Second order BDF method for FODE and FKS equations

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1 Introduction

2 The schemes and main results

Some preliminaries:

Below $a \in \mathbb{R}^{\mathbb{N}}$ is a sequence of the form $a = (a_0, a_1, \dots, a_m, \dots)$ where $a_m \in \mathbb{R}$. For $a \in \mathbb{R}^{\mathbb{N}}$, the generating function is given by

$$F_a(z) = \sum_{m=0}^{\infty} a_m z^m.$$

For $a, c \in \mathbb{R}^{\mathbb{N}}$, we define the convolution $a * c$ as

$$(a * c)_n = \sum_{m=0}^{n} a_m c_{n-m},$$

and clearly $F_{a*c} = F_a(z)F_c(z)$. The convolution identity is $\delta_d = (1, 0, \dots)$ whose generating function is 1. For a sequence $b(b_0 \neq 0)$ with generating function $F(z)$, the generation function of the convolution inverse of $b^{(-1)}$ is given by $1/F(z)$.

2.1 Numerical approximation of the Caputo derivative

Review of the first order scheme

The second order scheme:

Consider a time step k and $t^n = nk$. We assume that $T = Nk$ is a fixed constant. Let $u = (u_0, u_1, u_2, \dots) \in \mathbb{R}^{\mathbb{N}}$ be the sequence of nodal values of u.

Below, we given a second order backward differentiation scheme for $D_c^\gamma u$. For the discussions from here on, we will assume that u_0 and u_1 are given.

For $n \geq 1$, the derivative is computed by

$$D_c^\gamma u(t^{n+1}) \approx k^{-\gamma}(b^{n+1} * u)_{n+1} =: \mathcal{D}_k u.$$

Here $b^{n+1} = (b_m^{n+1})_{m=0}^{n+1}$ is a sequence with $n+2$ components. If we set $b_m^{n+1} = 0, m \geq n+2$, then $b^{n+1} \in \mathbb{R}^{\mathbb{N}}$. $b^{n+1} * u$ can be defined. $(b^{n+1} * u)_{n+1} = \sum_{m=0}^{n+1} b_m^{n+1} u_{n+1-m}$ is the $n+1$-th component of this convolution.

The sequences b^{n+1} are given as follows:
For $n = 1$,

$$\Gamma(2-\gamma)b_0^2 = -\frac{1}{2}2^{1-\gamma} + \frac{1}{2-\gamma}2^{2-\gamma}$$
$$\Gamma(2-\gamma)b_1^2 = 2 \cdot 2^{1-\gamma} - \frac{2}{2-\gamma}2^{2-\gamma}$$
$$\Gamma(2-\gamma)b_2^2 = -\frac{3}{2}2^{1-\gamma} + \frac{1}{2-\gamma}2^{2-\gamma}$$

For $n = 2$,

$$\Gamma(2-\gamma)b_0^3 = \frac{1}{2} + \frac{1}{2-\gamma}$$
$$\Gamma(2-\gamma)b_1^3 = -\frac{3}{2} - \frac{3}{2-\gamma} - \frac{1}{2}3^{1-\gamma} + \frac{1}{2-\gamma}3^{2-\gamma}$$
$$\Gamma(2-\gamma)b_2^3 = \frac{3}{2} + 2 \cdot 3^{1-\gamma} + \frac{3}{2-\gamma} - \frac{2}{2-\gamma}3^{2-\gamma}$$
$$\Gamma(2-\gamma)b_3^3 = -\frac{1}{2} - \frac{3}{2}3^{1-\gamma} + \frac{1}{2-\gamma}(3^{2-\gamma} - 1)$$

For $n \geq 3$:

$$\begin{aligned} \Gamma(2-\gamma)b_0^{n+1} &= \tfrac{1}{2} + \tfrac{1}{2-\gamma}, \\ \Gamma(2-\gamma)b_1^{n+1} &= -\tfrac{3}{2} + 2^{1-\gamma}\tfrac{1}{2} - \tfrac{3}{2-\gamma} + \tfrac{1}{2-\gamma}2^{2-\gamma} \end{aligned} \tag{1}$$

When $2 \leq m \leq n-2$, we have $\Gamma(2-\gamma)b_m^{n+1} = h(m)$ where the function h is given by

$$\begin{aligned} h(m) = &-\frac{1}{2}(m-2)^{1-\gamma} - \frac{3}{2}m^{1-\gamma} + \frac{3}{2}(m-1)^{1-\gamma} + \frac{1}{2}(m+1)^{1-\gamma} \\ &+ \frac{1}{2-\gamma}(m+1)^{2-\gamma} - \frac{3}{2-\gamma}m^{2-\gamma} + \frac{3}{2-\gamma}(m-1)^{2-\gamma} - \frac{1}{2-\gamma}(m-2)^{2-\gamma} \end{aligned} \tag{2}$$

For the last three coefficients,

$$\Gamma(2-\gamma)b_{n-1}^{n+1} = -\frac{1}{2}n^{1-\gamma} - \frac{1}{2}(n+1)^{1-\gamma} - \frac{1}{2-\gamma}[n^{2-\gamma} - (n+1)^{2-\gamma}] + h(n-1) \tag{3}$$
$$\Gamma(2-\gamma)b_n^{n+1} = h(n) + \frac{3}{2}n^{1-\gamma} + \frac{3}{2}(n+1)^{1-\gamma} + \frac{3}{2-\gamma}[n^{2-\gamma} - (n+1)^{2-\gamma}] \tag{4}$$
$$\Gamma(2-\gamma)b_{n+1}^{n+1} = -\frac{1}{2}(n-1)^{1-\gamma} - \frac{3}{2}(n+1)^{1-\gamma} - \frac{1}{2-\gamma}(n-1)^{2-\gamma} + \frac{1}{2-\gamma}(n+1)^{2-\gamma} \tag{5}$$

Remark 1. *In real simulation, we can compute u^1, for example using a first order scheme. The error for u^1 will then be $O(k^2)$ Need to confirm.. This is not as good as the*

$O(k^{3-\gamma})$ estimation below. An alternative way is to $L_1(t)$ on both I_0, I_1. The relations

$$D_c^\gamma u(t^1) \approx k^{-\gamma}\frac{1}{\Gamma(2-\gamma)}[(-\frac{1}{2}+\frac{1}{2-\gamma})u_2 + (2-\frac{2}{2-\gamma})u_1 + (-\frac{3}{2}+\frac{1}{2-\gamma})u_0],$$
$$D_c^\gamma u(t^2) \approx k^{-\gamma} b^2 * u$$

then form a system of equations for u^1, u^2. We then compute them all at once. The local truncation error is $O(k^{3-\gamma})$.

2.2 Main results on the second order BDF method for FODE

stability and accuracy results of the BDF method for $D_c^\gamma u = \lambda u$.
stability results on variant BDF method.

Theorem 1. *Suppose $u \in C^3([0,\infty), \mathbb{R})$. Then, $\exists C > 0$ independent of γ and n such that $\forall 1 \le n \le N-1$,*

$$|D_c^\gamma u(t^{n+1}) - k^{-\gamma}(b^{n+1} * u)_{n+1}| \le Ck^{3-\gamma}.$$

If we apply the scheme on the model equation $D_c^\gamma u = \lambda u$ and define $z = k^\gamma \lambda$ we have

$$(b_0^n - z) + \sum_{m=1}^{n} b_m^n \zeta_m^n = 0.$$

where $\zeta_n^m = u^{n-m}/u^n$. The characteristic polynomial is $(b_0^n - z) + \sum_{m=1}^n b_m^n \eta^m = 0$. As we shall see in Theorem .. below, there exists $b \in \mathbb{R}^{\mathbb{N}}$, such that $b_m^{n+1} = b_m$ for $m \le n-2$, and $b^{n+1} \to b$ in $l^p, p \ge 1$. Hence, when n is sufficiently large, this relation is roughly

$$f(z,\eta) = (b_0 - z) + \sum_{m=1}^{\infty} b_m \eta^m = 0.$$

$f = F_b(\eta) - z$. Clearly, we want $\eta \ge 1$. In other words, we need $f(z,\eta)$ to have no zeros in the unit disk.

Definition 1. *The stability region is $D = \{z \in \mathbb{C} : f(z,\eta)$ satisfies the root property$\}$*

Definition 2. *The scheme is called A-stable if the stability region contains the whole left half plane.*

Clearly, the A-stability is reduced to study of the generating function of b.

Theorem 2. *The second backward differentiation $\mathcal{D}_k$ is A-stable.*

Add the result saying that if $\langle u^{n+1}, \cdot\rangle \le 0$, then it is absolutely stable. The norm will not grow, as in the new reference.

Theorem 3. *Consider the FODE $D_c^\gamma u = A(u)$. Suppose $A_k u$ is a second order approximation for $A(u)$ such that $\exists \lambda \geq 0$,*

$$\langle u^{n+1}, (A_k u)^{n+1} \rangle \leq \lambda (\|u^n\|^2 + \|u^{n-1}\|^2).$$

The scheme given by

$$(\mathcal{D}_k u)^{n+1} = (A_k u)^{n+1}, \ n \geq 1$$

is l^2-stable, or in other words,

$$\sum_{m=0}^{n} |u_m|^2 k \leq C(T) E_\gamma (C_1 (nk)^\gamma)$$

*for all $n \leq N$, where E_γ is the Mittag-Leffler function.*Need to make precise the constants

2.3 Main results on the first/second order method for FKS

stability.
small data condition?

Consider the following fractional Keller-Segel equation:

$$\begin{aligned} D_c^\gamma \rho &= \Delta \rho - \nabla \cdot (\rho \nabla c) \\ -\Delta c &= \rho \end{aligned}$$

Proposition 1. *The first order scheme for the KS is stable with small initial data.*

Proposition 2. *The second order scheme for the KS is $l^2(L^2(\mathbb{R}^2))$-stable if the initial data is small.*

By the sign properties of of b^{n+1}, we have

Proposition 3. *For the FKS and the second order scheme with five point..* to complete*, $\exists \bar{\gamma}_0 \in (0,1)$, if $\gamma \leq \bar{\gamma}_0$ and $u_0 \geq 0, u_1 \geq 0$, then $u_m \geq 0$ for all $m \geq 0$.*

3 Construction of the numerical approximation of the Caputo derivative

derivation.
estimates on the coefficients.

To be convenient, we denote $I_m = [t^m, t^{m+1}]$.

Suppose u_m is the nodal value of u at t^m. The Lagrange interpolation on I_m is given by:

$$L_m(t) = u_{m-1} \frac{(t - t^m)(t - t^{m+1})}{2k^2} - u_m \frac{(t - t^{m-1})(t - t^{m+1})}{k^2} + u_{m+1} \frac{(t - t^m)(t - t^{m-1})}{2k^2}$$

Hence, we use the approximation for $m \geq 1$

$$u'(t) \approx L'_m(t) = u_{m-1}\frac{t - t^{m+1/2}}{k^2} - 2u_m\frac{t - t^m}{k^2} + u_{m+1}\frac{t - t^{m-1/2}}{k^2}, \ t \in I_m. \qquad (6)$$

For $t \in I_0$, L_0 will be the quadratic approximation using u_0, u_1, u_2, i.e., we set $L_0 = L_1$.

The numerical scheme is given by

$$\mathcal{D}_k u(t^{n+1}) \approx \frac{1}{\Gamma(1-\gamma)} \sum_{m=0}^{n} \int_{I_m} \frac{L'_m(s)}{(t^{n+1}-s)^\gamma} ds = k^{-\gamma} \sum_{m=0}^{n+1} b_m^{n+1} u_{n+1-m}. \qquad (7)$$

We call this formula 'backward differentiation' since $b_0^{n+1} > 0$. As we shall see the scheme tends to BDF2 as $\gamma \to 1$.

We define the coefficients C_m^p for $m \geq 1$ through:

$$k^\gamma(1-\gamma) \int_{I_m} \frac{L'_m(s)}{(t^{n+1}-s)^\gamma} ds = C_m^{m+1} u_{m+1} + C_m^m u_m + C_m^{m-1} u_{m-1}.$$

Hence,

$$\begin{aligned}
C_m^{m+1} = & \ -\tfrac{3}{2}(n-m)^{1-\gamma} + \tfrac{1}{2}(n-m+1)^{1-\gamma} - \tfrac{1}{2-\gamma}(n-m)^{2-\gamma} + \tfrac{1}{2-\gamma}(n-m+1)^{2-\gamma}, \\
C_m^m = & \ 2(n-m)^{1-\gamma} + \tfrac{2}{2-\gamma}(n-m)^{2-\gamma} - \tfrac{2}{2-\gamma}(n-m+1)^{2-\gamma}, \\
C_m^{m-1} = & \ -\tfrac{1}{2}(n-m)^{1-\gamma} - \tfrac{1}{2}(n-m+1)^{1-\gamma} - \tfrac{1}{2-\gamma}(n-m)^{2-\gamma} + \tfrac{1}{2-\gamma}(n-m+1)^{2-\gamma}.
\end{aligned}$$

These are only valid for $m \geq 1$.

For $m = 0$, we compute $k^\gamma(1-\gamma)\int_0^{t^1} \frac{L'_1(t)}{(t^{n+1}-s)^\gamma} ds$ where

$$L'_1(t) = u_0 \frac{t - t^{3/2}}{k^2} - 2u_1 \frac{t - t^1}{k^2} + u_2 \frac{t - t^{1/2}}{k^2}.$$

and find

$$\begin{aligned}
C_0^2 &= -\frac{1}{2}n^{1-\gamma} - \frac{1}{2}(n+1)^{1-\gamma} - \frac{1}{2-\gamma}[n^{2-\gamma} - (n+1)^{2-\gamma}],, \\
C_0^1 &= 2(n+1)^{1-\gamma} + \frac{2}{2-\gamma}[n^{2-\gamma} - (n+1)^{2-\gamma}], \\
C_0^0 &= \frac{1}{2}n^{1-\gamma} - \frac{3}{2}(n+1)^{1-\gamma} - \frac{1}{2-\gamma}[n^{2-\gamma} - (n+1)^{2-\gamma}]
\end{aligned}$$

Hence, by the definition, we have

$$D_c^\gamma u(t^{n+1}) \approx \frac{1}{k^\gamma} \sum_{m=0}^{n+1} b_m^{n+1} u_{n+1-m} =$$

$$\frac{1}{k^\gamma \Gamma(2-\gamma)}(C_0^0 u_0 + C_0^1 u_1 + C_0^2 u_2 + \sum_{m=1}^{n} (C_m^{m-1} u_{m-1} + C_m^m u_m + C_m^{m+1} u_{m+1}))$$

Using the explicit formulas, we obtain the coefficients listed in Section...

Theorem 4. *We have the following claims:*

1. *For all $n \geq 1$,*
$$\sum_{m=0}^{n+1} b_m^{n+1} = 0.$$
For all $n \geq 1$, $b_0^{n+1} > 0$, $b_1^{n+1} < 0$. For $n \geq 2$, $b_m^{n+1} < 0$, $m \geq 3$. $\exists \bar{\gamma}_0 \in (0,1)$ and $\bar{\gamma}_1 \in (\bar{\gamma}_0, 1)$ such that $b_2^{n+1} \leq 0$ for $n \geq 1, \gamma < \bar{\gamma}_0$ and $b_2^{n+1} > 0$ for $n \geq 1, \gamma > \bar{\gamma}_1$.
There exists a sequence $b \in \mathbb{R}^{\mathbb{N}}$ such that if $n \geq 2$, $b_m^{n+1} = b_m$ for $m \leq n-2$.

2. *When $n \geq 1$, as $\gamma \to 1$,*
$$b_0^{n+1} \to 3/2, b_1^{n+1} \to -2, b_2^{n+1} \to 1/2, b_m^{n+1} \to 0$$
and the scheme tends to BDF2; as $\gamma \to 0$,
$$b_0^{n+1} \to 1, b_m^{n+1} \to 0, b_{n+1}^{n+1} \to -1.$$

3. *As $n \to \infty$, $b_{n-1}^{n+1} = O(n^{-1-\gamma})$,$b_n^{n+1} = O(n^{-1-\gamma})$ and $b_{n+1}^{n+1} = O(n^{-\gamma})$. $b^{n+1} \to b$ pointwise and in l^p, $p \geq 1$.*
For the limiting sequence b, $b_0 > 0$, $b_m < 0$ for $m \geq 1, m \neq 2$, and
$$\sum_m b_m = 0, \; b_0 \geq -\frac{3}{4} b_1, \quad -b_1 \geq 4b_2.$$
$\exists \theta > 0$, $(4b_0 + 3b_1)/(1-\gamma) \leq \theta$ for all $\gamma \in (0,1)$. $\exists \gamma_0 \in (0,1)$ such that $b_2 \leq 0$ if $\gamma \leq \gamma_0$ and $b_2 > 0$ for $\gamma > \gamma_0$. When $m \geq 3$, b_m increases to zero and $b_m = \frac{1}{\Gamma(-\gamma)} \frac{1}{m^{1+\gamma}} \left(1 + O(\frac{1}{m})\right)$ as $m \to \infty$.

To make the statement clean. The proof of this theorem is put in the appendix.

4 Stability and convergence analysis

4.1 Local truncation error

Suppose u is C^3. We know estimate the local truncation error.

Proof of Theorem:

By the Taylor formula
$$f(t) = f(s) + (t-s)f'(s) + \frac{1}{2}(t-s)^2 f''(s) + \int_s^t \frac{1}{2}(t-\tau)^2 f'''(\tau) d\tau,$$
we find
$$R_m(s) = L'_m(s) - u_s(s) = \frac{s - t^{m+1/2}}{k^2} \int_s^{t^{m-1}} \frac{1}{2}(t^{m-1} - \tau)^2 u'''(\tau) d\tau$$
$$- 2\frac{s - t^m}{k^2} \int_s^{t^m} \frac{1}{2}(t^m - \tau)^2 u'''(\tau) d\tau + \frac{s - t^{m-1/2}}{k^2} \int_s^{t^{m+1}} \frac{1}{2}(t^{m+1} - \tau)^2 u'''(\tau) d\tau \quad (8)$$

The total error will be

$$r = \frac{1}{\Gamma(1-\gamma)} \left(r_0 + \sum_{m=1}^{n} \int_{I_m} \frac{R_m(s)}{(t^{n+1}-s)^\gamma} ds \right)$$

where

$$r_0 = \int_{I_0} \frac{R_1(s)}{(t^{n+1}-s)^\gamma} ds.$$

Direct estimate shows

$$r_0 \le Ck^2 \int_0^k \frac{1}{((n+1)k-s)^\gamma} ds \le C_1 k^{3-\gamma}.$$

where C_1 is independent of n, γ. If we use the same estimate, $|R_m| \le Ck^2$, then we obtain

$$r \le \frac{1}{\Gamma(1-\gamma)}(r_0 + Ck^2 \int_{t^1}^{t^{n+1}} \frac{1}{(t^{n+1}-s)^\gamma} ds) \le \frac{C}{\Gamma(2-\gamma)} T^{1-\gamma} k^2$$

The scheme is at least uniformly second order.

Better estimates

$$\frac{1}{\Gamma(1-\gamma)} \int_{t^m}^{t^{m+1}} \frac{R_m(s)}{(t^{n+1}-s)^\gamma} ds = I_1^m + I_2^m$$

where

$$I_1^m = \frac{1}{\Gamma(1-\gamma)} \frac{1}{2k^2} \int_{t^{m-1}}^{t^m} u'''(\tau)(t^{m+1}-\tau)^2 \int_{t^m}^{t^{m+1}} \frac{t^{m+1/2}-s}{(t^{n+1}-s)^\gamma} ds d\tau,$$

and $I_2^m = \frac{1}{2k^2\Gamma(1-\gamma)} \int_{t^m}^{t^{m+1}} u'''(\tau) P_m(\tau) d\tau$,

$$\begin{aligned} P_m(\tau) = (t^{m-1}-\tau)^2 \int_\tau^{t^{m+1}} \frac{t^{m+1/2}-s}{(t^{n+1}-s)^\gamma} ds \\ - 2(t^m-\tau)^2 \int_\tau^{t^{m+1}} \frac{t^m-s}{(t^{n+1}-s)^\gamma} ds + (t^{m+1}-\tau)^2 \int_{t^m}^\tau \frac{s-t^{m-1/2}}{(t^{n+1}-s)^\gamma} ds. \end{aligned}$$

Note that $\int_{t^m}^{t^{m+1}} \frac{t^{m+1/2}-s}{(t^{n+1}-s)^\gamma} ds$ is negative for all m, we find

$$|\sum_m I_1^m| \le \sum_m \frac{Ck}{\Gamma(1-\gamma)} \int_{t^m}^{t^{m+1}} \frac{s-t^{m+1/2}}{(t^{n+1}-s)^\gamma} ds$$

where $C \sim \sup |u'''|$ is independent of n, m, γ.

$$\int_{t^m}^{t^{m+1}} \frac{s-t^{m+1/2}}{(t^{n+1}-s)^\gamma} ds = \frac{k^{2-\gamma}}{1-\gamma} [\frac{1}{2-\gamma}((n-m+1)^{2-\gamma} - (n-m)^{2-\gamma}) - \frac{1}{2}((n-m+1)^{1-\gamma} + (n-m)^{1-\gamma})]$$

This number $\leq \frac{Ck^{2-\gamma}}{1-\gamma}(n-m+1/2)^{-1-\gamma}$ by Taylor expansion about $n-m+1/2$, where $C=\sup_\gamma \gamma(1-\gamma)$ is independent of m, γ, n. Hence,

$$|\sum_{m\geq 1} I_1^m| \leq \sum_{m=1}^{n} \frac{1}{\Gamma(1-\gamma)} \frac{Ck^{3-\gamma}}{1-\gamma}(n-m+1/2)^{-1-\gamma} \leq C_1 k^{3-\gamma}$$

where C_1 is independent of γ and n.

For I_2^m, in the appendix, we show that $P_m(\tau) \leq 0$ for all $m \geq 1$ and $\tau \in I_m$. Applying the integral mean value theorem, we obtain $\int_{t^m}^{t^{m+1}} u'''(\tau)P_m(\tau)d\tau = u'''(\xi)\int_{I_m} P_m(\tau)d\tau$. Direct computation shows

$$\begin{aligned}(1-\gamma)\int P_m(\tau)d\tau &= \frac{k^3}{2}k^{2-\gamma}(n-m)^{1-\gamma} + \frac{5}{3}\frac{1}{2-\gamma}(n-m)^{2-\gamma} \\ &+ (\frac{k^3}{3})k^{2-\gamma}[\frac{1}{2}(n-m+1)^{1-\gamma} + \frac{1}{2-\gamma}(n-m+1)^{2-\gamma}] \\ &+ \frac{2k^2}{(2-\gamma)(3-\gamma)}(n-m)^{3-\gamma}k^{3-\gamma} - \frac{2k^2}{(2-\gamma)(3-\gamma)}(n-m+1)^{3-\gamma}k^{3-\gamma}\end{aligned}$$

We do Taylor expansion about $n-m+1/2$. We find $2-\gamma$, $1-\gamma$, $-\gamma$ all cancel out. The nonzero power will be $(n-m+1/2)^{-1-\gamma}$, and hence summable.

Hence,

$$|\sum_{m\geq 1} I_2^m| \leq \sum_{1\leq m\leq n} \frac{1}{k^2\Gamma(1-\gamma)} \frac{C_2}{1-\gamma} k^{5-\gamma}(n-m+1/2)^{-1-\gamma}$$

Hence,

$$r \leq \frac{1}{\Gamma(1-\gamma)} r_0 + C_3 k^{3-\gamma} \leq C k^{3-\gamma},$$

where C is uniform for $\gamma \in [0,1]$ since $\Gamma(1-\gamma) \geq 1$.

4.2 A-stability

In the case $b_2 \leq 0$, the scheme is A-stable. This is because all coefficients except b_0 are all negative. $|b_0 - z| \leq \sum_{m=1}^{\infty}(-b_m^{\infty})|\eta|^m \leq b_0$ if $|\eta| \leq 1$.

Now, assume $b_2 > 0$. It would suffice to show $\inf_{z\in D(0,1)} Re(f(\eta, 0)) \geq 0$. Recall that $b_1 < 0, b_2 > 0$

Since $-|\sum_{m=3}^{\infty} b_m\eta^m| \geq -\sum_{m=3}^{\infty}|b_m| = \sum_{m=3}^{\infty} b_m = -(b_0+b_1+b_2)$, we find $Re(f(\eta,0)) \geq b_0 + Re(b_1\eta + b_2\eta^2) - (b_0+b_1+b_2)$

Setting $\eta = r\cos\theta$ results in the function

$$h(r,\theta) = |b_1|(1 - r\cos\theta) - b_2(1 - r^2\cos(2\theta)).$$

This function is positive for $\cos\theta \leq 0$ because $|b_1| \geq 2b_2$. For $\cos\theta \geq 0$, $h_r = -|b_1|\cos\theta + 2b_2 r\cos(2\theta) \leq 0$ since $r\cos(2\theta) \leq \cos(\theta)$. The minimum value is achieved on $r=1$.

Set $h(\theta) = |b_1|(1-\cos\theta) - b_2(1-\cos(2\theta))$ with $0 \leq \theta \leq \pi/2$. We find that $h(0)=0$, which is desired since $f(1,0)=0$. $h' = \sin\theta(|b_1| - 4b_2\cos\theta)$. Since $|b_1| > 4b_2$, $h > 0$ when $\theta \neq 0$. Hence, $h(\theta) > 0$ for $0 < \theta \leq \pi/2$.

4.3 Analysis of the FODE

Lemma 1. *Suppose $b = \{b_n\}$ is a sequence satisfying $\sum_{n=0}^{\infty} b_n = 0$ and $b_0 > 0$. Suppose further that $b_n = \frac{1}{\Gamma(-\gamma)} n^{-1-\gamma}(1 + O(\frac{1}{n}))$, where $0 < \gamma < 1$. Let $F(z)$ be its generating function $F(z) = \sum_{n=0}^{\infty} b_n z^n$. Then,*

1. $$F(z) - (1 - z)^{\gamma} = (1 - z)G(z)$$

   where $G(z)$ is bounded in the unit disk.

2. *Let $b^{(-1)}$ be the convolution inverse of b. Its generatating function $F(z)^{-1} \sim (1-z)^{-\gamma}$ and thus $b_n^{(-1)} = [z^n]F(z)^{-1} \sim \frac{1}{\Gamma(\gamma)} n^{\gamma-1}$*

Proof. Let $H(z) = F(z) - (1 - z)^{\gamma}$. Then, $H(1) = 0$. Consider the Taylor series of H:

$$H(z) = \sum_{n=0}^{\infty} d_n z^n.$$

By the asymptotic behavior of b and the asymptotic behavior of the coefficients of $(1-z)^{\gamma}$, we find

$$d_n = O(\frac{1}{n^{2+\gamma}}).$$

Now consider

$$\frac{H(z)}{1 - z} = \frac{H(z) - H(1)}{1 - z} = \sum \frac{d_n(z^n - 1)}{1 - z}.$$

Then, for each term, $|d_n z^n - d_n|(1 - z)^{-1} \leq Cnd_n$ where C is independent of n and $z \in D(0, 1)$. Since $\sum n|d_n|$ converges. Hence, $G(z) = H(z)/(1 - z)$ is bounded. The first claim is proved.

Using the first claim, we find that

$$F(z)^{-1} = (1 - z)^{-\gamma} \frac{1}{1 + (1 - z)^{1-\gamma} G(z)}$$

This implies that as $z \sim 1$, $F(z)^{-1} \sim (1 - z)^{-\gamma}$.

By Corollary VI.1 in [?], we have $b_n^{(-1)} = [z^n]F(z)^{-1} \sim \frac{1}{\Gamma(\gamma)} n^{\gamma-1}$. □

By the second statement, we are able to conclude:

Corollary 1. *If the sequence b satisfies the conditions in Lemma 1, then $\exists C > 0$ such that $|b_n^{(-1)}| \leq C \frac{1}{\Gamma(\gamma)} (n + 1)^{\gamma-1}$.*

We will then use the notation C_b to represent the sharp constant for this the sequence b.

The following discrete Gronwall inequality is important ([?]):

Lemma 2. *Let $a \in \mathbb{R}^{\mathbb{N}}$ and $a_i \geq 0, 0 \leq i \leq N$. If a satisfies*

$$a_n \leq B + \frac{M}{\Gamma(\gamma)} k^{\gamma} \sum_{m=0}^{n-1} (n-m)^{\gamma-1} a_m, \forall 0 \leq n \leq N,$$

where $B > 0$ and $M > 0$ are independent of n, k, γ, then,

$$a_n \leq B E_{\gamma}(M(nk)^{\gamma}), 0 \leq n \leq N.$$

The function E_{γ} is the Mittag-Leffler function.

Now, we prove an important lemma

Lemma 3. *Suppose $b = \{b_n\}$ is a sequence satisfying the properties above. Let $E = \{E^n\}$ be a nonnegative sequence. Let $b^{(-1)}$ be the convolution inverse of b, which has generating function $1/F(z)$. Let $k = T/N$ where N is a big integer.*

If one of the following two conditions is satisfied:
(i). $\exists \gamma_n \geq 0, \beta \geq 0$, $\gamma_n \leq C \frac{1}{\Gamma(1-\gamma)} k^{-\gamma} (1+n)^{-\gamma}$

$$k^{-\gamma} |(b * E)_{n+1}| \leq \gamma_n + \beta E^n, \forall 0 \leq n \leq N.$$

(ii). $b_n^{(-1)} \geq 0$ and $\exists \gamma_n \geq 0, \beta \geq 0$, $\gamma_n \leq C \frac{1}{\Gamma(1-\gamma)} k^{-\gamma} (1+n)^{-\gamma}$

$$k^{-\gamma} (b * E)_{n+1} \leq \gamma_n + \beta E^n, \forall 0 \leq n \leq N.$$

Then,

$$E^n \leq (C_b b_0 E_0 / \Gamma(\gamma) + C_b C) E_{\gamma}(C_b \beta (nk)^{\gamma}), \ \forall 0 \leq n \leq N.$$

Proof. Let $H_n = k^{-\gamma}(b * E)_n$ and consider the sequence $H = \{H_n\}$. Then clearly, we have $E^n = k^{\gamma}(b^{(-1)} * H)_n$ for all $n \geq 0$.

Recall that $|b_n^{(-1)}| \leq \frac{C_b}{\Gamma(\gamma)} (n+1)^{\gamma-1}$. For $0 \leq n \leq N$, if the first case happens, we have

$$\begin{aligned}
E^n &\leq k^{\gamma} \sum_{i=0}^{n} |b_{n-j}^{(-1)}| |H_j| \leq |b_n^{(-1)}| b_0 E_0 + C_b k^{\gamma} \sum_{j=1}^{n} \frac{1}{\Gamma(\gamma)} (n-j+1)^{\gamma-1} (\gamma_{j-1} + \beta E^{j-1}) \\
&\leq (|b_n^{(-1)}| b_0 E_0 + C_b C) + k^{\gamma} \frac{C_b \beta}{\Gamma(\gamma)} \sum_{j=0}^{n-1} (n-j)^{\gamma-1} E^j, \ \forall 0 \leq n \leq N
\end{aligned}$$

if the second case happens, then, we have

$$\begin{aligned}
E^n &\leq k^{\gamma} \sum_{j=0}^{n} b_{n-j}^{(-1)} H_j \leq b_n^{(-1)} b_0 E_0 + C_b k^{\gamma} \sum_{j=1}^{n} \frac{1}{\Gamma(\gamma)} (n-j+1)^{\gamma-1} (\gamma_{j-1} + \beta E^{j-1}) \\
&\leq (b_n^{(-1)} b_0 E_0 + C_b C) + \frac{C_b \beta}{\Gamma(\gamma)} \sum_{j=0}^{n-1} (n-j)^{\gamma-1} E^j, \ \forall 0 \leq n \leq N
\end{aligned}$$

Here, we have used the fact

$$\frac{1}{\Gamma(\gamma)\Gamma(1-\gamma)}k^{\gamma}\sum_{j=0}^{n-1}(n-j)^{\gamma-1}k^{-\gamma}(1+j)^{-\gamma}=\frac{1}{\Gamma(\gamma)\Gamma(1-\gamma)}\sum_{j=0}^{n-1}(1-\frac{j}{n})^{\gamma-1}(\frac{j+1}{n})^{-\gamma}\frac{1}{n}$$
$$\le\frac{1}{\Gamma(\gamma)\Gamma(1-\gamma)}\sum_{j=0}^{n-1}\int_{j/n}^{(j+1)/n}(1-x)^{\gamma-1}x^{-\gamma}dx=1$$

The discrete Gronwall inequality guarantees that E^n has the bound as indicated. □

We now prove theorem...

Proof. Now considering left hand side. The issue is that b_2 may be positive.

Consider that $n\ge 1$. Then, $b_m^{n+1}=b_m$ for $m\le n-2$.

The key point is to write

$$b_0u^{n+1}+b_1u^n+b_2u^{n-1}=-\frac{b_1}{2}(\frac{3}{2}u^{n+1}-2u^n+\frac{1}{2}u^{n-1})+(b_0+\frac{3}{4}b_1)u^{n+1}+(b_2+\frac{b_1}{4})u^{n-1}$$

Define the new sequence $c_0^{n+1}=b_0+\frac{3}{4}b_1>0$, $c_1^{n+1}=0$, $c_2^{n+1}=b_2+\frac{1}{4}b_2<0$, $c_m^{n+1}=b_m<0, m\ge 3$. $\sum_m c_m^{n+1}=0$ still holds. We also use c to mean the limiting sequence for c^{n+1}. By the technique used in...

$$\langle u^{n+1},\sum_m c_m^{n+1}u^{n+1-m}\rangle\ge\frac{1}{2}\sum_m c_m^{n+1}\|u^{n+1-m}\|^2.$$

Further,

$$\langle u^{n+1},\frac{3}{2}u^{n+1}-2u^n+\frac{1}{2}u^{n-1}\rangle\ge\frac{1}{4}(\|u^{n+1}\|_2^2-\|u^n\|_2^2+\|2u^{n+1}-u^n\|_2^2-\|2u^n-u^{n-1}\|_2^2)$$

Since $\langle u^{n+1},(\mathcal{D}_k u)^{n+1}\rangle\le\lambda(\|u^n\|^2+\|u^{n+1}\|^2)$ and $-b_1>0$, we have

$$-\frac{b_1}{8}k^{-\gamma}(\|u^{n+1}\|_2^2-\|u^n\|_2^2+\|2u^{n+1}-u^n\|_2^2-\|2u^n-u^{n-1}\|_2^2)$$
$$+\frac{1}{2}k^{-\gamma}\left(c_0\|u^{n+1}\|^2+c_2\|u^{n-1}\|^2+\sum_{m=3}^{n+1}c_m\|u^{n+1-m}\|^2\right)$$
$$\le k^{-\gamma}(b_{n-1}-b_{n-1}^{n+1})\|u^2\|^2+k^{-\gamma}(b_n-b_n^{n+1})\|u^1\|^2+k^{-\gamma}(b_{n+1}-b_{n+1}^{n+1})\|u^0\|^2+\lambda(\|u^n\|^2+\|u^{n-1}\|^2)$$

This is valid for all $n\ge 1$.

Set $F_n = \frac{1}{n+1}\sum_{m=0}^{n} \|u^m\|_2^2$.

$$-\frac{b_1}{8(n+2)}k^{-\gamma}((\|u^{n+1}\|_2^2 - \|u^1\|_2^2 + \|2u^{n+1} - u^n\|_2^2 - \|2u^1 - u^0\|_2^2)$$

$$+\frac{1}{2}k^{-\gamma}\left(c_0F_{n+1} + c_2\frac{n}{n+2}F_{n-1} + \sum_{m=3}^{n+1} c_m\frac{n+2-m}{n+2}F_{n+1-m}\right)$$

$$\le k^{-\gamma}\frac{1}{n+2}\sum_{m=1}^{n}(b_{m-1} - b_{m-1}^{m+1})\|u^2\|^2 + k^{-\gamma}\frac{1}{n+2}(\sum_{m=1}^{n}(b_m - b_m^{m+1}) + \frac{c_0}{2})\|u^1\|^2$$

$$+ k^{-\gamma}\frac{1}{n+2}(\frac{1}{2}c_0 + \sum_{m=1}^{n}(b_{m+1} - b_{m+1}^{m+1}))\|u^0\|^2 + 2\lambda F_n$$

By the explicit expressions

$$b_{n-1} - b_{n-1}^{n+1} = \frac{1}{\Gamma(2-\gamma)}(\frac{1}{2}n^{1-\gamma} + \frac{1}{2}(n+1)^{1-\gamma} + \frac{1}{2-\gamma}[n^{2-\gamma} - (n+1)^{2-\gamma}])$$

$$b_n - b_n^{n+1} = \frac{1}{\Gamma(2-\gamma)}(-\frac{3}{2}n^{1-\gamma} - \frac{3}{2}(n+1)^{1-\gamma} - \frac{3}{2-\gamma}[n^{2-\gamma} - (n+1)^{2-\gamma}])$$

$$b_{n+1} - b_{n+1}^{n+1} = \frac{1}{\Gamma(2-\gamma)}(\frac{3}{2}n^{1-\gamma} + \frac{1}{2}(n+2)^{1-\gamma} + \frac{1}{2-\gamma}[(n+2)^{2-\gamma} - 4(n+1)^{2-\gamma} + 3n^{2-\gamma}])$$

Taylor expanding $n^{1-\gamma}, (n+1)^{1-\gamma}$ at x yields

$$\left|\int_n^{n+1}(\frac{1}{2}n^{1-\gamma} + \frac{1}{2}(n+1)^{1-\gamma} - x^{1-\gamma})dx\right| \le \frac{1}{6}\gamma(1-\gamma)\frac{1}{n^{1+\gamma}}$$

Using this result, we find

$$|\frac{3}{2}n^{1-\gamma}+\frac{1}{2}(n+2)^{1-\gamma}+\frac{1}{2-\gamma}[(n+2)^{2-\gamma}-4(n+1)^{2-\gamma}+3n^{2-\gamma}]| \le \frac{4}{6}\gamma(1-\gamma)\frac{1}{n^{1+\gamma}}+(n+2)^{1-\gamma}-(n+1)^{1-\gamma}$$

Hence, the first two terms are controlled by

$$k^{-\gamma}\frac{1}{\Gamma(1-\gamma)}\frac{1+\gamma}{6(n+2)}\|u^2\|^2 + k^{-\gamma}\frac{1}{2(n+2)}(\frac{1+\gamma}{\Gamma(1-\gamma)} + c_0/6)\|u^1\|^2$$

The last term on right hand side is controlled by

$$k^{-\gamma}\frac{1}{n+2}(\frac{c_0}{2} + \frac{4}{6}\frac{1+\gamma}{\Gamma(1-\gamma)} + \frac{(n+2)^{1-\gamma} - 2^{1-\gamma}}{\Gamma(2-\gamma)})\|u^0\|^2$$

Noting the signs of the coefficients, we have

$$\frac{1}{2}k^{-\gamma}\left(c_0F_{n+1} + c_2F_{n-1} + \sum_{m=3}^{n+1} c_mF_{n+1-m}\right) \le -\frac{|b_1|k^{-\gamma}}{8|n+2|}\|u^{n+1}\|^2 +$$

$$\frac{k^{-\gamma}}{n+2}[\frac{\|u^2\|^2}{3\Gamma(1-\gamma)}+(\frac{5}{8}|b_1|+\frac{1}{\Gamma(1-\gamma)}+\frac{c_0}{12})\|u_1\|^2+(\frac{|b_1|}{8}+\frac{c_0}{2}+\frac{4}{3\Gamma(1-\gamma)}-\frac{2^{1-\gamma}}{\Gamma(2-\gamma)})\|u^0\|^2]$$

$$+\frac{1}{\Gamma(1-\gamma)(1-\gamma)}k^{-\gamma}(n+1)^{-\gamma}\|u^0\|^2 + 2\lambda F_n.$$

Using Lemma 3, we can show that F is bounded since $c = (b_0 + \frac{3}{4}b_1, 0, b_2 + \frac{b_1}{4}, b_3, \ldots)$ satisfies the conditions in the lemma. $\square$

Remark 2. *In the proof, we essentially use the sequence c to show the stability. The bound obtained depends on C_c. As $\gamma \to 1$, $c_0 \to 0$, and $C_c \to \infty$. Also, $\frac{1}{1-\gamma}$ blows up. The term $-k^{-\gamma}\|u^{n+1}\|^2$ in Equation .. becomes important to ensure the stability. One may combine these two to gain a uniform bound but we are not going to explore this.*

The condition on A_k says that A_k should have a kind of negativity. For example, if $A_k(u) = -\delta u^{n+1} + B(u^{n-1}, u^n)$ where $\delta > 0$ and $|B(u^{n-1}, u^n)| \le C(\|u^{n-1}\| + \|u^n\|)$, then the condition is satisfied. This theorem can be used to show that

Corollary 2. *The implicit second order scheme for $D_c^\gamma u = \lambda u, \lambda \le 0$ is l^2-stable.*

This agrees with the A-stability analysis. Actually, as stated in ..., we have more. Now, we list the proof here...

Using the tools above, we can actually show some results about the first order scheme: We denote the first order scheme as

$$(\mathscr{D}_k u)^{n+1} = k^{-\gamma}(a^{n+1} * u)_{n+1}.$$

As we have seen, the difference scheme is $(b^{n+1} * u)_{n+1}$ where b^{n+1} is a sequence with length $n+1$.

Theorem 5. *If E^n is a nonnegative sequence satisfying*

$$(\mathscr{D}_k E)^{n+1} \le \lambda E^n$$

then

$$E^n \le E^0 C(T) E_\gamma(C_1 (nk)^\gamma), \forall 0 \le n \le N.$$

Proof. Let $a = (a_0, a_1, \ldots)$ be the limit sequence.

As we know $a_0 > 0$ and $a_m < 0$ for all $m \ge 1$. Then, we find that all components of $a^{(-1)}$ are positive.

By what has been computed, a^{n+1} is exactly the same as the subsequence of a for the first n components.

$$k^{-\gamma}(a^{n+1} * E)_{n+1} = k^{-\gamma}(a * E)_{n+1} + k^{-\gamma}(a^{n+1}_{n+1} - a_{n+1})E^0 \le CE^n, \ \forall 0 \le n \le N.$$

Note that $a^{n+1}_{n+1} - a_{n+1} = \sum_{m=n+2}^\infty a_m = O(n^{-\gamma})$. Can make exact using the explicit expressions $\square$

Corollary 3. *Consider the FODE $D_c^\gamma u = A(u)$. Suppose $\mathscr{A}_k u$ is a first order approximation for $A(u)$ such that $\exists \lambda \ge 0$,*

$$\langle u^{n+1}, (\mathscr{A}_k u)^{n+1} \rangle \le \lambda (u^n)^2.$$

The scheme given by

$$(\mathcal{D}_k u)^{n+1} = (\mathscr{A}_k u)^{n+1}, \ n \ge 1$$

is stable.

Corollary 4. *Consider the FODE*

$$D_c^\gamma u = \lambda u.$$

The first order explicit scheme given by

$$(\mathscr{D}_k u)^{n+1} = \lambda u^n,$$

is stable for $\lambda \ge 0$.

The first order implicit scheme

$$(\mathscr{D}_k u)^{n+1} = \lambda u^{n+1},$$

is stable for $\lambda \le 0$.

Proof. Consider the explicit scheme and $\lambda \ge 0$. Since both the FODE and the scheme are linear. We can consider $u_0 \ge 0$. By the sign of the coefficients, we find that u^n are all nonnegative. The theorem then implies ....

For the implicit scheme, since $\langle u^{n+1}, \lambda u^{n+1}\rangle \le 0$. Using Corollary..., we find that ... □

4.4 Analysis of fractional KS

For the FKS, the continuous model,

Integrating by parts,

$$\frac{u(t)-u(0)}{t^\gamma} + \gamma \int_0^t \frac{u(t)-u(s)}{(t-s)^{1+\gamma}} ds = \dots$$

It is clear that the difference scheme is a kind of approximation for this. $b_0 \approx \frac{1}{t^\gamma} + \gamma \int_0^{t-k} \frac{1}{(t-s)^{1+\gamma}} ds$, etc..

Since

$$\langle u, \Delta u - \nabla \cdot (\rho \nabla c)\rangle = -\|\nabla u\|_2^2 + \frac{1}{2}\|\rho^3\|_1,$$

and $\|\rho^3\|_1 \le C\|\rho\|_1 \|\nabla \rho\|_2^2$ by Gargolidardo-Nirenberg inequality for dimension 2, we see that if the initial mass is small, then,

$$\langle u(t), \frac{u(t)-u(0)}{t^\gamma} + \gamma \int_0^t \frac{u(t)-u(s)}{(t-s)^{1+\gamma}} ds\rangle \le 0.$$

Since $a(a-b) \ge \frac{1}{2}(a^2 - b^2)$, then $\|u(t)\|_2^2$ decays.

For the semi-discrete scheme, we just verify the conditions....

We just verify the conditions in....

5 Numerical results

5.1 FODE

stability region plot with variant n.

convergence order test for $D_c^\gamma u = \lambda u$ with BDF and variant BDF methods, where exact solution is available.

convergence order test for $D_c^\gamma u = f(u)$, where reference solution is computed with fine mesh.

5.2 FKS

A Properties of the coefficients

We now give the proof of Theorem ...

Proof. If we set $u = 1$, then $u_s(s) - L_m'(s) = 0$ for all $m \geq 1$. Hence,

$$k^{-\gamma} \sum_{m=0}^{n+1} b_m^{n+1} = \mathcal{D}_k 1 = D_c^\gamma 1 = 0$$

for any $n \geq 1$.

By the explicit formulas, $b_2^2 = \frac{2^{1-\gamma}}{\Gamma(2-\gamma)}(\frac{2}{2-\gamma} - \frac{3}{2})$ and the inside is monotone which increases from $-1/2$ to $1/2$. For $n \geq 4$, the sign of $b_2^{n+1} = \frac{1}{\Gamma(2-\gamma)} h(2)$ is given by the discussion below. $b_2^4 = \frac{1}{\Gamma(2-\gamma)}[h(2) - \frac{1}{2}3^{1-\gamma} - \frac{1}{2}4^{1-\gamma} - \frac{1}{2-\gamma}(3^{2-\gamma} - 4^{2-\gamma})]$. The extra terms adding to $h(2)$ is nonpositive and is zero for $\gamma = 0, \gamma = 1$. By the property of $h(2)$ below, we find that b_2^4 is negative near $\gamma = 0$ and positive near $\gamma = 1$. Similarly, we find $\Gamma(2-\gamma) b_2^3 = h(2) + \frac{3}{2}(2^{1-\gamma} + 3^{1-\gamma}) + \frac{3}{2-\gamma}(2^{2-\gamma} - 3^{2-\gamma})$. The argument is similar as b_2^4. The existence of $\bar{\gamma}_0$ and $\bar{\gamma}_1$ is proved.

The signs of other coefficients when $n = 1, n = 2$ can be checked directly since the explicit expressions are simple enough. The other claims about $n = 1, n = 2$ in the theorem can also be checked directly.

We now focus on $n \geq 3$. $b_0^{n+1} > 0$ is obvious by the expressions of b_0^{n+1}. If $n \geq 2$, we have

$$\Gamma(2-\gamma) b_1^{n+1} = -1 + \frac{2^{1-\gamma}}{2} + (-\frac{1}{2} - \frac{3}{2-\gamma} + \frac{2^{2-\gamma}}{2-\gamma}) < 0.$$

The existence of b is obvious since b_m^{n+1} is independent of n when $n \geq 1$ and $m \leq n-1$.

Since $\Gamma(2-\gamma) \geq 0$ and $\Gamma(2-\gamma) \to 1$ as $\gamma \to 1$ or $\gamma \to 0$, the properties of b_m can be reduced to considering

$$h(m) = -\frac{1}{2}(m-2)^{1-\gamma} - \frac{3}{2}m^{1-\gamma} + \frac{3}{2}(m-1)^{1-\gamma} + \frac{1}{2}(m+1)^{1-\gamma}$$
$$+ \frac{1}{2-\gamma}(m+1)^{2-\gamma} - \frac{3}{2-\gamma}m^{2-\gamma} + \frac{3}{2-\gamma}(m-1)^{2-\gamma} - \frac{1}{2-\gamma}(m-2)^{2-\gamma}.$$

Then,

$$h(2) = -\frac{3}{2}2^{1-\gamma} + \frac{3}{2} + \frac{1}{2}3^{1-\gamma} + \frac{1}{2-\gamma}3^{2-\gamma} + \frac{3}{2-\gamma} - \frac{3}{2-\gamma}2^{2-\gamma}.$$

As $\gamma \to 0$, $h(2) \to 0$ and $h(2) \to 1/2$ as $\gamma \to 1$. Consider $H_2(\gamma) = (2-\gamma)h(2) = 3(\gamma-6)2^{-\gamma} + (12-3\gamma/2)3^{-\gamma} + (6-3\gamma/2)$. It's easy to see $H_2'(0) < 0$. Further,

$$H_2''(\gamma) = 3^{-\gamma}[3\ln 3 + (12-3\gamma/2)(\ln 3)^2 - 6(3/2)^{\gamma}\ln 2 + (3/2)^{\gamma}(\gamma-6)(\ln 2)^2]$$
$$\geq 3^{-\gamma}[3\ln 3 + (12-3\gamma/2)(\ln 3)^2 - 9\ln 2 + \frac{3}{2}(\gamma-6)(\ln 2)^2]$$

The inside is a linear function which is positive at both $\gamma = 0$ and $\gamma = 1$. Hence, $\exists \gamma_0 > 0$ such that $H_2(\gamma) < 0$ when $\gamma \in (0, \gamma_0)$ and $H_2(\gamma) > 0$ when $\gamma > \gamma_0$. Then, $h(2)$ has the same sign since $2-\gamma > 0$.

For $m \geq 3$, we find $h(m) \to 0$ as $\gamma \to 0$ or $\gamma \to 1$. Setting $g = \frac{1}{2-\gamma}x^{2-\gamma} + \frac{1}{2}x^{1-\gamma}$, we have $h(m) = -g(m-2) + 3g(m-1) - 3g(m) + g(m+1)$. $g''' < 0$ for $x \geq 1$. Hence,

$$h(m) = \int_{m-2}^{m-1} g'dx - 2\int_{m-1}^{m} g'dx + \int_{m}^{m+1} g'dx < 0,$$

because $g''' < 0$ implies that g' is concave. $h(m)$ increases for $m \geq 4$ since $g'''' > 0$ for $x > 3/2$. Direct computation shows that $b_3 < b_4$.Need to confirm. It is clear that $\lim_{m\to\infty} b_m = 0$. By Taylor expansion about $m - 1/2$, we find

$$h(m) = -(1-\gamma)\gamma m^{-1-\gamma}(1 + O(1/m)),\ m \to \infty.$$

Now ,consider $n-1$, $n=3$ and $n=4$ are different, though the formula is uniform. Consider $h_1(n-1)$ where $n \geq 4$. $h_1(2)$ corresponds to b_2^{3+1} which has been discussed. Then, $h_2(n)$ and $h_3(n+1)$

The last four terms equal to

$$\frac{1}{2}n^{1-\gamma} + \frac{1}{2}(n+1)^{1-\gamma} - \int_{n}^{n+1} x^{1-\gamma}dx < 0$$

because $x^{1-\gamma}$ is a concave function. If $n = 2$, as $\gamma \to 1$, $\tilde{h}(n) \to 1/2$ and as $\gamma \to 0$, $\tilde{h}(n) \to 0$. Hence, it is clear that $\tilde{h}(2)$ is negative if γ is close to 0 and positive if γ is close to 1. If $n \geq 3$, $\tilde{h}(n) < 0$. By Taylor expansion about $n + 1/2$, the last four terms add to $O(n^{-1-\gamma})$. It is also clear that when $n \geq 3$, as $\gamma \to 0, 1$, $\tilde{h}(n) \to 0$.

Now, consider $\bar{h}(n+1)$ for $n \geq 2$ where

$$\bar{h}(n+1) \;=\; -(n-1)^{1-\gamma}\frac{1}{2} + \frac{1}{2}n^{1-\gamma} - \frac{1}{2-\gamma}(n-1)^{2-\gamma} + \frac{1}{2-\gamma}n^{2-\gamma} - (n+1)^{1-\gamma}.$$

As $\gamma \to 1$, $\bar{h}(n+1) \to 0$ and as $\gamma \to 1$, $\bar{h}(n+1) \to -1$.

We find

$$\begin{aligned}\bar{h}(n+1) &= \int_{n-1}^{n} x^{1-\gamma}dx - (n+1)^{1-\gamma} + \frac{1}{2}n^{1-\gamma} - \frac{1}{2}(n-1)^{1-\gamma} \\ &\qquad\qquad < -(n+1)^{1-\gamma} + \frac{3}{2}n^{1-\gamma} - \frac{1}{2}(n-1)^{1-\gamma} < 0\end{aligned}$$

Further, as $n \to \infty$, by Taylor expansion about n, we find that $\bar{h}(n+1) = O(n^{-\gamma})$.

Now, we compute directly

$$\begin{aligned}\Gamma(2-\gamma)(b_0 + \frac{3}{4}b_1) &= -\frac{5}{8} - \frac{5}{4}\frac{1}{2-\gamma} + \frac{3}{4}2^{-\gamma} + \frac{3}{2-\gamma}2^{-\gamma} =: g_1(\gamma) \\ \Gamma(2-\gamma)(|b_1| - 4b_2) &= -\frac{9}{2} - \frac{8-\gamma}{2-\gamma}6\cdot 3^{-\gamma} + \frac{6-\gamma}{2-\gamma}11\cdot 2^{-\gamma} - \frac{9}{2-\gamma} =: g_2(\gamma)\end{aligned}$$

$g_1 = \frac{3}{2-\gamma}(2^{-\gamma} - \frac{1}{2}) + \frac{1}{4(2-\gamma)} + \frac{3}{4}2^{-\gamma} - \frac{5}{8} > \frac{1}{4(2-\gamma)} + \frac{3}{4}2^{-\gamma} - \frac{5}{8} := \tilde{g}_1$. $\tilde{g}_1$ is a convex function and $\tilde{g}_1(1) = 0$, $\tilde{g}_1'(1) < 0$, then $\tilde{g}_1 > 0$. $g_2(0) = g_2(1) = 0$. Note that $[(2-\gamma)g_2]'' = 3^{-\gamma}[-12\ln 3 - 6(8-\gamma)\ln(3)^2 + 22\cdot 1.5^{\gamma}\ln 2 + 11(6-\gamma)1.5^{\gamma}(\ln 2)^2]$. Clearly, $-12\ln 3 - 6(8-\gamma)\ln(3)^2 + 22\cdot 1.5^{\gamma}\ln 2 + 11(6-\gamma)1.5^{\gamma}(\ln 2)^2 < -12\ln 3 - 6(8-\gamma)\ln(3)^2 + 33\ln 2 + 16.5(6-\gamma)(\ln 2)^2$. The right hand side is a linear function and the values of this linear function at two endpoints are negative. Hence, $[(2-\gamma)g_2]'' < 0$. Hence, $(2-\gamma)g_2$ is concave and $g_2 > 0$.

Then, the third part of the theorem and the second part of the theorem for $n \geq 2$ are proved. □

B The negativity of P_m

Lemma 4. *$P_m(\tau) \leq 0$ for all $m \geq 1$ and $\tau \in I_m$.*

Proof.

$$\begin{aligned}P_m(\tau) = (t^{m-1} - \tau)^2 k^{2-\gamma}[\frac{1}{2}(n-m)^{1-\gamma} + \frac{1}{2-\gamma}(n-m)^{2-\gamma}] + \\ (-2)(t^m - \tau)^2 k^{2-\gamma}[(n-m)^{1-\gamma} + \frac{1}{2-\gamma}(n-m)^{2-\gamma}] \\ + (t^{m+1} - \tau)^2 k^{2-\gamma}[\frac{1}{2}(n-m+1)^{1-\gamma} + \frac{1}{2-\gamma}(n-m+1)^{2-\gamma}] \\ - \frac{2k^2}{2-\gamma}(t^{n+1} - \tau)^{2-\gamma}\end{aligned}$$

$P_m(\tau = t^{m+1}) = 0$ and $P_m(\tau = t^m) = k^2 \int_{I_m} \frac{t^{m+1/2}-s}{(t^{n+1}-s)^\gamma} ds < 0$.

We find that

$$
\begin{aligned}
(1-\gamma)P' = 2(\tau - t^{m-1})k^{2-\gamma}[\frac{1}{2}(n-m)^{1-\gamma} + \frac{1}{2-\gamma}(n-m)^{2-\gamma}] + \\
(-2)2(\tau - t^m)k^{2-\gamma}[(n-m)^{1-\gamma} + \frac{1}{2-\gamma}(n-m)^{2-\gamma}] \\
+ 2(\tau - t^{m+1})k^{2-\gamma}[\frac{1}{2}(n-m+1)^{1-\gamma} + \frac{1}{2-\gamma}(n-m+1)^{2-\gamma}] \\
+ 2k^2(t^{n+1} - \tau)^{1-\gamma}
\end{aligned}
$$

We can show that $P'(t^m) < 0$. $P'(t^{m+1}) = 0$.

Further,

$$
\begin{aligned}
(1-\gamma)P''(t^{m+1})/k^{2-\gamma} &= -3(n-m)^{1-\gamma} - \frac{2}{2-\gamma}(n-m)^{2-\gamma} + \\
&+ [(n-m+1)^{1-\gamma} + \frac{2}{2-\gamma}(n-m+1)^{2-\gamma}] - 2(1-\gamma)(n-m)^{-\gamma} \\
&= (n-m+1)^{1-\gamma} - 3(n-m)^{1-\gamma} + 2\int_{n-m}^{n-m+1} x^{1-\gamma} dx - 2(1-\gamma)(n-m)^{-\gamma}
\end{aligned}
$$

Using the inequality $x^{1-\gamma} \leq (n-m)^{1-\gamma} + (1-\gamma)(n-m)^{-\gamma}(x-(n-m))$ since the function is concave, we find

$$
(1-\gamma)P''(t^{m+1})/k^{2-\gamma} \leq (n-m+1)^{1-\gamma} - (n-m)^{1-\gamma} - (1-\gamma)(n-m)^{-\gamma} \leq 0.
$$

Hence, P'' could be positive on $\tau \in (t^m, t_0)$ and negative on (t_0, t^{m+1}) or all negative on (t^m, t^{m+1}). Together with the fact $P'(t^{m+1}) = 0$, we know either P either first decreases and then increases or increases for all time. Since $P(t^{m+1}) = 0$ and $P(t^m) < 0$, we find that $P \leq 0, \tau \in (t^m, t^{m+1})$. $\square$