Regularization of backwards diffusion by fractional time derivatives

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joint work with
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Reconstruction Methods for Inverse Problems,
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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

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

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

Quasi-reversibility

Replace diffusion equation

$$u_t - \mathbb{L}u = 0$$

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

$$\varepsilon u_{tt} + u_t - \mathbb{L}u = 0 \qquad u_t - \mathbb{L}u + \varepsilon \mathbb{L}^2 u = 0$$

drawback: additional boundary and/or initial conditions needed.

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

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

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

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

$$\partial_t^\alpha u_t - \mathbb{L}u = 0$$

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

fractional derivatives and Mittag-Leffler functions

Fractional derivatives

Abel fractional integral operator

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

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

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

or

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

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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 $\rightsquigarrow$ appropriate for prescribing initial values

Nonlocal and causal character of these derivatives provides them with a "memory" $\rightsquigarrow$ initial values are tied to later values and can therfore be better reconstructed backwards in time.

Diffusion as limit of continuous time random walk

1-d random walk:
PDF $p_j(t)$ for the probability of being at position j at time t:

$$p_j(t+\Delta t) = \frac{1}{2}p_{j-1}(t) + \frac{1}{2}p_{j+1}(t),$$

where jumps to the left and right are equally likely;
Δt is a fixed time step. Δx is a fixed jump distance.

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Rearranging:

$$\frac{p_j(t + \Delta t) - p_j(t)}{\Delta t} = \frac{(\Delta x)^2}{2\Delta t} \frac{p_{j-1}(t) - 2p_j(t) + p_{j+1}(t)}{(\Delta x)^2}$$

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as $\Delta x \to 0, \Delta t \to 0$ leads to the diffusion equation

$$\partial_t p(x,t) = K \partial_{xx} p(x,t),$$

The limit is taken such that $0 < K = \lim_{\Delta x \to 0, \Delta t \to 0} \frac{(\Delta x)^2}{2\Delta t} < \infty$

$K \ldots$ diffusion coefficient – it couples the spatial and time scales.

Subdiffusion as limit of continuous time random walk

slightly more general setting:
Assume that the temporal and spatial increments

$$\Delta t_n = t_n - t_{n-1} \quad \text{and} \quad \Delta x_n = x_n - x_{n-1}$$

are iid random variables, with PDFs $\psi(t)$ and $\lambda(x)$,
– the *waiting time* and *jump length distribution*, respectively, i.e.,

$$P(a < \Delta t_n < b) = \int_a^b \psi(t)\, dt, \qquad P(a < \Delta x_n < b) = \int_a^b \lambda(x)\, dx.$$

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CTRW processes can be categorized by the characteristic waiting time T and the jump length variance Σ^2 being finite or diverging.

$$T =: E[\Delta t_n] = \int_0^\infty t\psi(t)dt, \quad \Sigma^2 =: E[(\Delta x_n)^2] = \int_{-\infty}^\infty x^2\lambda(x)dx.$$

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Case $0 < T < \infty$, $0 < \Sigma < \infty$: $\rightsquigarrow$ classical diffusion;
Case $T = \infty$, $0 < \Sigma < \infty$: $\rightsquigarrow$ subdiffusion,
in particular $\psi(t) \sim t^{-1+\alpha}$, $0 < \Sigma < \infty$: $\rightsquigarrow$ $\partial_t^\alpha u = K\partial_{xx}p(x,t)$

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.

Mittag-Leffler functions

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

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

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 $|z| \to \infty$

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

Mittag-Leffler functions

For $x \to +\infty$

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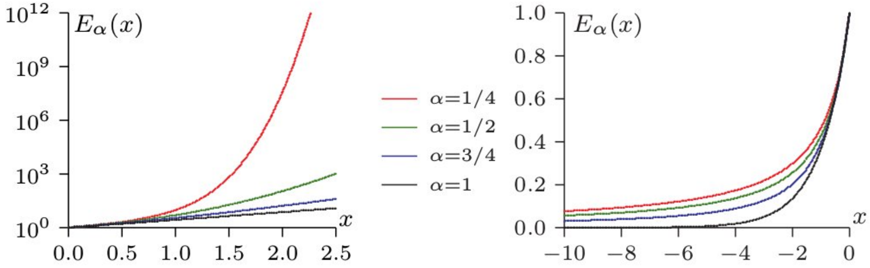
On the positive real axis, $E_{\alpha,\beta}$ grows superexponetially.
On the negative real axis, $E_{\alpha,\beta}$ decreases only linearly.



regularization based on subdiffusion

Plain 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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in terms of Fourier coefficients:

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

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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 (truncated SVD):

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

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replace ∂_t by ∂_t^α with $\alpha < 1$ ($\rightsquigarrow$ regularization parameter)

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

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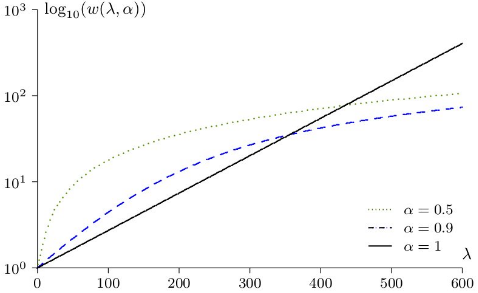

$\rightsquigarrow$ more stable for large frequencies, less stable for small frequencies

Split frequency subdiffusion regularization

backwards diffusion $u_t + Au = 0,\ u(x,T) = \underbrace{u_T}_{\in C^\infty(\Omega)} \approx \overbrace{\underbrace{u_T^\delta}_{\in L^2(\Omega)}}^{\text{noisy}} \approx \overbrace{\underbrace{\tilde{u}_T^\delta}_{\in H^2(\Omega)}}^{\text{smoothed}}$,

in terms of Fourier coefficients:

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backwards diffusion on small frequencies, subdiffusion on large frequencies

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

$\rightsquigarrow$ regularization parameters α, K

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:

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

backwards diffusion on small frequencies, subdiffusion on larger frequencies

$$\langle u_{0,\alpha}^\delta, \phi_j \rangle = \begin{cases} w(\lambda_j, 1)\langle u_T^\delta, \phi_j \rangle & \text{for } j \le K_1 \\ w(\lambda_j, \alpha_1)\langle \tilde{u}_T^\delta, \phi_j \rangle & \text{for } K_1 + 1 \le j \le K_2 \\ \dots & \\ w(\lambda_j, \alpha_i)\langle \tilde{u}_T^\delta, \phi_j \rangle & \text{for } K_i + 1 \le j \le K_{i+1} \\ \dots & \end{cases}$$

$\rightsquigarrow$ 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., $\lambda_j \to \lambda_j^\beta$:

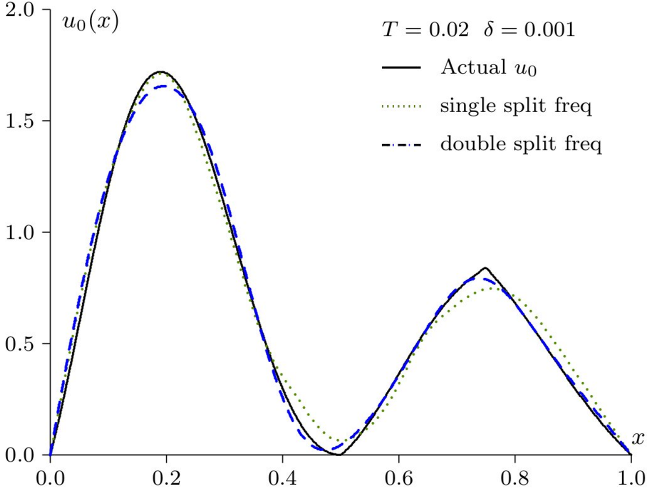
$$u_t + Au = 0 \quad \rightsquigarrow \quad (I + \varepsilon A^\beta) \partial_t^\alpha u + Au = 0$$

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

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

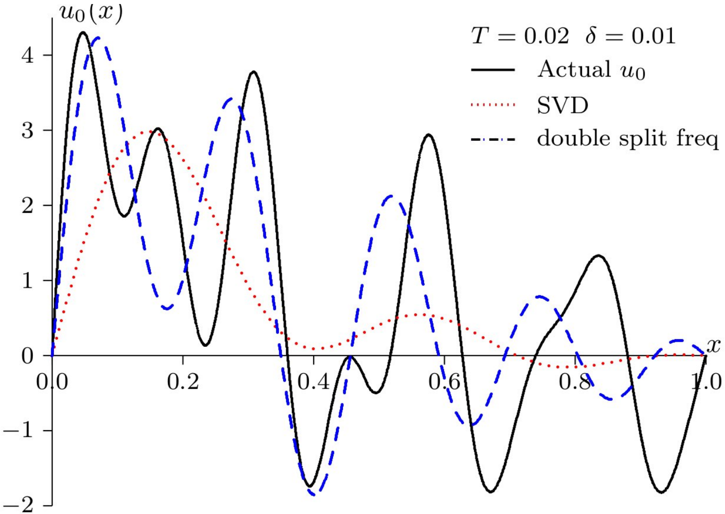
reconstructions - numerical experiments

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



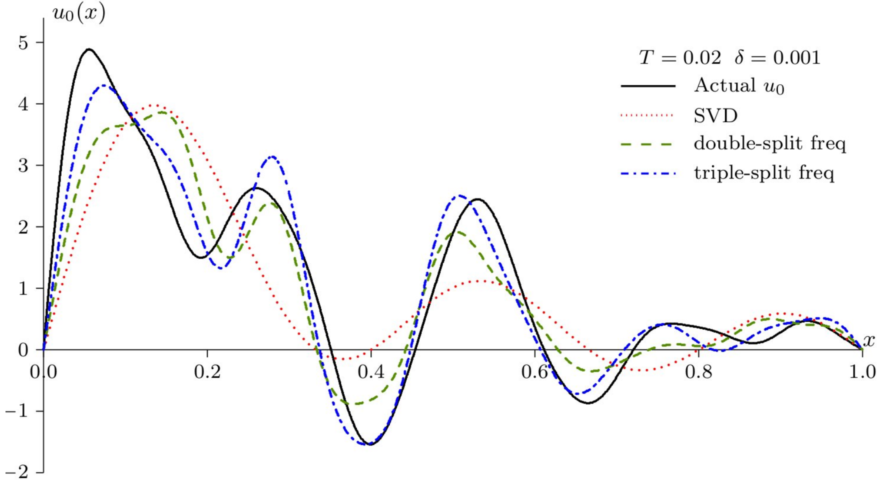
Reconstructions from single and double split frequency method.
single split: $K_1 = 4$ and $\alpha = 0.92$;
double split: $K_1 = 4$, $K_2 = 10$ and $\alpha_1 = 0.999$, $\alpha_2 = 0.92$.

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



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

Test case 3: u_0 with $\lambda_j \neq 0$, $j = 1, \ldots, 7, 10 \ldots, 15$; $\delta = 0.1$



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

convergence analysis

Plain 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:

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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 $0 < \alpha \leq 1$ *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 $\quad \partial_t^{\alpha} u + \lambda u = 0.$

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

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 $\left|\frac{\exp(-\lambda T)}{E_{\alpha,1}(-\lambda T^\alpha)} - 1\right| \leq \tilde{C}\lambda^{1+1/p}$

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:

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$\rightsquigarrow$ exponential instability.

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backwards subdiffusion

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

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

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

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

Pre-smoothing the data

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

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 $i_* \sim T^{-2}\log\left(\frac{\|u_0\|_{L^2(\Omega)}}{\delta}\right)$ *yields* $\|u_T - \tilde{u}_T^\delta\|_{L^2(\Omega)} \leq C_1\delta$,

$$\|u_T - \tilde{u}_T^\delta\|_{H^s(\Omega)} \sim \|A^{s/2}(u_T - \tilde{u}_T^\delta)\|_{L^2(\Omega)} \leq \frac{C_2}{T}\,\delta\sqrt{\log\left(\frac{\|u_0\|_{L^2(\Omega)}}{\delta}\right)} =: \tilde{\delta}$$

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

Note that Tikhonov regularization would not properly pre-smooth noisy versions of C^∞ data, due to saturation.

Convergence with a priori choice of α

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

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*

$$\underline{\tau}\tilde{\delta} \leq \| \exp(-AT)u_0^\delta(\cdot;\alpha) - \tilde{u}_T^\delta \| \leq \overline{\tau}\tilde{\delta}$$

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

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

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 implies a logarithmic 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:

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

backwards diffusion on small frequencies, subdiffusion on large frequencies

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

$\rightsquigarrow$ regularization parameters α, K

Convergence with a posteriori choice of K and α

First choose K:

$$K = \min\{k \in \mathbb{N} \, : \, \| \exp(\mathbb{L}T) u^{\delta}_{0,If} - u^{\delta}_T \| \leq \tau\delta\} \qquad (1)$$

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

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

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 $s \geq 2(1 + \frac{1}{p})$, 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

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

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  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
- can be improved by spitting frequencies (using eigensystem) and treating different parts of the frequency range by different time differentiation orders α

Thank you for your attention!