Regularization of backwards diffusion by fractional time derivatives

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joint work with
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Outline

- backwards diffusion and quasi reversibility
- fractional derivatives and Mittag-Leffler functions
- regularization based on subdiffusion
- reconstructions - numerical experiments
- convergence analysis

backwards diffusion and quasi reversibility

Backwards diffusion

Reconstruct initial data $u_0(x) = u(x,0)$ in

$$\begin{aligned} u_t - \mathbb{L}u &= 0, \quad (x,t) \in \Omega \times (0,T) + \text{boundary conditions} \\ u(x,0) &= u_0 \quad x \in \Omega \end{aligned}$$

from final time values

$$u(x,T) = u_T(x) \quad x \in \Omega$$

where $\mathbb{L}$ is a uniformly elliptic second order partial differential operator defined in a C^2 domain Ω with sufficiently smooth coefficients.

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- This is a classical inverse problem.
- More recent applications are, e.g.:
  - identification of airborne contaminants
  - imaging with acoustic or elastic waves in the presence of strong attenuation
  - deblurring

Quasi-reversibility

Replace diffusion equation

$$u_t - \mathbb{L}u = 0\,, \quad u(T) = u_T$$

by a nearby differential equation, e.g.,
[Làttes & Lions 1969] weakly damped wave or beam equation

$$\varepsilon u_{tt} + u_t - \mathbb{L}u = 0\,, \quad u(T) = u_T \qquad u_t - \mathbb{L}u + \varepsilon\mathbb{L}^2 u = 0\,, \quad u(T) = u_T$$

drawback: additional boundary and/or initial conditions needed.

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[Showalter 1974,'75,'76] add inviscid term

$$(I - \epsilon\mathbb{L})u_t^\epsilon - \mathbb{L}u^\epsilon = 0, \,, \quad u(T) = u_T$$

see also the proof of the Hille-Phillips-Yosida Theorem.

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[Ames, Clark, Epperson, Oppenheimer, 1998; '94] quasi-final value

$$u_t - \mathbb{L}u = 0\,, \quad \epsilon u(0) + u(T) = u_T$$

This is in fact Tikhonov/Lavrentiev regularization and not causality preserving.

Quasi-reversibility

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by a nearby differential equation.

Here: Replace u_t by a fractional time derivative of order $\alpha < 1$

$$\partial_t^\alpha u_t - \mathbb{L}u = 0\,, \quad u(T) = u_T$$

with $\alpha < 1$, i.e., replace diffusion by subdiffusion.

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This is natural in view of modeling (both diffusion and subdiffusion are limits of continuous time random walks)
and causality preserving.

fractional derivatives and Mittag-Leffler functions

Fractional derivatives

Abel fractional integral operator

$$I_a^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t \frac{f(s)}{(t-s)^{1-\alpha}}\, ds$$

Then a fractional (time) derivative can be defined by either

$${}_a^R D_t^\alpha f = \frac{d}{dt} I_a^{1-\alpha} f \quad \text{Riemann-Liouville derivative}$$

or

$${}_a^C D_t^\alpha f = I_a^{1-\alpha} \frac{df}{ds} \quad \text{Djrbashian-Caputo derivative}$$

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- R-L is defined on a larger function space, but derivative of constant is nonzero; singularity at initial time *a*
- D-C maps constants to zero ⇝ appropriate for prescribing initial values

Nonlocal and causal character of these derivatives provides them with a “memory” ⇝ initial values are tied to later values and can therfore be better reconstructed backwards in time.

Mittag-Leffler functions: solutions to ODEs/PDEs

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)} \qquad \alpha > 0,\ \beta \in \mathbb{R}, \quad z \in \mathbb{C},$$

generalizes exponential $E_{1,1}(z) = e^z$; $\qquad E_\alpha := E_{\alpha,1}$

[Djrbashian 1966,'93, Jin&Rundell 2015, Gorenflo&Kilbas&Mainardi&Rogosin 2014]

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Lemma

For $0 < \alpha \leq 1$ *and* $x, t > 0$, $\lambda > 0$

$$\alpha\,\lambda \frac{d}{dx} E_{\alpha,1}(-\lambda x) = -E_{\alpha,\alpha}(-\lambda x).$$

Consequently, $u(t) := E_{\alpha,1}(-\lambda t^\alpha)$ solves fractional ODE $\quad \partial_t^\alpha u + \lambda u = 0$.

Mittag-Leffler functions: asymptotics

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Theorem (Djrbashian, 1966,'93)

Let $\alpha \in (0,2)$, $\beta \in \mathbb{R}$, *and* $\mu \in (\alpha\pi/2, \min(\pi, \alpha\pi))$, *and* $N \in \mathbb{N}$. *Then for* $|\arg(z)| \leq \mu$ *with* $|z| \to \infty$,

$$E_{\alpha,\beta}(z) \sim \frac{1}{\alpha} z^{\frac{1-\beta}{\alpha}} e^{z^{\frac{1}{\alpha}}}$$

and for $\mu \leq |\arg(z)| \leq \pi$ *with* $|z| \to \infty$

$$E_{\alpha,\beta}(z) = -\sum_{k=1}^{N} \frac{1}{\Gamma(\beta - \alpha k)} \frac{1}{z^k} + O\left(\frac{1}{z^{N+1}}\right).$$

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For $x \to +\infty$

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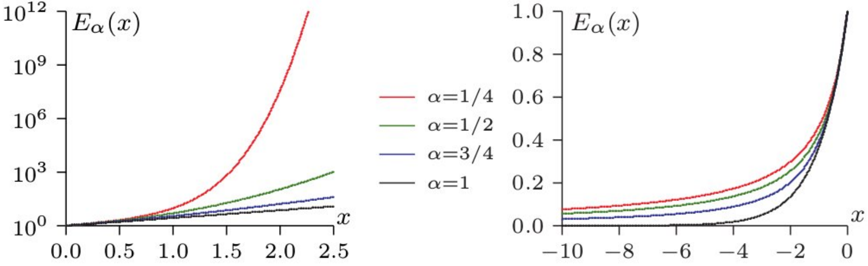
On the positive real axis, $E_{\alpha,\beta}$ grows superexponetially.
On the negative real axis, $E_{\alpha,\beta}$ decreases only linearly.



regularization based on subdiffusion

Subdiffusion regularization — the quasi-reversibility paradigm

Replace diffusion equation

$$u_t + Au = 0$$

by subdiffusion equation

$$\partial_t^\alpha u_t + Au = 0$$

with $\alpha < 1$, $\alpha \nearrow 1$ (regularization parameter);
note that $\lim_{\alpha \to 1^-} \partial_t^\alpha u = u_t$ but i.g. $\lim_{\alpha \to 1^+} \partial_t^\alpha u \neq u_t$

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- numerical computations based on finite element - finite difference approximations, see, e.g., [Langlands, Henry 2005; Lin, Xu, 2007; Jin, Lazarov, Zhou, 2013, 2016; Alikhanov 2015; Mustapha, Abdallah, Furati 2015]

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- analysis based on separation of variables and properties of Mittag-Leffler functions

Solution representation by separation of variables

1-d ODE:

$$u'(t) + \lambda u(t) = 0\,, \qquad u(T) = e^{-\lambda T} u(0)\,, \qquad u(0) = e^{\lambda T} u(T)$$

PDE with elliptic operator $A = -\mathbb{L}$
with eigensystem $\lambda_j \nearrow \infty$, $\phi_j \in H^2(\Omega) \cap H_0^1(\Omega)$, $j \in \mathbb{N}$:

$$u_t(t) + Au(t) = 0\,, \qquad u(x,0) = \sum_{j=1}^{\infty} e^{\lambda_j T} \langle u(\cdot, T), \phi_j \rangle \phi_j(x)$$

exponential amplification of noise in Fourier coefficients $\langle u(\cdot, T), \phi_j \rangle$

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replace diffusion by subdiffusion:

1-d ODE:

$$\partial_t^\alpha u(t)+\lambda u(t)=0\,,\quad u(T)=E_{\alpha,1}(-\lambda T^\alpha)u(0)\,,\quad u(0)=\frac{u(T)}{E_{\alpha,1}(-\lambda T^\alpha)}$$

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where $E_{\alpha,1}$ is a Mittag-Leffler function.

Plain subdiffusion regularization

backwards diffusion $u_t + Au = 0$,

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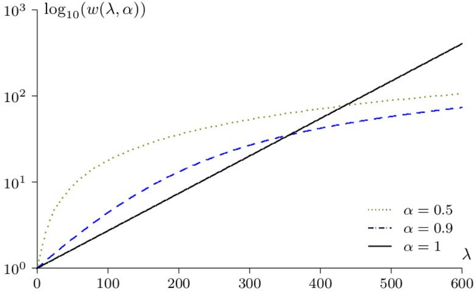

$\rightsquigarrow$ more stable for large frequencies, less stable for small frequencies

Split frequency subdiffusion regularization

backwards diffusion $u_t + Au = 0$, $u(x, T) = u_T \approx u_T^\delta \approx \tilde{u}_T^\delta$,
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backwards diffusion on small frequencies, subdiffusion on large frequencies

$$\langle u_{0,\alpha}^\delta, \phi_j\rangle = \begin{cases} w(\lambda_j, 1)\langle u_T^\delta, \phi_j\rangle & \text{for } j \le K \\ w(\lambda_j, \alpha)\langle \tilde{u}_T^\delta, \phi_j\rangle & \text{for } j \ge K+1 \end{cases} \ \text{ with } \ w(\lambda,\alpha) = \frac{1}{E_{\alpha,1}(-\lambda T^\alpha)}$$

$\rightsquigarrow$ regularization parameters α, K

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numerical computations:

- perform truncated SVD on $P_{lo}\, u_T^\delta$ $\quad\rightsquigarrow\quad$ $P_{lo}\, u_{0,\alpha,K}^\delta$
- backpropagate $P_{hi}\, \tilde{u}_T^\delta$ by subdiffusion PDE $\quad\rightsquigarrow\quad$ $P_{hi}\, u_{0,\alpha,K}^\delta$

where $P_{lo} = P_{\text{span}\{\phi_1,\ldots,\phi_K\}}$, $P_{hi} = I - P_{lo}$
... projections onto low and high frequencies, respectively

Multiple split frequency subdiffusion regularization

backwards diffusion $u_t + Au = 0,\ u(x,T) = u_T \approx u_T^\delta \approx \tilde{u}_T^\delta$,
in terms of Fourier coefficients:

$$\langle u_0, \phi_j\rangle = w(\lambda_j)\langle u_T^\delta, \phi_j\rangle \ \text{ for } j \le K \ \text{ with } \quad w(\lambda) = e^{\lambda T} = \frac{1}{e^{-\lambda T}}$$

backwards diffusion on small frequencies, subdiffusion on larger frequencies

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$\rightsquigarrow$ regularization parameters $\alpha_1 > \alpha_2 > \cdots > \alpha_\ell,\ \ K_1 < K_2 < \cdots < K_{\ell+1}$

Other regularization approaches based on fractional derivatives

- add fracional time derivative:

  $$u_t + Au = 0 \quad \rightsquigarrow \quad u_t + \varepsilon \partial_t^\alpha u + Au = 0$$

  amplification factors
  $w(\lambda, \alpha, \beta, \varepsilon) = \left(\mathcal{L}^{-1} \left(\frac{1+\epsilon s^{\alpha-1}}{s+\epsilon s^\alpha + \lambda} \right) \right)^{-1} \sim \frac{\pi T^\alpha \Gamma(1-\alpha)}{\sin(\alpha\pi)} \frac{1}{\epsilon} \lambda$
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- add fractional space derivative A^β, e.g., $\lambda_j \to \lambda_j^\beta$:

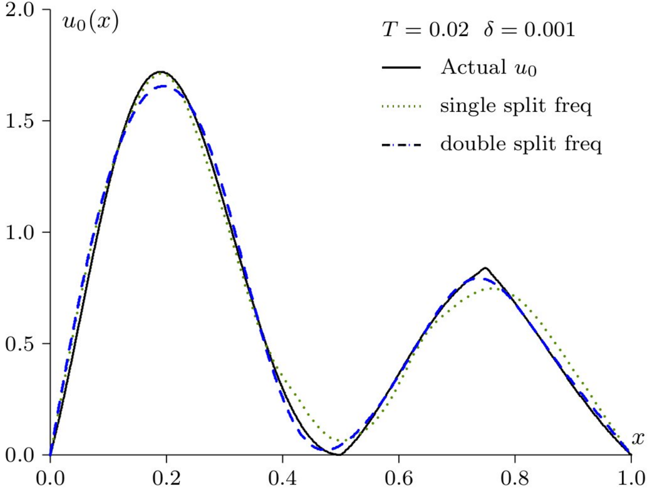
$$u_t + Au = 0 \quad \rightsquigarrow \quad (I + \varepsilon A^\beta)\partial_t^\alpha u + Au = 0$$

  amplification factors $\quad w(\lambda, \alpha, \beta, \varepsilon) = \frac{1}{E_{\alpha,1}(-\frac{\lambda}{1+\varepsilon\lambda^\beta} T^\alpha)}$

  regularization parameters $\alpha, \beta, \varepsilon$

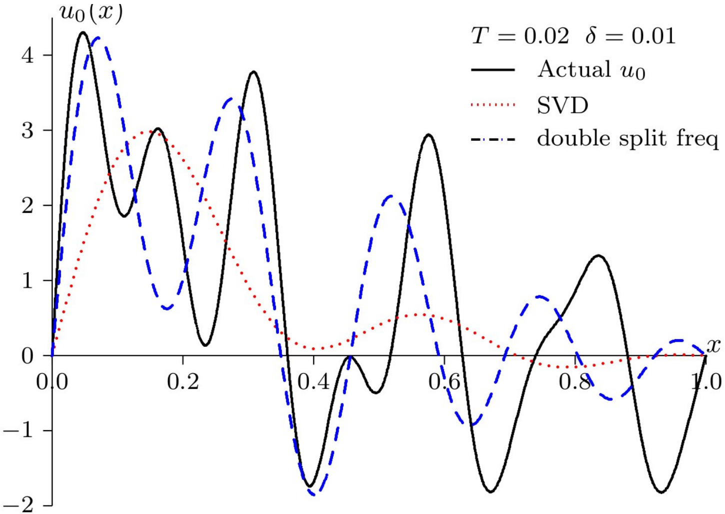
reconstructions - numerical experiments

Test case 1: u_0 with kink; $\delta = 0.1\%$



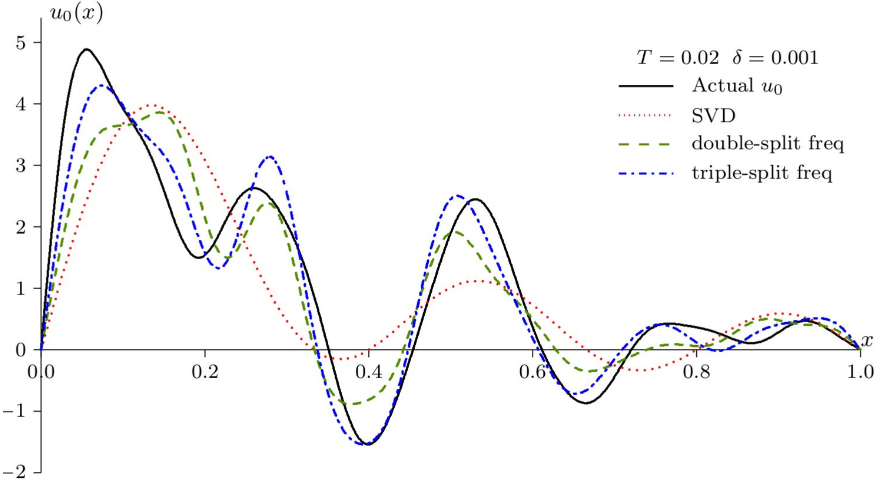
Reconstructions from single and double split frequency method.
single split: $K_1 = 4$ and $\alpha = 0.92$;
double split: $K_1 = 4$, $K_2 = 10$ and $\alpha_1 = 0.999$, $\alpha_2 = 0.92$.

Test case 2: u_0 with $\langle u_0, \phi_j \rangle \neq 0$, $j = 1, \ldots, 7, 10 \ldots, 15$; $\delta = 1\%$



Reconstructions from truncated SVD, single and double split frequency method.

Test case 3: u_0 with $\langle u_0, \phi_j \rangle \neq 0$, $j = 1, \ldots, 7, 10 \ldots, 15$; $\delta = 1\%$



Reconstructions from truncated SVD, single, double, and triple split frequency method.

convergence analysis

Plain subdiffusion regularization

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Properties of the Mittag-Leffler function $E_{\alpha,1}(-\lambda x)$ (I)

[Djrbashian 1966,'93, Jin&Rundell 2015, Gorenflo&Kilbas&Mainardi&Rogosin 2014]

Lemma

For $0 < \alpha < 1$ *and* $x > 0$

$$\frac{1}{1+\Gamma(1-\alpha)x} \leq E_{\alpha,1}(-x) \leq \frac{1}{1+\Gamma(1+\alpha)^{-1}x}$$

Consequently, we have the stability estimate $\frac{1}{E_{\alpha,1}(-\lambda T^{\alpha})} \leq \bar{C}\frac{\lambda}{1-\alpha}$

Properties of the Mittag-Leffler function $E_{\alpha,1}(-\lambda x)$ (II)

Lemma (BK&Rundell 2018)

For any $\alpha_0 \in (0,1)$ *and* $p \in [1, \frac{1}{1-\alpha_0})$, *there exists* $C = C(\alpha_0, p) > 0$ *such that for all* $\lambda \geq \lambda_1$, $\alpha \in [\alpha_0, 1)$

$$|E_{\alpha,1}(-\lambda T^{\alpha}) - \exp(-\lambda T)| \leq C\lambda^{1/p}(1-\alpha)\,.$$

Consequently, we have the convergence rate $\left|\dfrac{\exp(-\lambda T)}{E_{\alpha,1}(-\lambda T^{\alpha})} - 1\right| \leq \tilde{C}\lambda^{1+1/p}$

with α_0, α, p, λ_1, λ as above, $\tilde{C} = \tilde{C}(\alpha_0, p) > 0$.

Exponential ill-posedness $\longrightarrow$ mild ill-posedness

backwards diffusion:

$$\langle u_0, \phi_j \rangle = w(\lambda_j) \langle u_T, \phi_j \rangle \quad \text{with} \quad w(\lambda) = e^{\lambda T} = \frac{1}{e^{-\lambda T}}$$

$\rightsquigarrow$ exponential instability.

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backwards subdiffusion

$$\langle u_{0,\alpha}^{\delta}, \phi_j \rangle = w(\lambda_j, \alpha) \langle \tilde{u}_T^{\delta}, \phi_j \rangle \quad \text{with} \quad w(\lambda, \alpha) = \frac{1}{E_{\alpha,1}(-\lambda T^{\alpha})}$$

stability estimate $\quad \dfrac{1}{E_{\alpha,1}(-\lambda T^{\alpha})} \leq \dfrac{\bar{C}}{1-\alpha} \lambda$

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and Sobolev norm equivalence $\quad \|v\|_{H^s(\Omega)} \sim \sum_{j=1}^{\infty} \lambda_j^s \langle v, \phi_j \rangle^2$

$\Longrightarrow$ $H^2 - L^2$ stability of backwards subdiffusion,
with a stability constant that degenerates as $\alpha \nearrow 1$.

Pre-smoothing the data

$$u(x,T) = \underbrace{u_T}_{\in C^\infty(\Omega)} \approx \overbrace{\underbrace{u_T^\delta}_{\in L^2(\Omega)}}^{\text{noisy}} \underset{\substack{\uparrow \\ \text{mildly ill-posed}}}{\approx} \overbrace{\underbrace{\tilde{u}_T^\delta}_{\in H^2(\Omega)}}^{\text{smoothed}}$$

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Here an exponential source condition is satisfied.

Tikhonov regularization would not properly pre-smooth due to saturation.

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Use Landweber iteration for defining $\tilde{u}_T^\delta = v^{(i_*)}$

$$v^{(i+1)} = v^{(i)} - \mu A^{-s/2}(v^{(i)} - u_T^\delta), \qquad v^{(0)} = 0,$$

with $\mu > 0$ chosen so that $\mu \|A^{-s/2}\|_{L^2 \to L^2} \leq 1$.

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Lemma (BK&Rundell 2018; pre-smoothing)

A choice of $i_* \sim T^{-2} \log\left(\frac{1}{\delta}\right)$ *yields* $\|u_T - \tilde{u}_T^\delta\|_{L^2(\Omega)} \leq C_1 \delta$,

$$\|u_T - \tilde{u}_T^\delta\|_{H^s(\Omega)} \sim \|A^{s/2}(u_T - \tilde{u}_T^\delta)\|_{L^2(\Omega)} \leq \frac{C_2}{T}\,\delta \sqrt{\log\left(\frac{1}{\delta}\right)} =: \tilde{\delta}$$

for some $C_1, C_2 > 0$ *independent of* T *and* δ.

Convergence with a priori choice of α

$$Fu_0 = u_T$$

with forward operator $F = \exp(-AT)$

Theorem (BK&Rundell 2018)

Let $u_0 \in L^2(\Omega)$, $A^{1+1/p}u_0 \in L^2(\Omega)$ *for some* $p \in (1,\infty)$, $\tilde{u}_T^\delta = v^{(i_*)}$ *as in pre-smoothing Lemma with* $s \geq 2(1+\frac{1}{p})$, *and assume that* $\alpha = \alpha(\tilde{\delta})$ *is chosen such that*

$$\alpha(\tilde{\delta}) \nearrow 1 \text{ and } \frac{\tilde{\delta}}{1-\alpha(\tilde{\delta})} \to 0\,, \qquad \text{as } \tilde{\delta} \to 0\,,$$

Then

$$\|u^\delta_{0,\alpha(\tilde{\delta})} - u_0\|_{L^2(\Omega)} \to 0\,, \qquad \text{as } \tilde{\delta} \to 0\,.$$

Backwards time fractional diffusion is a regularization method.

Convergence with a posteriori choice of α

$$Fu_0 = u_T$$

with forward operator $F = \exp(-AT)$

Theorem (BK&Rundell 2018)

Let $u_0 \in L^2(\Omega)$, $A^{1+1/p} u_0 \in L^2(\Omega)$ for some $p \in (1, \infty)$, $\tilde{u}_T^\delta = v^{(i_*)}$ as in pre-smoothing Lemma with $s \geq 2(1 + \frac{1}{p})$, and assume that $\alpha = \alpha(\tilde{u}_T^\delta, \tilde{\delta})$ is chosen according to

$$\underline{\tau}\tilde{\delta} \leq \|Fu_0^\delta(\cdot; \alpha) - \tilde{u}_T^\delta\| \leq \overline{\tau}\tilde{\delta}$$

(discrepancy principle) with fixed $1 < \underline{\tau} < \overline{\tau}$.
Then

$$u^\delta_{0,\alpha(\tilde{\delta})} \rightharpoonup u_0 \text{ in } L^2(\Omega)\,, \qquad \text{as } \tilde{\delta} \to 0\,.$$

Backwards time fractional diffusion is a regularization method.

Convergence rates

Theorem (BK&Rundell 2018)

Let $u_0 \in L^2(\Omega)$, $A^{1+1/p+\max\{1/p,q\}} u_0 \in L^2(\Omega)$ *for some* $p \in (1,\infty)$, $q > 0$, $\tilde{u}_T^\delta = v^{(i_*)}$ *as in pre-smoothing Lemma with* $s \geq 2(1+\frac{1}{p})$, *and assume that* $\alpha = \alpha(\tilde{u}_T^\delta, \tilde{\delta})$ *is chosen according to*

$$1 - \alpha(\tilde{\delta}) \sim \sqrt{\tilde{\delta}}\,, \qquad \text{as } \tilde{\delta} \to 0\,.$$

Then

$$\|u^\delta_{0,\alpha(\tilde{\delta})} - u_0\|_{L^2(\Omega)} = O\left(\log(\tfrac{1}{\delta})^{-2q}\right)\,, \qquad \text{as } \delta \to 0\,.$$

In the noise free case we have

$$\|u^0_{0,\alpha} - u_0\|_{L^2(\Omega)} = O\left(\log(\tfrac{1}{1-\alpha})^{-2q}\right)\,, \qquad \text{as } \alpha \nearrow 1\,.$$

Finite Sobolev regularity (≡ log-source condition) implies log rate.

Split frequency subdiffusion regularization

backwards diffusion $u_t + Au = 0$, $u(x,T) = u_T \approx u_T^\delta \approx \tilde{u}_T^\delta$,
in terms of Fourier coefficients:

$$\langle u_0, \phi_j \rangle = w(\lambda_j) \langle u_T^\delta, \phi_j \rangle \quad \text{for } j \le K \quad \text{with} \qquad w(\lambda) = e^{\lambda T} = \frac{1}{e^{-\lambda T}}$$

backwards diffusion on small frequencies, subdiffusion on large frequencies

$$\langle u_{0,\alpha}^\delta, \phi_j \rangle = \begin{cases} w(\lambda_j, 1) \langle u_T^\delta, \phi_j \rangle & \text{for } j \le K \\ w(\lambda_j, \alpha) \langle \tilde{u}_T^\delta, \phi_j \rangle & \text{for } j \ge K+1 \end{cases} \quad \text{with} \quad w(\lambda, \alpha) = \frac{1}{E_{\alpha,1}(-\lambda T^\alpha)}$$

$\rightsquigarrow$ regularization parameters α, K

Convergence with a posteriori choice of K and α

First choose K:

$$K = \min\{k \in \mathbb{N} \, : \, \| \exp(\mathbb{L}T)u^{\delta}_{0,lf} - u^{\delta}_{T} \| \le \tau\delta\} \tag{1}$$

for some fixed $\tau > 1$. Then choose α

$$\underline{\tau}\tilde{\delta} \le \| \exp(-AT)u^{\delta}_{0,\alpha,K} - u^{\delta}_{T} \| \le \overline{\tau}\tilde{\delta}\,. \tag{2}$$

Theorem (BK&Rundell 2018)

Let $u_0 \in L^2(\Omega)$, $A^{1+1/p}u_0 \in L^2(\Omega)$ for some $p \in (1, \infty)$, $\tilde{u}^{\delta}_{T} = v^{(i_*)}$ as in pre-smoothing Lemma with $s \ge 2(1 + \frac{1}{p})$, and assume that $K = K(u^{\delta}_{T}, \delta)$ and $\alpha = \alpha(\tilde{u}^{\delta}_{T}, \tilde{\delta})$ are chosen according to (1) and (2). Then

$$u^{\delta}_{0,\alpha(\tilde{u}^{\delta}_{T},\tilde{\delta}),K(u^{\delta}_{T},\delta)} \rightharpoonup u_0 \text{ in } L^2(\Omega)\,, \qquad \text{as } \delta \to 0\,.$$

Split frequency backwards time fractional diffusion is a regularization method.

Conclusions and remarks

- based on the paradigm of quasi-reversibility,
  backwards subdiffusion (with pre-smoothing) is a regularizer for backwards diffusion

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- based on the paradigm of quasi-reversibility, backwards subdiffusion (with pre-smoothing) is a regularizer for backwards diffusion
- can be implemented without explicit use of eigensystem by just numerical solution of time-fractional PDE
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→ prove numerically observed superiority to TSVD for appropriate classes of initial data(?)

Thank you for your attention!