Petrov-Galerkin method for fractional advection-dispersion equations

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Outline

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Why fractional derivatives ?

"Fractional" order differential operators appear naturally in:

- Trace theory of functions in Sobolev classes (Sobolev imbedding)
- Theory of special classes analytic functions (Dzhrbashyan)
- Modeling various phenomena (e.g. particle movement in heterogeneous media)
- Modeling materials with memory (e.g. viscoelasticity, Bagley-Torvik eqn., [1])
- Heavily tailed Levy flights of particles
- Other non-local models, e.g. peridynamics (deformable media with fractures)

The most important characterization of these operators is that they are **non-local**.

Why fractional derivatives ?

Microscopic particle's motion: if $x(t)$ is the particle trajectory in time then the following relation between the mean-square displacement $\langle x^2(t)\rangle$ in time are used:

1. standard diffusion – $\langle x^2(t)\rangle \sim D\, t$, D diffusion/dispersion coefficient (Brownian)
2. sub-diffusion – $\langle x^2(t)\rangle \sim D\, t^\alpha$, $0 < \alpha < 1$, cont. time random walks (CTRW)
3. super-diffusion – $\langle |x(t)|^{2\alpha}\rangle \sim D\, t$, $0.5 < \alpha < 1$ (Levy flights).

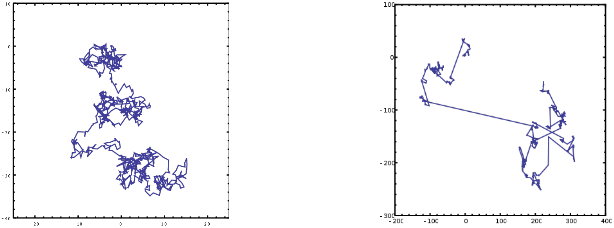

Figure: Brownian (left) versus Levy flights (right) trajectories

Fractional order elliptic operators

There are many ways to define fractional order differential equations (and operators). They are not equivalent, but many of them are inter-related.

The simplest case would be the fractional Laplacian in a bounded domain $\Omega \subset R^d$ with Dirichlet boundary conditions:

$$(-\Delta)^\alpha u = f(x), \quad x \in \Omega \quad \text{by definition} \quad (-\Delta)^\alpha u = \sum_{j=1}^{\infty} \lambda_j^\alpha (u, \psi_j)\psi_j$$

where $\alpha \in (0,1)$ and (λ_j, ψ_j) are the eigenpairs of $-\Delta$.

It is obvious how to define the fractional order of general self-adjoint elliptic operator L^α:

$$Lu := -\nabla \cdot \big(a(x)\nabla u\big) + q(x)u,$$

where $a(x)$ is an SPD $d \times d$ matrix and $q(x) \geq 0$.

Fractional integrals on the interval $(0, 1)$

In this talk I'll be using **Riemann-Liouville and Caputo** fractional derivatives. They are used in various models as derivatives in time, space, or both. To defined these we shall need some preliminary information about fractional integrals.

For positive integers n we define the integral, that plays essential role in the analysis:

$$({}_0I_x^n f)(x) = \frac{1}{(n-1)!} \int_0^x (x-t)^{n-1} f(t)\, dt.$$

The following two properties give the relation between differentiation and integration:

$$\left({}_0I_x^n \frac{d^n f}{dx^n}\right)(x) = f(x) - \sum_{j=0}^{n-1} \frac{x^j}{j!} \frac{d^j f}{dx^j}(0) \quad \text{and} \quad \frac{d^n}{dx^n}\left({}_0I_x^n f(x)\right) = f(x),$$

which shows that in the class of functions satisfying the conditions $f^{(j)}(0) = 0$, $j = 0, \dots, n-1$, the integration operator is both right and left inverse of differentiation.

Fractional integrals on the interval $(0, 1)$

Now we generalize the integration operator to any positive β:

$$({}_0I_x^\beta f)(x) = \frac{1}{\Gamma(\beta)} \int_0^x (x-t)^{\beta-1} f(t)\, dt.$$

This is the left sided fractional integral. The right sided integral is given by

$$({}_xI_1^\beta f)(x) = \frac{1}{\Gamma(\beta)} \int_x^1 (t-x)^{\beta-1} f(t)\, dt.$$

The following formula for change of integration order is valid [10, p. 76, Lemma 2.7]

$$({}_0I_x^\gamma \psi, \varphi) = (\psi, {}_xI_1^\gamma \varphi) \quad \forall \psi, \varphi \in L^2(0,1), \tag{1}$$

where $(\cdot, \cdot)$ denotes the $L^2(0,1)$ inner product.

Fractional derivatives:

For any positive β with $n-1<\beta<n$, the (formal) left-sided **Riemann-Liouville** fractional derivative and **Caputo** fractional derivative of order β are defined by

$$ {}_0^R D_x^\beta u = \frac{d^n}{dx^n}\left({}_0 I_x^{n-\beta} u\right) \quad \text{and} \quad {}_0^C D_x^\beta u = {}_0 I_x^{n-\beta}\left(\frac{d^n u}{dx^n}\right), \tag{2} $$

and the right-sided Riemann-Liouville derivative ${}_x^R D_1^\beta$ and Caputo derivative ${}_x^C D_1^\beta$ of order β, respectively, by

$$ {}_x^R D_1^\beta u = (-1)^n \frac{d^n}{dx^n}\left({}_x I_1^{n-\beta} u\right) \quad \text{and} \quad {}_x^C D_1^\beta u = (-1)^n {}_x I_1^{n-\beta}\left(\frac{d^n u}{dx^n}\right). $$

Fractional Order PDE Problems

These are used these mostly in two cases:

1. $$0 < \beta < 1: \quad {}_0^R D_x^\beta u = \frac{d}{dx}\left({}_0I_x^{1-\beta} u\right) \quad \text{and} \quad {}_0^C D_x^\beta u = {}_0I_x^{1-\beta}\left(\frac{du}{dx}\right)$$
2. $$1 < \beta < 2: \quad {}_0^R D_x^\beta u = \frac{d^2}{dx^2}\left({}_0I_x^{2-\beta} u\right) \quad \text{and} \quad {}_0^C D_x^\beta u = {}_0I_x^{2-\beta}\left(\frac{d^2 u}{dx^2}\right)$$

Other definitions include **Riesz derivative** (a symmetric variant of these two), e.g.

$$D^\beta u = \frac{1}{2}\frac{d^2}{dx^2}\left({}_0I_x^{2-\beta} u + {}_xI_1^{2-\beta} u\right)$$

Note that these fractional derivatives could be used for functions of two variables $u(x, t)$ in **time, space, or in both, time and space**.

Fractional Order PDE Problems

Examples of fractional order PDEs:
(a) Sub-diffusion problem: for given $f(x,t)$, $u_0(x)$, and $0 < \alpha < 1$ find $u(x,t)$ such that

$$\begin{aligned} {}_0^C D_t^\alpha u - \Delta u &= f(x,t), \quad x \in \Omega, 0 < t \le T, \\ u(x,t) &= 0, \quad x \in \partial\Omega, \quad 0 < t \le T, \\ u(x,0) &= u_0(x), \quad x \in \Omega. \end{aligned}$$

Note that $\alpha = 1$ corresponds to the **standard diffusion** problem.

(b) Fractional wave problem: for given $f(x,t)$, $u_0(x)$, $u_1(x)$ and $1 < \alpha < 2$ find $u(x,t)$ such that

$$\begin{aligned} {}_0^C D_t^\alpha u - \Delta u &= f(x,t), \quad x \in \Omega, 0 < t \le T, \\ u(x,t) &= 0, \quad x \in \partial\Omega, \quad 0 < t \le T, \\ u(x,0) &= u_0(x), \quad u_t(x,0) = u_1(x) \quad x \in \Omega. \end{aligned}$$

Fractional Order PDE Problems

The problems pose various challenges when one tries to solve them numerically:

- Non-locality in time, i.e. the solution at t depends directly on the solution for all time less that t; i.e. **memory effects** are build in the model;
- Solution is less regular that the standard diffusion problem, this means that the fractional order differential operators have different **smoothing** properties.

Indeed, the solution is substantially different compared to the solution of the standard diffusion $\alpha = 1$ problem !

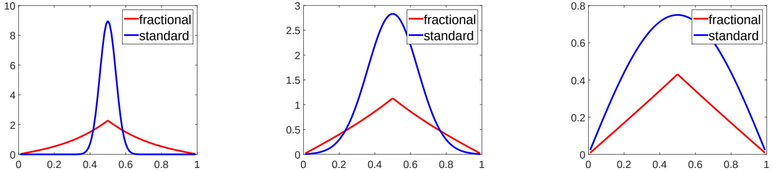

Figure: Solution profile for the sub-diffusion equation for $t = 0.001$, $t = 0.01$ and $t = 0.1$ with initial data $\delta(x - \frac{1}{2})$ in 1-D for $\alpha = 0.7$ (red) and $\alpha = 1$ (blue)

General Non-Local Operators

Recall the definition of the fractional in time derivative of order $0 < \alpha < 1$:

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u'(s) ds$$

Important property of this operator: **history dependence** !
Now extend $u(t)$ as $u(0)$ for $-\infty < t < 0$ and rewrite the above definition as

$$\partial_t^\alpha u(t) = \lim_{\epsilon \to 0} \int_\epsilon^\infty \frac{u(t) - u(t-s)}{s} \frac{1}{\Gamma(1-\alpha)} s^{-\alpha} ds.$$

Now replace the kernel $s^{-\alpha}/\Gamma(1-\alpha)$ by a general function $\rho_\delta(s)$ and instead define

$$\mathcal{G}_\delta u(t) = \lim_{\epsilon \to 0} \int_\epsilon^\infty \frac{u(t) - u(t-s)}{s} \rho_\delta(s) ds$$

General Non-Local Operators

Thus, we have defined a new nonlocal operator

$$\mathcal{G}_\delta u(t) = \lim_{\epsilon\to 0}\int_\epsilon^\infty \frac{u(t)-u(t-s)}{s}\rho_\delta(s)ds$$

where:

- $\rho_\delta(s)$ is a non-negative radial type of function;
- $\rho_\delta(s)$ may have a singularity at the origin;
- $\rho_\delta(s)$ has a compact support in $(0,\delta)$ and satisfies

$$\int_0^\delta \rho_\delta(s)ds = 1.$$

Here δ is the length of the history dependence or space horizon. These are the general models in peridynamics (a formulation of continuum mechanics that is oriented toward deformations with discontinuities due to fractures).

Note: $\mathcal{G}_\delta u(t) = \partial_t^\alpha u, \;\; t>0, \;\; \delta=\infty, \;\; \rho_\delta(s) = \frac{\alpha}{\Gamma(1-\alpha)}s^{-\alpha}$

Fractional Advection-Dispersion Equation $1 < \alpha < 2$

In this talk we shall consider the following one-dimensional fractional boundary value problem: find $u(x)$, $0 < x < 1$, such that

$$\begin{aligned} -{}_0D_x^\alpha u + bu' + qu &= f, \quad x \in D = (0,1), \\ u(0) = u(1) &= 0, \end{aligned} \tag{3}$$

- $f \in L^2(D)$ or a suitable subspace, $b \in W^{1,\infty}(D)$, $q \in L^\infty(D)$
- ${}_0D_x^\alpha$, $\alpha \in (3/2, 2)$: left-sided Riemann-Liouville or Caputo fractional derivative
- $\alpha \to 2$, (3) $\to$ steady advection-dispersion equation.

The most popular is model where u is the concentration of a chemical transported in porous media. This is a steady state variant of 1-D time-dependent problem:

$$\frac{\partial u}{\partial t} - {}_0D_x^\alpha u + bu' + qu = f, \quad x \in D = (0,1).$$

Fractional Advection-Dispersion Equation

One can formulate also a multidimensional advection-dispersion problem

$$\frac{\partial u}{\partial t} + \mathcal{L}^\alpha u + \mathbf{b} \cdot \nabla u + qu = f, \quad x \in \Omega, \quad \mathcal{L}^\alpha = (-\Delta)^\alpha.$$

Different definition of $\mathcal{L}^\alpha$ is: extend u by zero in the whole $\mathbb{R}^n$, take its Fourier transform $\widehat{u}(\xi)$ and define the Fourier transform of $\mathcal{L}^\alpha u$ as

$$-\widehat{\mathcal{L}^\alpha u} = \int_{\|\theta\|=1} (i\xi \cdot \theta)^\alpha M(d\theta)\, \widehat{u}(\xi),$$

where $M(d\theta)$ is a probability measure on the unit sphere $\{x \in \mathbb{R}^n : \|x\| = 1\}$.

Here are some example of models involving anomalous diffusion:

- ultra-cold atoms [14],
- single particle movements in cytoplasm [13],
- DNA sequences [2],
- see Tarasov's review [15] for more models

Review

There has been considerable interest in this kind of problems:

- Ervin and Roop [4], $b = 0$, variational formulation on $\widetilde{H}^{\alpha/2}(D) \times \widetilde{H}^{\alpha/2}(D)$, finite element method, full regularity assumption
- Jin et al [7], $b = 0$, sharp regularity pickup, $\widetilde{H}^{\alpha/2}(D)$ and $L^2(D)$ error estimates (suboptimal);
- Zayernouri et al [17], Petrov-Galerkin formulations for fractional ODEs and PDEs, with a Riemann-Liouville derivative in time.
- Chen et al [3], generalized Jacobi polynomials for approximating FBVPs without any lower order term (suboptimal);
- Stynes and Gracia [11, 12], Caputo, particular mixed boundary condition, finite difference method, comparison principle,optimal error estimate
- Jin et al [9, 6], RL, reformulate the variational problem, compensate the singularity, improve the approximation.

Goal of our works

- develop a well-posed variational (weak) formulation;
- discuss the existence of strong solution;
- establish sharp regularity pickup;
- develop stable numerical schemes based on finite element method
- derive optimal error estimates in terms with the data regularity.

Fractional calculus: Functional Spaces

For any $\beta \geq 0$

- $H^\beta(D)$: the Sobolev space of fractional order β on the unit interval D;
- $\widetilde{H}^\beta(D)$: the set of functions in $H^\beta(D)$ whose extension by zero to $\mathbb{R}$ is in $H^\beta(\mathbb{R})$;
- $\widetilde{H}_L^\beta(D)$ (respectively, $\widetilde{H}_R^\beta(D)$): the set of functions u whose extension by zero, denoted by $\tilde{u}$, is in $H^\beta(-\infty, 1)$ (respectively, $H^\beta(0, \infty)$);
- $u \in \widetilde{H}_L^\beta(D)$, we set $\|u\|_{\widetilde{H}_L^\beta(D)} := \|\tilde{u}\|_{H^\beta(-\infty,1)}$, and similarly the norm in $\widetilde{H}_R^\beta(D)$.

Note that for $\beta < \frac{1}{2}$ all these spaces are essentially the same since the trace at a point is not defined.

Fractional calculus:

Theorem

(a) *The integral operators* ${}_0I_x^\beta$ *and* ${}_xI_1^\beta$ *satisfy the semigroup property; e.g.* ${}_0I_x^{\alpha+\beta} = ({}_0I_x^\alpha)({}_0I_x^\beta)$

(b) *The operators* ${}_0^RD_x^\beta$ *and* ${}_x^RD_1^\beta$ *extend continuously to operators from* $\widetilde{H}_L^\beta(D)$ *and* $\widetilde{H}_R^\beta(D)$*, respectively, to* $L^2(D)$*.*

(c) *For any* $s, \beta \geq 0$*, the operator* ${}_0I_x^\beta$ *is bounded from* $\widetilde{H}_L^s(D)$ *to* $\widetilde{H}_L^{\beta+s}(D)$*, and* ${}_xI_1^\beta$ *is bounded from* $\widetilde{H}_R^s(D)$ *to* $\widetilde{H}_R^{\beta+s}(D)$*.*

Fractional calculus:

Lemma

For $u \in \widetilde{H}_L^1(D)$ and $\beta \in (0,1)$,

$$({}_0I_x^{1-\beta} u)' = {}_0I_x^{1-\beta}(u')$$

Similarly, for $u \in \widetilde{H}_R^1(D)$ and $\beta \in (0,1)$,

$$({}_xI_1^{1-\beta} u)' = -{}_xI_1^{1-\beta}(u').$$

Remark: We know that for $\beta \in (1/2, 1)$ functions $u \in \widetilde{H}_L^\beta(D)$ satisfy $u(0) = 0$ and then ${}_0^RD_x^\beta u = {}_0^CD_x^\beta u$, thus, ${}_0I_x^{1-\beta}(u') = ({}_0I_x^{1-\beta} u)'$.

Outline

Riemann-Liouville case: $b, q \equiv 0$

Let begin with the trivial case $b, q \equiv 0$ and $f \in L^2(D)$, i.e.,

$$-{}_0^R D_x^\alpha u = f \text{ in } D = (0,1) \quad u(0) = u(1) = 0$$

so that the solution can be written explicitely

$$u = -({}_0I_x^\alpha f)(x) + ({}_0I_x^\alpha f)(1)x^{\alpha-1}. \tag{4}$$

This innocently looking solution has some very important properties:

1. Even for very smooth data f the solution contains a singular part $x^{\alpha-1}$
2. $u \in \widetilde{H}_L^{\alpha-1+\beta}(D), \quad \beta \in [2-\alpha, 1/2)$
3. **only for** $\alpha \in (3/2, 2)$ **we have** $u \in \widetilde{H}^1(D)$ **!**

Riemann-Liouville case: $b, q \equiv 0$

Keep the fact **only for** $\alpha \in (3/2, 2)$ **we have** $u \in \widetilde{H}^1(D)$ **!**

Further, for $\varphi \in C_0^\infty(D)$, the following identity holds

$$\begin{aligned}({}_0^R D_x^\alpha u, \varphi) &= (({}_0 I_x^{2-\alpha} u)'', \varphi) = -(({}_0 I_x^{2-\alpha} u)', \varphi') \\ &= -({}_0 I_x^{2-\alpha} u', \varphi') = -(u', {}_x I_1^{2-\alpha} \varphi') = (u', {}_x^R D_1^{\alpha-1} \varphi).\end{aligned}$$

This **motivates us** to define a bilinear form $a(\cdot,\cdot) : \widetilde{H}^1(D) \times \widetilde{H}^{\alpha-1}(D) \to \mathbb{R}$ by

$$a(u, \varphi) := -(u', {}_x^R D_1^{\alpha-1} \varphi). \tag{5}$$

Riemann-Liouville case: $b, q \equiv 0$

Lemma

The bilinear form $a(\cdot,\cdot)$ in (5) satisfies the inf-sup condition:

$$\sup_{\varphi \in \widetilde{H}^{\alpha-1}(D)} \frac{a(u,\varphi)}{\|\varphi\|_{\widetilde{H}^{\alpha-1}(D)}} \geq c_0 \|u'\|_{L^2(D)},$$

and further for $\varphi \in \widetilde{H}^{\alpha-1}(D)$

$$a(u,\varphi) = 0 \ \ \text{for all} \ \ u \in \widetilde{H}^1(D) \ \ \Rightarrow \ \ \varphi = 0.$$

Let $U = \widetilde{H}^1(D)$ and $V = \widetilde{H}^{\alpha-1}(D)$. Note that the functions in V and U satisfy BC at both ends of D !

Given a $F \in V^*$, there exists a unique solution $u \in U$ such that

$$a(u,\varphi) = \langle F, \varphi \rangle \quad \forall \varphi \in V.$$

Riemann-Liouville case

We now turn to the general case of $b, q \not\equiv 0$ in (3).

Variational formulation: given any $F \in V^*$, find $u \in U$ such that for any $\varphi \in V$

$$A(u, \varphi) = \langle F, \varphi \rangle, \tag{6}$$

where the bilinear form $A(\cdot, \cdot) : U \times V \to \mathbb{R}$ is defined by

$$A(u, \varphi) = a(u, \varphi) + (bu', \varphi) + (qu, \varphi).$$

To study the bilinear form $A(\cdot, \cdot)$, we make the following assumption.

Assumption

Let the bilinear form $A(u, \varphi)$ with $u \in U$ and $\varphi \in V$ satisfy

(a) *The problem of finding $u \in U$ such that $A(u, \varphi) = 0$ for all $\varphi \in V$ has only the trivial solution $u \equiv 0$.*

(a*) *The problem of finding $\varphi \in V$ such that $A(u, \varphi) = 0$ for all $u \in U$ has only the trivial solution $\varphi \equiv 0$.*

Riemann-Liouville case

Theorem

Let $b, q \in L^\infty(D)$ and Assumption 2.1 hold. Then for any $F \in V^*$, there exists a unique solution $u \in U$ to (6), which satisfies

$$c_0 \|u\|_U \le \sup_{\varphi \in V} \frac{A(u, \varphi)}{\|\varphi\|_V} \quad \forall u \in U. \tag{7}$$

Proof.

Use Petree-Tartar's Lemma. □

Riemann-Liouville case

Theorem

Let $b, q \in L^\infty(D)$ and $f \in L^2(D)$, and Assumption 2.1 hold. Then there exists a unique solution $u \in \widetilde{H}_L^{\alpha-1+\beta}(D) \cap \widetilde{H}^1(D)$ to problem (6) for any $\beta \in [2-\alpha, 1/2)$ and it satisfies

$$\|u\|_{\widetilde{H}_L^{\alpha-1+\beta}(D)} \le c\|f\|_{L^2(D)}.$$

Note that the maximum smoothness we can get is $H^{\alpha-\frac{1}{2}}(D)$ but not $H^\alpha(D)$!

Proof.

- By the inf-sup condition (7) in Theorem 4, we have $\|u\|_{\widetilde{H}^1(D)} \le c\|f\|_{V^*}$.
- Regularity pickup. Rewrite the problem into $-{}_0^R D_x^\alpha u = \widetilde{f}$ with $\widetilde{f} = f - bu' - qu$.

□

Adjoint problem

Adjoint problem in the Riemann-Liouville case:

For a given $F \in U^*$, find $w \in V$ such that

$$A(\varphi, w) = \langle \varphi, F \rangle \quad \forall \varphi \in U. \tag{8}$$

Example: $b, q = 0$ and $F = f \in L^2(D)$. Then the adjoint problem has a strong form

$$-{}_x^R D_1^\alpha u = f, \quad \text{with} \;\; w(0) = w(1) = 0.$$

The solution is $u = -({}_xI_1^\alpha f)(x) + ({}_xI_1^\alpha f)(0)(1-x)^{\alpha-1} \in \widetilde{H}_R^{\alpha-1+\beta}(D)$.

Theorem

Let $b \in W^{1,\infty}(D)$, $q \in L^\infty(D)$ and $F = f \in L^2(D)$ and Assumption 2.1 hold. Then there exists a unique solution $w \in \widetilde{H}_R^{\alpha-1+\beta}(D) \cap \widetilde{H}^{\alpha-1}(D)$ to problem (8) for any $\beta \in [2-\alpha, 1/2)$ and it satisfies

$$\|w\|_{\widetilde{H}_R^{\alpha-1+\beta}(D)} \le c\|f\|_{L^2(D)}.$$

Caputo case:

Now we consider the Caputo case and let us begin with $b, q \equiv 0$, i.e.,

$$-{}_0^C D_x^\alpha u = f \text{ in } (0,1) \quad u(0) = u(1) = 0.$$

$$\text{solution}: \quad u = -{}_x I_1^\alpha f(x) + ({}_x I_1^\alpha f)(0)x \in H^\alpha. \tag{9}$$

Let $g = -{}_x I_1^\alpha f(x) \in \widetilde{H}_L^\alpha(D)$, then $u = g(x) + u'(0)x$. Hence for any $\varphi \in \widetilde{C}_R^\infty(D)$

$$\begin{aligned}({}_0I_x^{2-\alpha} u'', \varphi) &= (({}_0I_x^{2-\alpha} g')', \varphi) = -({}_0I_x^{2-\alpha} g', \varphi') = -(g', {}_x I_1^{2-\alpha} \varphi') \\ &= -(u', ({}_x I_1^{2-\alpha} \varphi)') + u'(0)({}_x I_1^{2-\alpha} \varphi)(0)\end{aligned}$$

Define

$$W = \widetilde{H}_R^{\alpha-1}(D) \cap \{\varphi : (\varphi, x^{1-\alpha}) = 0\}$$

and introduce $a(\cdot,\cdot) : U \times W \to \mathbb{R}$ s.t.

$$a(u, \varphi) = -(u', {}_x^R D_1^{\alpha-1} \varphi). \tag{10}$$

in the Caputo case, it involves an integral constraint $(\varphi, x^{1-\alpha}) = 0$.

Caputo case:

Lemma

The bilinear form $a(\cdot,\cdot)$ *in* (10) *satisfies the inf-sup condition:*

$$\sup_{\varphi\in \widetilde{H}_R^{\alpha-1}(D)} \frac{a(u,\varphi)}{\|\varphi\|_{\widetilde{H}_R^{\alpha-1}(D)}} \geq c_0\|u'\|_{L^2(D)}.$$

Further, it holds for $\varphi \in W$

$$a(u,\varphi) = 0 \ \ \textit{for all} \ \ u \in U \quad \Rightarrow \quad \varphi = 0.$$

Given a $F \in W^*$, there exists a unique solution $u \in U$ such that

$$a(u,\varphi) = \langle F,\varphi\rangle \quad \forall \varphi \in W.$$

Caputo case:

We next consider the case $b, q \neq 0$. Then the variational formulation reads

$$A(u, \varphi) = \langle F, \varphi \rangle \quad \forall \varphi \in W, \tag{11}$$

where the bilinear form $A(\cdot, \cdot) : U \times W \to \mathbb{R}$ is given by

$$A(u, \varphi) = a(u, \varphi) + (bu', \varphi) + (qu, \varphi).$$

To analyze the formulation (11), like before, we assume the unique solvability.

Assumption

Let the bilinear form $A(u, \varphi)$ with $u \in U, \quad \varphi \in W$ satisfy

(b) *The problem of finding $u \in U$ such that $A(u, \varphi) = 0$ for all $\varphi \in W$ has only the trivial solution $u \equiv 0$.*

(b*) *The problem of finding $\varphi \in W$ such that $A(u, \varphi) = 0$ for all $u \in U$ has only the trivial solution $\varphi \equiv 0$.*

Caputo case:

Theorem

Let $s \in [0, 1/2)$ and Assumption 2.2 hold. Suppose that $\langle F, v\rangle = (f, v)$ for some $f \in \widetilde{H}_L^s(D)$, and $b, q \in L^\infty(D) \cap H^s(D)$. Then the solution $u \in U$ of (11) is in $\widetilde{H}^1(D) \cap H^{\alpha+s}(D)$ and further it satisfies

$$\|u\|_{H^{\alpha+s}(D)} \le c\|f\|_{\widetilde{H}_L^s(D)}.$$

Proof.

- Existence, uniqueness and $\widetilde{H}^1(D)$-stability of solution follow from Petree-Tartar's lemma and BNB condition;
- regularity pickup, write $-{}_0^C D_x^\alpha u = \widetilde{f} = f - bu' - qu$.

□

The solution regularity differs significantly for these two fractional derivatives.

Adjoint problem

Adjoint problem in the Caputo case:

For a given $F \in U^*$, find $w \in W$ such that

$$A(\varphi, w) = \langle \varphi, F \rangle \quad \forall \varphi \in U. \tag{12}$$

Example: $b, q = 0$ and $F = f \in L^2(D)$. Then the adjoint problem has a strong form

$$-{}_x^R D_1^\alpha w = f, \quad \text{with} \;\; w(1) = 0 \text{ and } (w, x^{1-\alpha}) = 0.$$

The solution is $w = -({}_x I_1^\alpha f)(x) + c_f (1-x)^{\alpha-1} \in \widetilde{H}_R^{\alpha-1+\beta}(D)$.

Theorem

Let Assumption 2.2 hold, and $b \in W^{1,\infty}(D)$, $q \in L^\infty(D)$. Then with $F = f \in L^2(D)$, then the solution w to (12) is in $\widetilde{H}^1(D) \cap \widetilde{H}_R^{\alpha-1+\beta}(D)$ for any $\beta \in [2-\alpha, 1/2)$ and

$$\|w\|_{\widetilde{H}_R^{\alpha-1+\beta}(D)} \le c \|f\|_{L^2(D)}.$$

The adjoint problem is Riemann-Liouville type!!!

Outline

Finite element method

Idea:

- trial space: continuous piecewise linear finite elements
- test space:"shifted" fractional powers of the form $(x_{i+1} - x)_+^{\alpha-1}$.
- derive estimates in the $L^2(D)$ and $H^1(D)$ norm.

Distinct features:

- $L^2(D)$-error estimate is optimal;
- the stiffness matrix of the leading term is diagonal, and the resulting linear system is nearly well conditioned.

Finite element method

- Consider a uniform partition of the domain $D = (0,1)$. Let $h = 1/m$ be the mesh size, $m \in \mathbb{N}$, and denote the nodes by $x_i = ih$, $i = 0, \ldots, m$.
- Let U_h be the set of continuous piecewise linear functions, $U_h \subset U$.
- The "shifted" fractional powers, $1 \le i \le m$:

$$\phi_i(x) = \left\{ \begin{array}{cc} (x_i - x)^{\alpha-1} & x \le x_i \\ 0 & x > x_i \end{array} \right\} := (x_i - x)^{\alpha-1} \chi_{[0,x_i]}(x),$$

where χ_S denotes the characteristic function of the set S.

Choice of the FE spaces

Observations:

- $\phi_i(x) = \Gamma(\alpha)_x I_1^{\alpha-1}\chi_{[0,x_i]}(x)$, i.e., the fractionalization of piecewise constant functions, i.e. the fractional derivative $-{}_x^R D_1^{\alpha-1}\phi_i$ is piecewise constant.
- Clearly, $\phi_i \in \widetilde{H}_R^{\alpha-1+\beta}(D)$ for any $\beta \in [2-\alpha, 1/2)$.
- Clearly, this choice of the solution spaces is related to the works of
  (a) Tikhonov & Samarskii 1958 - 1961 on the exact difference schemes
  (b) Babuska, 1983 - 1994 (and co-authors) on generalized FEM

The essence is that for the solution space one uses **piece-wise local solutions** of a suitable differential problem.

Approximation properties of the FE spaces

Then we define $V_h \subset V$ and $W_h \subset W$

$$V_h = \text{span}\{\phi_i\}_{i=1}^m \cap V \quad \text{and} \quad W_h = \text{span}\{\phi_i\}_{i=1}^m \cap W,$$

as the test space for the **Riemann-Liouville and Caputo** derivative, respectively.

Lemma

Let the mesh $\mathcal{T}_h$ be quasi-uniform and $1 \le \gamma \le 2$, and $\delta = \alpha - 1 \in (1/2, 1)$. If $u \in H^\gamma(D) \cap \widetilde{H}^1(D)$, then

$$\inf_{\psi_h \in U_h} \|u - \psi_h\|_{\widetilde{H}^1(D)} \le ch^{\gamma-1}\|u\|_{H^\gamma(D)}.$$

Further, if $u \in \widetilde{H}_R^\gamma(D) \cap V$, then

$$\inf_{\psi_h \in V_h} \|{}_x^R D_1^\delta (u - \psi_h)\|_{L^2(D)} \le ch^{\min(1,\gamma-\delta)}\|u\|_{H^\gamma(D)}.$$

Similarly, if $u \in \widetilde{H}_R^\gamma(D) \cap W$, then

$$\inf_{\psi_h \in W_h} \|{}_x^R D_1^\delta (u - \psi_h)\|_{L^2(D)} \le ch^{\min(1,\gamma-\delta)}\|u\|_{H^\gamma(D)}.$$

Petrov-Galerkin FEM in the Riemann-Liouville case

Petrov-Galerkin FEM in the Riemann-Liouville case: given a $F \in V^*$, find $u_h \in U_h$ s.t.

$$A(u_h, \varphi_h) = \langle F, \varphi_h \rangle \quad \forall \varphi_h \in V_h. \tag{13}$$

A first lemma shows the stability of the discrete problem (13) in case of $b, q \equiv 0$.

Lemma

Let $a(\cdot,\cdot)$ be the bilinear form defined in (5)*. Then there holds*

$$\sup_{\varphi_h \in V_h} \frac{a(\psi_h, \varphi_h)}{\|\varphi_h\|_V} \geq c\|\psi_h\|_U \quad \forall \psi_h \in U_h, \tag{14}$$

and the finite element problem: Find $u_h \in U_h$ such that

$$a(u_h, \varphi_h) = (f, \varphi_h) \quad \forall \varphi_h \in V_h,$$

has a unique solution.

Petrov-Galerkin FEM in the Riemann-Liouville case

$$\text{Ritz projection } R_h: \; V \to V_h \quad a(\psi_h, R_h\varphi) = a(\psi_h, \varphi) \quad \forall \psi_h \in U_h.$$

Recall we are studying the case $\frac{3}{2} < \alpha < 2$!!!

Lemma

The projection R_h is well-defined and satisfies for any $\beta \in (2-\alpha, 1/2)$

$$\begin{aligned} \|R_h\varphi\|_{\widetilde{H}^{\alpha-1}(D)} &\leq c\|\varphi\|_{\widetilde{H}^{\alpha-1}(D)}, \\ \|\varphi - R_h\varphi\|_{L^2(D)} &\leq ch^{\alpha-2+\beta}\|\varphi\|_{\widetilde{H}^{\alpha-1}(D)}. \end{aligned} \tag{15}$$

This Lemma says that for $\alpha = \frac{3}{2} + \epsilon$, $\epsilon > 0$ small, we get very low accuracy of the Ritz projection in L^2-norm, namely

$$\|\varphi - R_h\varphi\|_{L^2(D)} = O(h^\epsilon).$$

Petrov-Galerkin FEM in the Riemann-Liouville case

Lemma

Let Assumption 2.1 hold, $f \in L^2(D)$, and $b, q \in L^\infty(D)$. Then there exists an $h_0 > 0$ such that for all $h \le h_0$ and a constant $c > 0$

$$c\|\psi_h\|_U \le \sup_{\varphi_h \in V_h} \frac{A(\psi_h, \varphi_h)}{\|\varphi_h\|_V} \quad \forall \psi_h \in U_h. \tag{16}$$

For such h, the finite element problem: Find $u_h \in U_h$ such that

$$A(u_h, \varphi_h) = (f, \varphi_h) \quad \forall \varphi_h \in U_h, \tag{17}$$

has a unique solution.

Proof.

Use "kickback technique" of Schatz, 1974. □

Error estimates in the Riemann-Liouville case

Some estimates for the adjoint problem:

Lemma

Let Assumption 2.1 hold, $f \in L^2(D)$, $b \in W^{1,\infty}(D)$ and $q \in L^\infty(D)$. Let w be the solution of the adjoint problem (8). Then there holds

$$\inf_{\psi_h \in V_h} \|w - \psi_h\|_{L^2(D)} + \inf_{\psi_h \in V_h} \|{}_x^R D_1^{\alpha-1}(w - \psi_h)\|_{L^2(D)} \le ch\|f\|_{L^2(D)}. \qquad (18)$$

Observation:

- The approximation is better than usual cases due to the specific singularity behavior of the dual solution;
- The $L^2(D)$-estimate in the lemma is not sharp, but it is sufficient for our desired result.

Main theorem

Theorem

Let Assumption 2.1 hold, $f \in L^2(D)$, $b \in W^{1,\infty}(D)$, and $q \in L^\infty(D)$. Then there is an $h_0 > 0$ such that for all $h \le h_0$, the solution u_h to the finite element problem (17) *satisfies for any $\beta \in (2-\alpha, 1/2)$,*

$$\|u - u_h\|_{L^2(D)} + h\|(u-u_h)'\|_{L^2(D)} \le ch^{\alpha-1+\beta}\|f\|_{L^2(D)}.$$

Proof.

- The error estimate in the $\widetilde{H}^1(D)$-norm follows from Cea's lemma, inf-sup condition and Galerkin orthogonality.
- The error estimate in the L^2-norm follows from duality argument and approximation on the joint solution.

$\square$

Petrov-Galerkin FEM in the Caputo case

For Caputo, the Petrov-Galerkin finite element problem is to find $u_h \in U_h$ such that

$$A(u_h, \varphi_h) = \langle F, \varphi_h \rangle \quad \forall \varphi_h \in W_h. \tag{19}$$

Here $F \in W^*$ is a bounded linear functional on W.

Arguments is similar as those in the R-L case.

Theorem

Let Assumption 2.2 hold, $f \in \widetilde{H}_L^s(D)$, $b \in W^{1,\infty}(D)$ and $q \in L^\infty(D) \cap H^s(D)$. Then there is an h_0 such that for all $h \leq h_0$, the solution u_h to (19) satisfies

$$\|u - u_h\|_{L^2(D)} + h\|(u - u_h)'\|_{L^2(D)} \leq ch^{\min(\alpha+s,2)}\|f\|_{\widetilde{H}_L^s(D)}.$$

Compare with R-L case when $s = 0$:

$$\|u - u_h\|_{L^2(D)} + h\|(u - u_h)'\|_{L^2(D)} \leq ch^{\alpha-1+\beta}\|f\|_{L^2(D)}.$$

(a) The source term $f = x \in \widetilde{H}_L^s(D)$ for $s \in (1, 3/2)$.

(b) The source term $f = x^{-1/4} \in \widetilde{H}_L^s(D)$ $s \in (0, 1/4)$.

Table: Numerical results for example (a) with the R-L derivative and $b, q = 0$.

α	m	10	20	40	80	160	rate
1.6	L^2	3.10e-3	1.39e-3	6.42e-4	2.99e-4	1.39e-4	$\approx$ 1.10 (1.10)
	H^1	1.67e-1	1.50e-1	1.35e-1	1.21e-1	1.07e-1	$\approx$ 0.17 (0.10)
1.75	L^2	1.25e-3	4.62e-4	1.84e-4	7.55e-5	3.15e-5	$\approx$ 1.27 (1.25)
	H^1	5.03e-2	3.89e-2	3.14e-2	2.57e-2	2.10e-2	$\approx$ 0.29 (0.25)
1.9	L^2	6.40e-4	1.72e-4	4.92e-5	1.53e-5	5.14e-6	$\approx$ 1.53 (1.40)
	H^1	2.08e-2	1.15e-2	6.81e-3	4.38e-3	3.01e-3	$\approx$ 0.50 (0.40)

Table: Numerical results for example (a) with the Caputo derivative and $b, q = 0$.

α	m	10	20	40	80	160	rate
1.6	L^2	6.88e-4	1.72e-4	4.30e-5	1.08e-5	2.69e-6	$\approx$ 2.00 (2.00)
	H^1	2.18e-2	1.09e-2	5.45e-3	2.72e-3	1.33e-3	$\approx$ 1.02 (1.00)
1.75	L^2	6.28e-4	1.57e-4	3.93e-5	9.81e-6	2.45e-6	$\approx$ 2.00 (2.00)
	H^1	1.99e-2	9.93e-3	4.97e-3	2.48e-3	1.22e-3	$\approx$ 1.02 (1.00)
1.9	L^2	5.67e-4	1.42e-4	3.54e-5	8.86e-6	2.21e-6	$\approx$ 2.00 (2.00)
	H^1	1.79e-2	8.97e-3	4.48e-3	2.24e-3	1.10e-3	$\approx$ 1.02 (1.00)

observation: in case $b, q = 0$, the finite element solution is exactly the nodal interpolation, i.e.

$$u_h(x_i) = u(x_i), \quad i = 0, 1, 2, ..., m.$$

Table: Example (a) with the R-L derivative and $b = e^x$, $q = x(1-x)$.

α	m	10	20	40	80	160	rate
1.6	L^2	2.67e-3	9.41e-4	3.89e-4	1.74e-4	8.01e-5	$\approx$ 1.13 (1.10)
	H^1	1.22e-1	9.14e-2	7.93e-2	6.65e-2	5.81e-2	$\approx$ 0.20 (0.10)
1.75	L^2	1.23e-3	3.69e-4	1.28e-4	4.92e-5	2.00e-5	$\approx$ 1.29 (1.25)
	H^1	5.25e-2	3.18e-2	2.18e-2	1.65e-2	1.31e-2	$\approx$ 0.33 (0.25)
1.9	L^2	7.49e-4	1.92e-4	5.05e-5	1.40e-5	4.20e-6	$\approx$ 1.66 (1.40)
	H^1	3.02e-2	1.55e-2	8.10e-3	4.44e-3	2.61e-3	$\approx$ 0.70 (0.40)

Table: Example (a) with the Caputo derivative and $b = e^x$, $q = x(1-x)$.

α	m	10	20	40	80	160	rate
1.6	L^2	1.91e-3	4.92e-4	1.25e-4	3.18e-5	8.03e-6	$\approx$ 1.99 (2.00)
	H^1	7.12e-2	3.59e-2	1.80e-2	9.00e-3	4.50e-3	$\approx$ 1.03 (1.00)
1.75	L^2	1.03e-3	2.59e-4	6.49e-5	1.62e-5	4.06e-6	$\approx$ 2.00 (2.00)
	H^1	4.18e-2	2.10e-2	1.05e-2	5.27e-3	2.63e-3	$\approx$ 1.00 (1.00)
1.9	L^2	7.22e-4	1.81e-4	4.53e-5	1.13e-5	2.83e-6	$\approx$ 2.00 (2.00)
	H^1	2.88e-2	1.45e-2	7.25e-3	3.62e-3	1.81e-3	$\approx$ 1.02 (1.00)

Example (a)

One distinct feature: the stiffness matrix for the leading term is diagonal, and the resulting linear system is well conditioned.

Table: The condition number of the linear system for $b(x) = e^x$, $q(x) = x(1-x)$.

Deriv. type	$\alpha \backslash m$	20	40	80	160	320	640	1280
	1.55	2.98	3.48	4.26	4.30	4.57	4.84	5.00
R-L	1.75	2.06	2.22	2.33	2.40	2.45	2.48	2.50
	1.95	1.63	1.68	1.71	1.73	1.74	1.74	1.75
	1.55	2.75	3.20	3.57	3.89	4.16	4.39	4.60
Caputo	1.75	2.02	2.17	2.27	2.34	2.39	2.42	2.44
	1.95	1.63	1.68	1.71	1.73	1.73	1.74	1.74

Example (b)

Table: Example (b) with the R-L derivative and $b = e^x$, $q = x(1-x)$.

α	m	10	20	40	80	160	rate
1.6	L^2	1.07-2	4.61e-3	2.04e-3	9.18e-4	4.18e-4	$\approx$ 1.13 (1.10)
	H^1	5.03e-1	4.38e-1	3.87e-1	3.42e-1	2.99e-1	$\approx$ 0.20 (0.10)
1.75	L^2	4.62e-3	1.71e-3	6.60e-4	2.63e-4	1.07e-4	$\approx$ 1.30 (1.25)
	H^1	1.76e-1	1.33e-1	1.05e-1	8.47e-2	6.83e-2	$\approx$ 0.32 (0.25)
1.9	L^2	2.02e-3	5.93e-4	1.82e-4	5.87e-5	1.99e-5	$\approx$ 1.53 (1.40)
	H^1	7.05e-2	4.12e-2	2.54e-2	1.66e-2	1.14e-2	$\approx$ 0.52 (0.40)

Table: Example (b) with the Caputo derivative and $b = e^x$, $q = x(1-x)$.

α	m	10	20	40	80	160	rate
1.6	L^2	1.84e-3	4.92e-4	1.31e-4	3.51e-5	9.46e-6	$\approx$ 1.89 (1.85)
	H^1	7.47e-2	3.87e-2	2.01e-2	1.05e-2	5.54e-3	$\approx$ 0.94 (0.85)
1.75	L^2	1.56e-3	4.05e-4	1.05e-4	2.72e-5	7.04e-6	$\approx$ 1.97 (2.00)
	H^1	5.92e-2	3.04e-2	1.56e-2	7.99e-3	4.09e-3	$\approx$ 0.99 (1.00)
1.9	L^2	1.39e-3	3.54e-4	8.99e-5	2.28e-5	5.74e-6	$\approx$ 1.99 (2.00)
	H^1	5.02e-2	2.55e-2	1.29e-2	6.49e-3	3.27e-3	$\approx$ 1.03 (1.00)

Conclusion

Conclusion and remarks:

(1) novel Petrov-Galerkin formulations for FBVPs involving a convection term;

(2) the well-posedness and sharp regularity pickup of the formulations are established;

(3) a new finite element method was also developed;

(4) numerically, it leads to a diagonal stiffness matrix for the leading term;

(5) theoretically, admits derive optimal $L^2(D)$ and $H^1(D)$ error estimates;

(6) the technique can be used to improve the result for the time-dependent problem discussed in [8] for R-L case. The Caputo case is still open...

(7) other techniques, such as singularity reconstruction technique in [9], can be used to improve the result further.

Outstanding issues and future works

(1) optimal L^2-error estimate for piecewise linear approximations;
(2) what if $\alpha \in (1, 3/2)$, especially for Caputo derivative ???
(3) convection-dominated problem;
(4) nonlocal model in higher dimension;
(5) time-dependent problems;
(6) space-time formulations and adaptivity

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Thank you for your attention !!!