Exponential Integrators for Fractional Differential Equations

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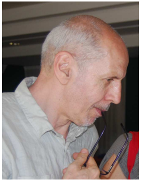
Outline and acknowledgements

1. Introduction to FDEs
2. Exponential integrators for FDEs
3. Example: a linear fractional Schrödinger equation



Igor Moret
Univeristy of Trieste - Italy

Marina Popolizio
Salento Univeristy - Italy

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Fractional derivative and FDEs

Fractional differential equations

$$D_{t_0}^{\alpha} y(t) = f(t, y(t))$$

$\alpha > 0$ is the order of the derivative operator

Caputo's definition of the fractional derivative

$$D_{t_0}^{\alpha} y(t) = \frac{1}{\Gamma(m-\alpha)} \int_{t_0}^{t} (t-s)^{m-\alpha-1} y^{(m)}(s) ds$$

- Coupled with initial conditions of Cauchy type $D^k y(t_0) = y_{0,k}$

✓ $\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt$ is the Euler gamma function $\Gamma(z+1) = z\Gamma(z)$

✓ $m = \lceil \alpha \rceil$ the smallest integer such that $m > \alpha$

✓ $y^{(m)}(s)$ classical derivative of integer order

Fields of applications

Polarization processes in disordered materials (polymers, biological tissues, etc.)

Control theory

Sedimentology

Finance

Mechanics (viscoelasticity and viscoplasticity)

Several other fields

Systems of linear FDEs

$$D_{t_0}^{\alpha} U(t) = A \cdot U(t) + F(t, U(t))$$

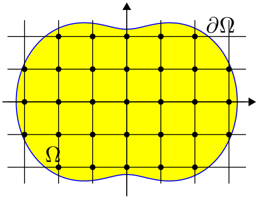
Linear term

$A \cdot U(t)$ stiff
A large and sparse

Non linear term

$F(t, U(t))$ non stiff

Usually from time–fractional PDEs



$$\frac{\partial^{\alpha}}{\partial t^{\alpha}} u(t,x) = \nu \nabla^2 u(t,x) + f(t,x)$$

$$\text{I.C.}: \; u(t_0, x) = u_0(x)$$

$$\text{B.C.}: \; u(t,x) = g(t,x), t > t_0, \; x \in \partial\Omega$$

Exponential integrators for ODEs

$$U'(t) = AU(t) + F(t, U(t)), \qquad U(0) = U_0$$

1. Methods based on the V.o.C. formula

$$U(t) = e^{tA}U_0 + \int_0^t e^{(t-\tau)A}F(\tau, U(\tau))\, d\tau$$

2. Discretization applied just to $F(\tau, U(\tau))$
3. Numerical evaluation of e^{tA} or φ–functions

Advantages: stability (stiff term evaluated exactly) with explicit schemes

Generalization to fractional order problems: change points 1) and 3) !

M. Hochbruck, Ostermann, A., Exponential integrators, *Acta Numerica*, 19, 209–286, 2010

The variation–of–constant formula for FDEs

$$D_{t_0}^{\alpha} U(t) = AU(t) + F(t) \qquad 0 < \alpha < 1$$

$\Downarrow$ *in the Laplace transform domain*

$$s^{\alpha} \hat{U}(s) - s^{\alpha-1} U_0 = A\hat{U}(s) + \hat{F}(s)$$

$\Downarrow$ *solve w.r.t. $\hat{U}(s)$*

$$\hat{U}(s) = s^{\alpha-1}\big(s^{\alpha} I - A\big)^{-1} U_0 + \big(s^{\alpha} I - A\big)^{-1} \hat{F}(s)$$

$\Downarrow$ *in the time domain*

$$\text{V.o.C. :} \quad U(t) = e_{\alpha,1}(t; A) U_0 + \int_0^t e_{\alpha,\alpha}(t-\tau; A) F(\tau)\, d\tau$$

$$e_{\alpha,\beta}(t; z) = \mathcal{L}^{-1}\left(\frac{s^{\alpha-\beta}}{s^{\alpha} - z}; t\right)$$

The variation–of–constant formula for FDEs

$$\text{V.o.C. :} \quad U(t) = e_{\alpha,1}(t; A)U_0 + \int_0^t e_{\alpha,\alpha}(t-\tau; A)F(\tau, U(\tau))\, d\tau$$

The kernel $e_{\alpha,\beta}(t; A)$ and the Mittag–Leffler (ML) function:

$$e_{\alpha,\beta}(t; A) = t^{\beta-1}E_{\alpha,\beta}(t^{\alpha}A) \qquad E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}$$

Some properties of the $e_{\alpha,\beta}$ function:

- Generalizes exponential $e_{1,1}(t; A) = e^{tA}$ and φ–functions
- No semigroup property $e_{\alpha,\beta}(t+s; A) \neq e_{\alpha,\beta}(t; A)e_{\alpha,\beta}(s; A)$

Polynomial approximation of $F(\tau, U(\tau))$:

$$U_n = e_{\alpha,1}(t; A)U_0 + h^{\alpha} \sum_{j=0}^{n-1} W_{\alpha}(n-j; h^{\alpha}A)\nabla^{\ell}F_{j+1}$$

Numerical evaluation of the ML function

$$e_{\alpha,\beta}(t;\lambda) = t^{\beta-1}E_{\alpha,\beta}(t^{\alpha}\lambda), \quad E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}$$

Convergence of the series can be extremely slow !

Some challenging problems: fast and accurate evaluation of $e_{\alpha,\beta}(t;\lambda)$
extension to matrix arguments

Method based on the Laplace transform

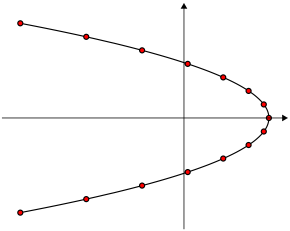
$$\mathcal{L}\Big(e_{\alpha,\beta}(t;\lambda)\,;\,s\Big) = \frac{s^{\alpha-\beta}}{s^{\alpha}-\lambda} \qquad e_{\alpha,\beta}(t,\lambda) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} e^{st}\frac{s^{\alpha-\beta}}{s^{\alpha}-\lambda}ds,$$

Numerical evaluation of the ML function

$$e_{\alpha,\beta}(t,\lambda) = \frac{1}{2\pi i}\int_{\mathcal{C}} e^{st}\frac{s^{\alpha-\beta}}{s^{\alpha}-\lambda}ds,$$

Parabolic contour + trapezoidal rule :

- simplicity of the contour
  $\mathcal{C} : z(u) = \mu(iu+1)^2$
- accurate estimation of the error
- fast computation and good accuracy
- matrix arguments via Schur decomposition



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Garrappa R., Numerical evaluation of two and three parameters Mittag–Leffler functions. *Submitted*

The fractional Schrödinger equation

$$i\hbar \frac{d}{dt}\psi = -\frac{\hbar^2}{2\widehat{m}}\nabla_x^2\psi + V(x)\psi,$$

$\widehat{m}$ particle mass - $V(x)$ potential energy

Two generalizations to fractional order:

1) $$i\hbar T_p^{\alpha-1}\, {}_0D_t^{\alpha}\psi = -\frac{\hbar^2}{2\widehat{m}}\nabla_x^2\psi + V(x)\psi$$

2) $$i^{\alpha}\hbar T_p^{\alpha-1}\, {}_0D_t^{\alpha}\psi = -\frac{\hbar^2}{2\widehat{m}}\nabla_x^2\psi + V(x)\psi$$

Main difference (active debate among physics): i or i^{α} ?

Different numerical issues

Naber M., Time fractional Schrödinger equation, *J. Math. Phys.*, 45(8), 3339–3352 (2004)

The fractional Schrödinger equation

$$ {}_0D_t^{\alpha} Y(t) = (-i)^{\eta} A Y(t) \qquad \eta \in \{\alpha, 1\} $$

Matrix A: discretization of the Hamiltonian

$$ A \approx \frac{1}{\hbar T_p^{\alpha-1}} \left(-\frac{\hbar^2}{2\widehat{m}} \nabla_x^2 + V(x) \right) $$

Exact solution:

$0 < \alpha < 1$: $Y(t) = e_{\alpha,1}(t; (-i)^{\eta} A) Y^{(0)}$

$1 < \alpha < 2$: $Y(t) = e_{\alpha,1}(t; (-i)^{\eta} A) Y^{(0)} + e_{\alpha,2}(t; (-i)^{\eta} A) Y^{(1)}$

Approximation of the Mittag–Leffler function with matrix arguments

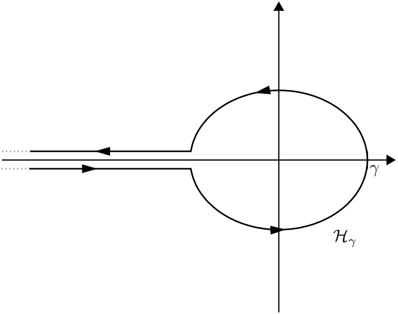
The ML function $e_{\alpha,1}(t;(-i)^\eta z)$ with complex arguments

$$e_{\alpha,\beta}(t;z) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} e^{st}\mathcal{E}_{\alpha,\beta}(s;z)ds$$

$$\Downarrow$$

$$e_{\alpha,\beta}(t;z) = \frac{1}{2\pi i}\int_{\mathcal{H}_\gamma} e^{st}\mathcal{E}_{\alpha,\beta}(s;z)ds$$

$$\Downarrow \gamma \to 0$$



$$e_{\alpha,\beta}(t;z) = \underbrace{\lim_{\gamma\to 0}\frac{1}{2\pi i}\int_{\mathcal{H}_\gamma} e^{st}\mathcal{E}_{\alpha,\beta}(s;z)ds}_{F^{(1)}_{\alpha,\beta}(t;z)} + \underbrace{\sum_{s^\star\in S} Res\big(e^{st}\mathcal{E}_{\alpha,\beta}(s;z),s^\star\big)}_{F^{(2)}_{\alpha,\beta}(t;z)}$$

$$e_{\alpha,\beta}(t;z) = F^{(1)}_{\alpha,\beta}(t;z) + F^{(2)}_{\alpha,\beta}(t;z)$$

The function $F^{(1)}_{\alpha,\beta}(t;z)$ and its behavior

$$e_{\alpha,\beta}(t;z) = F^{(1)}_{\alpha,\beta}(t;z) + F^{(2)}_{\alpha,\beta}(t;z)$$

$$\begin{aligned} F^{(1)}_{\alpha,\beta}(t;z) \quad = \quad & \frac{e^{i\beta\pi}}{2\pi i} G_{\alpha,\beta-\alpha}(t;\bar{z}) - \frac{e^{-i\beta\pi}}{2\pi i} G_{\alpha,\beta-\alpha}(t;z) \\ & - \frac{\bar{z} e^{-i(\alpha-\beta)\pi}}{2\pi i} G_{\alpha,\beta}(t;\bar{z}) + \frac{\bar{z} e^{i(\alpha-\beta)\pi}}{2\pi i} G_{\alpha,\beta}(t;z) \end{aligned}$$

$$G_{\alpha,\beta}(t;z) = \int_0^{+\infty} e^{-rt} K_{\alpha,\beta}(r;z) dr, \quad K_{\alpha,\beta}(r;z) = \frac{r^{\alpha-\beta}}{r^{2\alpha} - 2r^{\alpha}\Phi_{\alpha}(z) + |z|^2}$$

Bernstein's theorem: since $\Phi_{\alpha}(z) < |z|$ and $K_{\alpha,\beta}(r;z) \ge 0$, $G_{\alpha,\beta}(t;z)$ are monotonic (and also their derivatives).

$F^{(1)}_{\alpha,\beta}(t;z)$ is a regular function: no oscillatory behavior

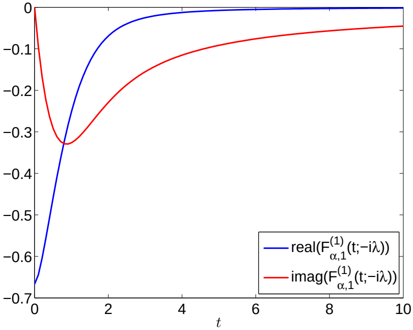
The function $F^{(1)}_{\alpha,\beta}(t;z)$ and its behavior

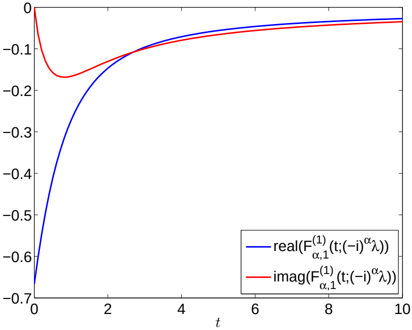
Equation 1)

$$F^{(1)}_{\alpha,1}(t; -i\lambda)$$

Equation 2)

$$F^{(1)}_{\alpha,1}(t; (-i)^{\alpha}\lambda)$$





The function $F^{(2)}_{\alpha,\beta}(t;z)$ and its behavior

$$e_{\alpha,\beta}(t;z) = F^{(1)}_{\alpha,\beta}(t;z) + F^{(2)}_{\alpha,\beta}(t;z)$$

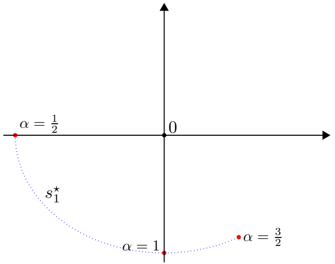
$$F^{(2)}_{\alpha,\beta}(t;z) = \sum_{s^\star \in S} Res\bigl(e^{st}\mathcal{E}_{\alpha,\beta}(s;z), s^\star\bigr) = \frac{1}{\alpha}\sum_{s^\star \in S} e^{ts^\star}(s^\star)^{1-\beta}.$$

Number and locations of poles of $\mathcal{E}_{\alpha,\beta}(s;z)$

$$s^\star_j = \bigl((-i)^\eta \lambda\bigr)^{1/\alpha} = \lambda^{1/\alpha} e^{i\frac{(4j-\eta)}{2\alpha}\pi}, \quad j \in \mathbb{Z}.$$

Only poles in the main Riemann sheet: $-\pi < \arg(s^\star_j) \le \pi$

The function $F^{(2)}_{\alpha,\beta}(t;z)$ for $z=-i\lambda$

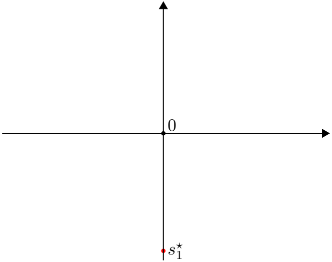
$0<\alpha\le\frac{1}{2}$	$\frac{1}{2}<\alpha\le\frac{3}{2}$
No poles	One pole at $s_1^\star=\lambda^{1/\alpha}e^{-i\frac{\pi}{2\alpha}}$
	
$F^{(2)}_{\alpha,\beta}(t;-i\lambda)=0$	$F^{(2)}_{\alpha,\beta}(t;-i\lambda)=\frac{1}{\alpha}e^{ts_1^\star}$

Two poles at $s_1^\star=\lambda^{1/\alpha}e^{-i\frac{\pi}{2\alpha}}$ and $s_2^\star=\lambda^{1/\alpha}e^{-i\frac{3\pi}{2\alpha}}$ when $\frac{3}{2}\le\alpha<2$

The function $F^{(2)}_{\alpha,\beta}(t;z)$ for $z=(-i)^\alpha\lambda$

$0<\alpha<\frac{4}{3}$

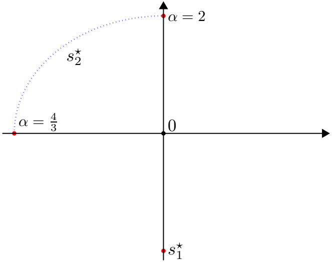
1 pole $s_1^\star = -i\lambda^{1/\alpha}$



$$F^{(2)}_{\alpha,\beta}(t;-i^\alpha\lambda) = \frac{1}{\alpha}e^{-it\lambda^{1/\alpha}}$$

$\frac{4}{3}\le\alpha<2$

2 poles $s_1^\star = -i\lambda^{1/\alpha}$
$s_2^\star = \lambda^{1/\alpha}e^{-i\frac{(4-\alpha)\pi}{2\alpha}}$



$$F^{(2)}_{\alpha,\beta}(t;-i^\alpha\lambda) = \frac{e^{-it\lambda^{\frac{1}{\alpha}}}+e^{ts_2^\star}}{\alpha}$$

Oscillations of $e_{\alpha,1}(t; z)$

Equation 1)	
	$z = -i\lambda$
$0 < \alpha \leq \frac{1}{2}$	Over-damped (no osccillations)
$\frac{1}{2} < \alpha < 1$	Damped (return to equilibrium after oscillations)
$1 < \alpha < 2$	Unstable behavior

Equation 2)	
	$z = (-i)^{\alpha}\lambda$
$0 < \alpha < \frac{4}{3}$	Undamped persisting oscillations
$\frac{4}{3} \leq \alpha < 2$	Undamped persisting oscillations + Damped

$\alpha \approx 1$ is interesting from the physical point of view

Krylov subspace methods

Approximation of $e_{\alpha,1}(t; -iA)v$ and $e_{\alpha,1}(t; (-i)^{\alpha}A)v$

A real, positive and symmetric matrix $\quad \sigma(A) \subset [a, +\infty)$, $a > 0$

Size of A: $2,500 \times 2,500$

Krylov subspace methods (Projection w.r.t A and not $(-i)^{\eta}A$)

$$e_{\alpha,1}(t; (-i)^{\eta}A)v \approx V_m e_{\alpha,1}(t; (-i)^{\eta}H_m)e_1$$

Polynomial: $\mathbb{K} = K_m(A, v)$

Rational: $\mathbb{K} = K_m(Z, v), \quad Z = (\delta I + A)^{-1} \quad \delta > 0$

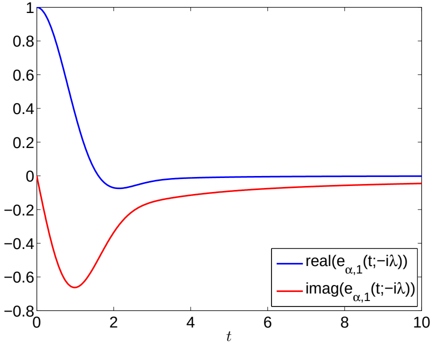
A-priori estimation of the error

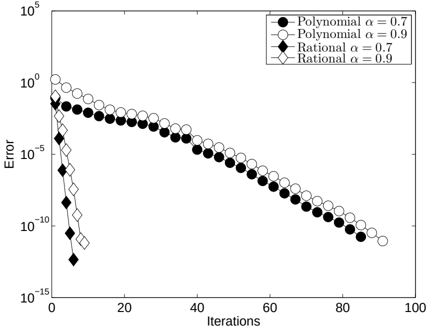
Comparison with numerical results

Garrappa R., Moret I. and Popolizio M., Sovling the time–fractional Schrödinger equation by Krylov projection methods. *J. Comput. Phys.*, in press (available on-line)

Evaluation of $e_{\alpha,1}(t; -iA)v$

Damped oscillations with return to equilibrium when $\frac{1}{2} < \alpha < 1$



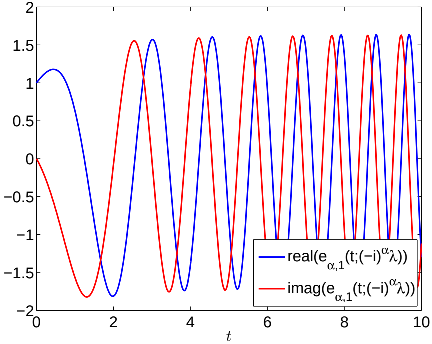


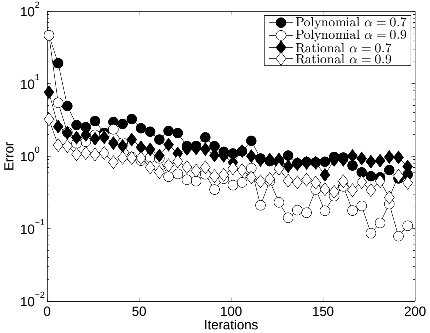
$$\text{Polynomial:} \quad Err_m \le C \frac{\|(t^\alpha A)^m v\|}{(\alpha m)^{\alpha m}} e^{\alpha m}$$

$$\text{Rational:} \quad Err_m \le C \frac{\|Av\|}{\delta} \left[\exp(t\delta^{\frac{1}{\alpha}}) q_\alpha^m + \sqrt{\cos\mu}\, e^{-mC_{\alpha,t,\delta}} \right] \qquad 0 < q_\alpha < 1$$

Evaluation of $e_{\alpha,1}(t;(-i)^{\alpha}A)v$

Persisting oscillations for $0 < \alpha < 1$

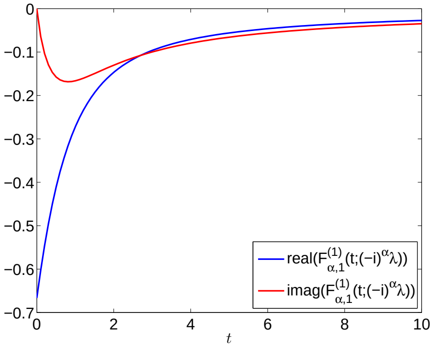


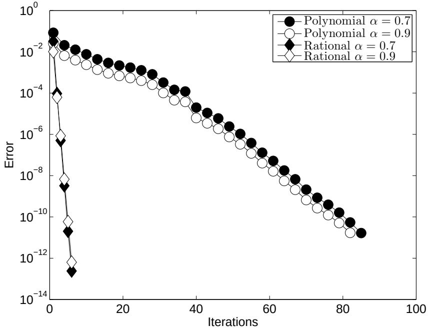


$$e_{\alpha,1}(t;(-i)^{\alpha}A) = F^{(1)}_{\alpha,1}(t;(-i)^{\alpha}A) + F^{(2)}_{\alpha,1}(t;(-i)^{\alpha}A)$$

Evaluation of $e_{\alpha,1}(t;(-i)^\alpha A)v$

$$e_{\alpha,1}(t;(-i)^\alpha A) = F^{(1)}_{\alpha,1}(t;(-i)^\alpha A) + F^{(2)}_{\alpha,1}(t;(-i)^\alpha A)$$



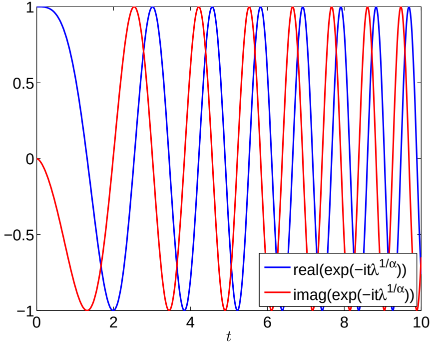


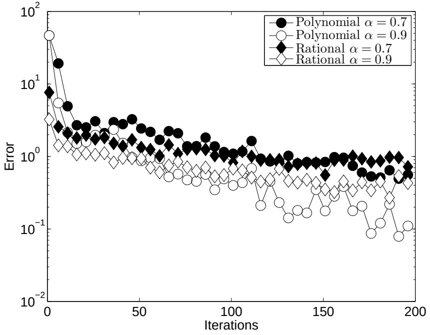
Polynomial: $Err_m \le C \dfrac{\|Av\|}{a} \exp(tC_{A,\alpha}) \exp\left(-m\sqrt{2/R}\right) \qquad R = \mathcal{K}(A) - 1$

Rational: $Err_m \le C \dfrac{\|Av\|}{a} \exp(tC_{A,\alpha}) \left(3^{-m} + B_{A,\alpha,t,m} \exp(-mD_{A,\alpha,t,m})\right)$

Evaluation of $e_{\alpha,1}(t;(-i)^\alpha A)v$

$$e_{\alpha,1}(t;(-i)^\alpha A) = F^{(1)}_{\alpha,1}(t;(-i)^\alpha A) + F^{(2)}_{\alpha,1}(t;(-i)^\alpha A) \qquad F^{(2)}_{\alpha,1}(t;(-i)^\alpha A) = \frac{1}{\alpha}\exp\left(-itA^{\frac{1}{\alpha}}\right)$$





$$\text{Polynomial:}\quad Err_m \le C\frac{\|A^2 v\|}{a^2}\exp(tC_{A,\alpha})\left(\exp\left(-m\sqrt{\frac{2}{R}}\right)+\left(\frac{\sqrt{2R}}{m}\right)^{\frac{2(2\alpha-1)}{2-\alpha}}\right)$$

$$\text{Rational:}\quad Err_m \le C\frac{\|A^2 v\|}{a^2}\exp(tC_{A,\alpha})\left(3^{-m}+B_\alpha m^{-\frac{2(2\alpha-1)}{\alpha+2}}\right)$$

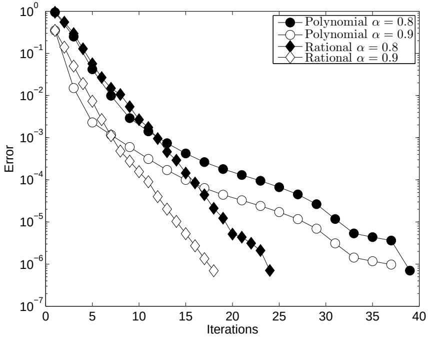
Evaluation of $e_{\alpha,1}(t; (-i)^{\alpha} A)v$

Alternative approach:

$$y_{\alpha}(t) = F_{\alpha,1}^{(1)}(t; (-i)^{\alpha} A)v + \widetilde{y}_{\alpha}(t), \qquad \widetilde{y}_{\alpha}(t) = \frac{1}{\alpha} e^{-itA^{1/\alpha}} v$$

$$\begin{cases} \widetilde{y}_{\alpha}(t_{n+1}) = e^{-ihA^{1/\alpha}} \widetilde{y}_{\alpha}(t_n) \\ \widetilde{y}_0 = \frac{1}{\alpha} v \end{cases}$$

$$h = 0.0001$$



Main issues (related to the computational cost):

- Efficient generation of $K_m(A, v)$ and $K_m((\delta I + A)^{-1}, v)$
- Balancing of m and h

Some references

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