{1}{2}<\nu<1$,

$$\|u-u_L^k\|_{B^\alpha(\mathbb{D})} \lesssim N^{-2-\bar{k}} + \inf_{v_L(t,\cdot)\in V_h} \|u-v_L\|_{H^\alpha(I,H_{\mathcal{L}}(\Omega))}.$$

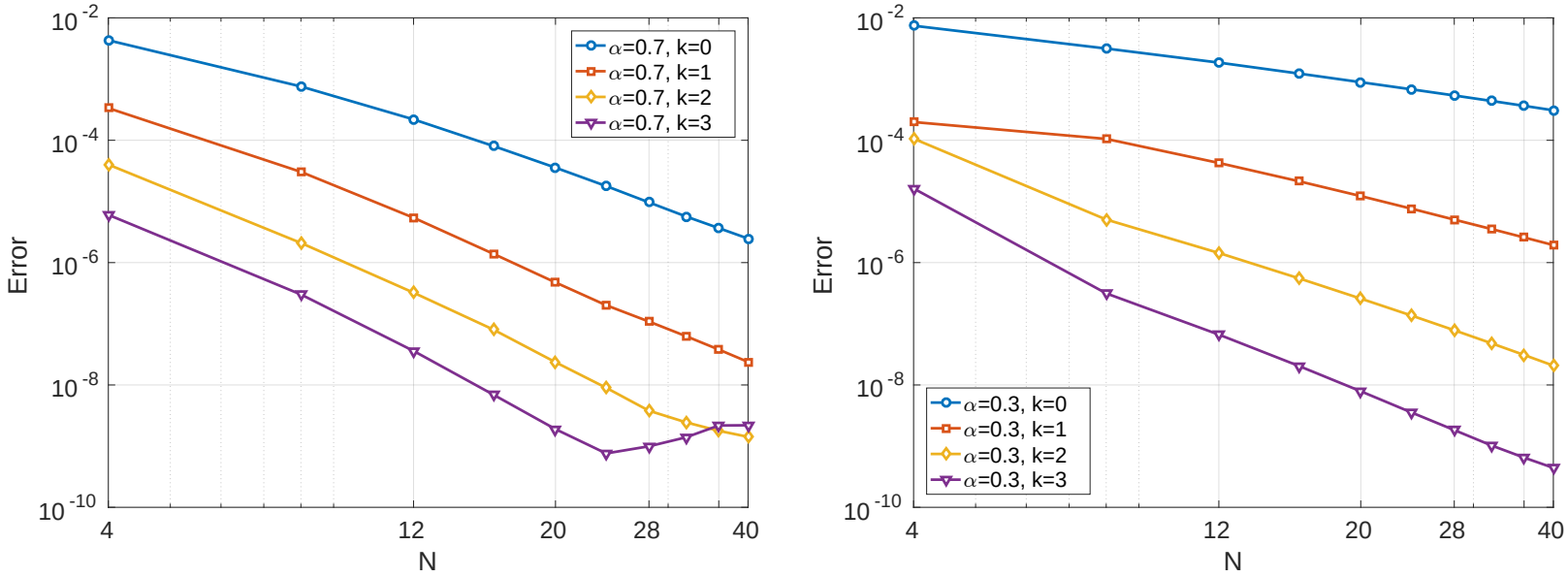

Figure: Errors in B^{α} against various N and α.

Extension to nonlinear problems

Consider now the nonlinear fractional PDEs:

$$ {}_0D_t^\alpha v(x,t) + \mathcal{L}v(x,t) + \mathcal{N}(v(x,t)) = g; \qquad v(x,0) = 0. $$

Let us denote

$$ \mathcal{A}(u,v) := ({}_0D_t^\alpha u, v)_{\mathbb{D}} + (\mathcal{L}^{\frac{1}{2}} u, \mathcal{L}^{\frac{1}{2}} v)_{\mathbb{D}} + (\mathcal{N}(u), v)_{\mathbb{D}}. $$

Petrov-Galerkin Approximation: Find $u_L \in V_h \otimes \mathcal{F}_N^{(\alpha)}$ s.t.

$$ \mathcal{A}(u_L, v_L) = (g, v_L)_{\mathbb{D}}, \quad \forall v_L \in V_h \otimes \mathcal{P}_N. $$

- The above nonlinear system can be solved by using Newton iteration which requires solving linear fractional PDEs with variable coefficients.
- We can use, as a preconditioner, the fast solver for linear fractional PDEs with constant coefficients. So the overall algorithm is still very efficient.

Time fractional Allen-Cahn equation

$$ {}_0^C D_t^\alpha u(x,t) - \epsilon^2 \Delta u(x,t) + f(u(x,t)) = 0, \qquad \forall (x,t) \in \Omega, $$

with the initial condition $u_0(x) = \begin{cases} 1, & 0 \le x \le 1, \\ -1, & -1 \le x < 0. \end{cases}$

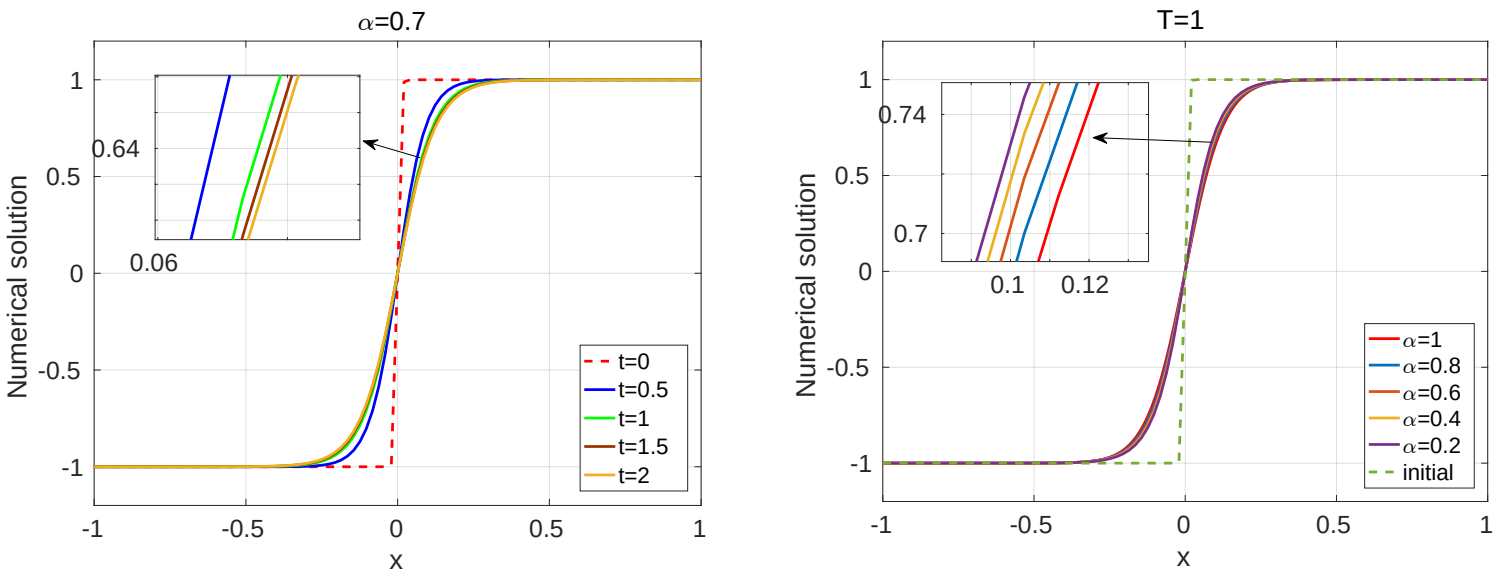

Figure: Solution profile. Left: $\alpha = 0.7$, $\epsilon = 0.1$ at various t; Right: $\epsilon = 0.1$ at $T = 1$ with various α.

Concluding remarks

Part I. We developed efficient numerical methods for fractional Laplacian in bounded domains:

- we adopt the Caffarelli-Silverstre extension and developed efficient and accurate Laguerre-spectral method to deal with the singularity in the extended direction:
  - The method is not intrusive and can be applied to any discretization in space.
  - The method is much more efficient and easy to implement than using a finite-element approach in the extended direction.
  - The approach presented here can be extended to more general fractional elliptic equations.

Part II. We developed efficient space-time Petrov-Galerkin method for time fractional PDEs using the following two new approaches:

- We use the QZ decomposition which leads to accurate decompositions for non-symmetric matrices.
- We enrich the GJF approximation space by adding leading singular terms to resolve the weak singularity at $t = 0$.

Our Petrov-Galerkin method enjoys the following advantages:

- Accuracy: the enriched spectral method with a small number of modes can effectively resolve the weak singularity at $t = 0$.
- Efficiency: the total cost is dominated by a small number of elliptic solvers in space variables.
- Flexibility: one can use any Galerkin type discretization in space.

Some future directions:

- How to effectively deal with fractional Laplacian in integral form with the Caffarelli-Silvestre extention?
- The space-time Petrov-Galerkin method is only effective for simulation of short-times or smooth evolutions. How to develop an efficient space-time method with a spectral-element discretization in-time?

Thank you!