An introduction to fractional calculus

Fundamental ideas and numerics

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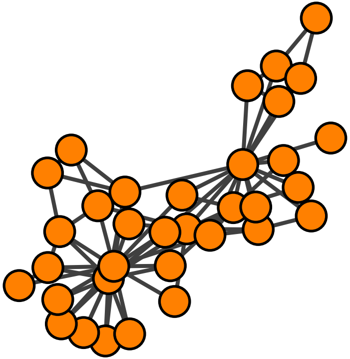
Questions in Complex Networks



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We are interested in tasks in **exploratory data analysis**, that is analyzing the data to summarize their main characteristics:

- Divide the nodes into groups that are in the same community (clustering),
- Find the “most relevant” nodes in the network (centrality),
- Find the “most relevant” edge in the network (edge centrality)
- Individuation of motifs, computation of fluxes, maximum cuts, *etc.*

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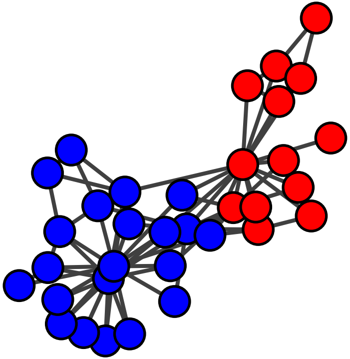

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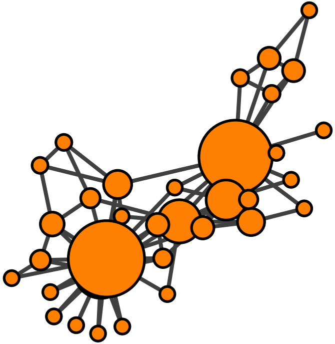

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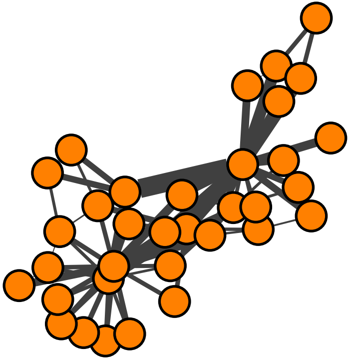

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Notation

Network

A *network* $G = (V, E)$ is defined as a pair of sets: a set $V = \{1, 2, \ldots, n\}$ of *nodes* and a set $E \subset V \times V$ of *edges* between them.

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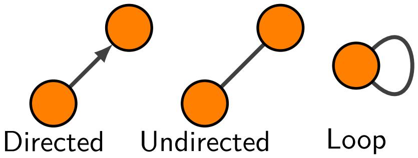
Directed/Undirected

If $\forall (i, j) \in E$ then $(j, i) \in E$ the network is said to be *undirected* is *directed* otherwise.



An edge from a node to itself is called a *loop*.

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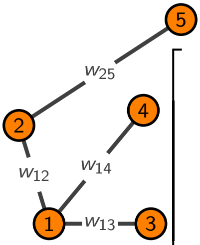


$$\begin{bmatrix} 0 & w_{12} & w_{13} & w_{14} & 0 \\ w_{12} & 0 & 0 & 0 & w_{25} \\ w_{13} & 0 & 0 & 0 & 0 \\ w_{14} & 0 & 0 & 0 & 0 \\ 0 & w_{25} & 0 & 0 & 0 \end{bmatrix}$$

Adjacency Matrix

We represent a Network via its *adjacency matrix* $A = (a_{ij}) \in \mathbb{R}^{n \times n}$, entrywise defined as

$$a_{ij} = \begin{cases} w_{ij} & \text{if } (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$$

where $w_{ij} > 0$ is the weight of edge (i, j).

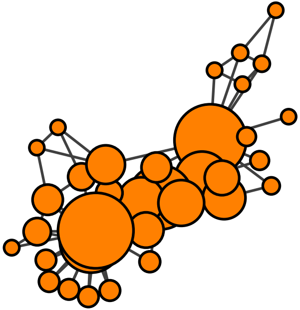
★ Centrality Measures: the limiting cases

- **Degree centrality:**

$$d_i = \sum_{j=1}^{n} a_{ij} = (A\mathbf{1})_i$$

- **Eigenvector centrality:** $\rho(A) > 0$ the spectral radius of the irreducible $A \geq 0$

$$x_i = \frac{1}{\rho(A)} \sum_{j=1}^{n} a_{ij} x_j$$



Degree centrality is oblivious to the whole topology of the network.

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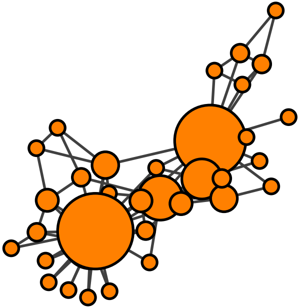


Eigenvector centrality considers both the number of neighbors and their importance when assigning scores to nodes.

Walk based centralities and Matrix Functions

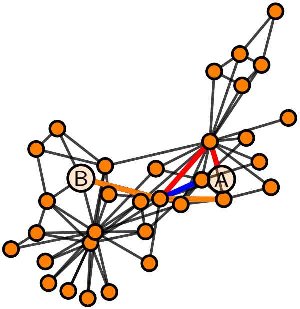
Consider the **analytic function** f in $\{z \in \mathbb{C} : |z| < R_f\}$:

$$f(z) = \sum_{r=0}^{\infty} c_r z^r, \qquad c_r \geq 0$$

then under suitable hypothesis on the spectrum of A we can write:

$$f(A) = \sum_{r=0}^{\infty} c_r A^r.$$

$(A^r)_{i_1,i_{r+1}}$ is the number of walks from i_1 to i_{r+1}.



A *walk* of length r is a sequence of $r+1$ nodes $i_1, i_2, \ldots, i_{r+1}$ such that $(i_\ell, i_{\ell+1}) \in E$ for all $\ell = 1, \ldots, r$.

Walk based centralities and Matrix Functions

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$(A^r)_{i_1,i_{r+1}}$ is the number of walks from i_1 to i_{r+1}.

- $(f(A))_{ij}$ is a **weighted sum** of the number of **all walks** of any length that start from node i and end at node j,
- $c_r \longrightarrow 0$ as r increases thus **walks of longer lengths** are considered to be **less important**,
- The most popular functions used in networks science are $f(z) = e^z$ and $f(z) = (1+z)^{-1}$.

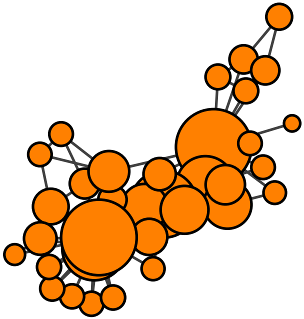
Walk based centralities

- **Subgraph centrality:**

$$s_i(f) = \mathbf{e}_i^T f(A)\mathbf{e}_i = \sum_{r=0}^{\infty} c_r (A^r)_{ii}.$$

- **Total** (node) **communicability:**

$$t_i(f) = \sum_{j=1}^{n} (f(A))_{ij} = \sum_{j=1}^{n} \sum_{r=0}^{\infty} c_r (A^r)_{ij}$$



Subgraph centrality accounts for the returnability of information from a node to itself: it is a weighted count of all the subgraphs node i is involved in.

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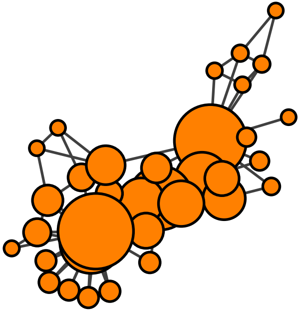


For the **total comunicability** the importance of a node depends on how well it communicates with the whole network, itself included

The Mittag-Leffler Function

The *Mittag–Leffler (ML) function* is an analytic functions given, $\forall \alpha, \beta > 0$, by

$$E_{\alpha,\beta}(z) = \sum_{r=0}^{\infty} c_r(\alpha,\beta) z^r = \sum_{r=0}^{\infty} \frac{z^r}{\Gamma(\alpha r + \beta)},$$

where

- $c_r(\alpha, \beta) = \Gamma(\alpha r + \beta)^{-1}$,
- $\Gamma(z)$ is the *Euler Gamma function*:

$$\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t} dt.$$

For particular choices of $\alpha, \beta > 0$, the ML function $E_{\alpha,\beta}(z)$ has a nice closed form descriptions.

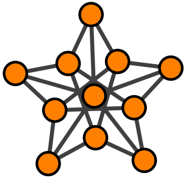
α	β	Function
0	1	$(1-z)^{-1}$ Resolvent
1	1	$\exp(z)$ Exponential
$\frac{1}{2}$	1	$\exp(z^2)\,\mathrm{erfc}(-z)$ Error Function[1]
2	1	$\cosh(\sqrt{z})$ Hyperbolic Cosine
2	2	$\sinh(\sqrt{z})/\sqrt{z}$ Hyperbolic Sine
4	1	$\frac{1}{2}[\cos(z^{1/4}) + \cosh(z^{1/4})]$
1	$k \geq 2$	$z^{1-k}(e^z - \sum_{r=0}^{k-2} \frac{z^r}{r!})$ $\varphi_{k-1}(z) = \sum_{r=0}^{\infty} \frac{z^r}{(r+k-1)!}$

The Mittag-Leffler Function: other occurrences

Another use of it is in the case $E_{1,2}(z) = \psi_1(z)$ for computing the **non-backtracking exponential generating function** for simple graphs (Arrigo et al. 2018) is:

$$\sum_{r=0}^{\infty} \frac{p_r(A)}{r!} = \begin{bmatrix} I & 0 \end{bmatrix} \psi_1(Y) \begin{bmatrix} A \\ A^2 - D \end{bmatrix} + I,$$

where $p_r(A)$ is a matrix whose entries represent the number of non-backtracking walks of length r between any two given nodes



Backtracking walk

A walk is *backtracking* if it contains at least one pair of successive edeges of the form $i \mapsto j$, $j \mapsto i$. We say that is *non-backtracking* otherwise.

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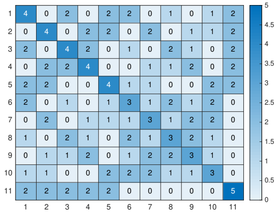
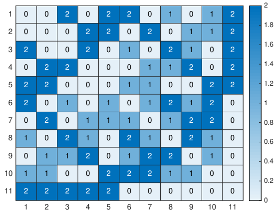


A^2



$p_2(A)$

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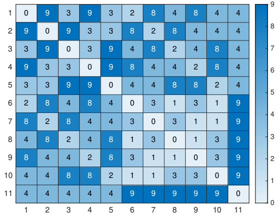
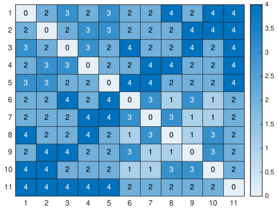


A^3



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where $p_r(A)$ is a matrix whose entries represent the number of non-backtracking walks of length r between any two given nodes $D = \mathrm{diag}(A)$, and Y is the first companion linearization of the matrix polynomial $(D - I) - A\lambda + I\lambda^2$:

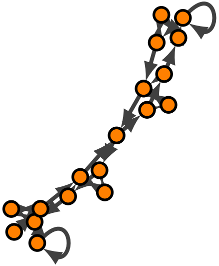
$$Y = \begin{bmatrix} 0 & I \\ I - D & A \end{bmatrix}.$$

The Mittag-Leffler Function: other occurrences

To compute **centrality** and **communicability** indices for **directed networks**, if A is the adjacency matrix of a directed graph, then

$$\mathcal{A} = \begin{bmatrix} O & A \\ A^T & O \end{bmatrix} \Rightarrow \exp(\mathcal{A}) = \begin{bmatrix} \cosh(\sqrt{AA^T}) & A(\sqrt{A^TA})^\dagger \sinh(\sqrt{A^TA}) \\ \sinh(\sqrt{A^TA})(\sqrt{A^TA})^\dagger A^T & \cosh(\sqrt{A^TA})) \end{bmatrix}$$

Centrality and communicability indices for directed networks defined by exploiting the representation of such networks as bipartite graphs; details in (Benzi, Estrada, and Klymko 2013).



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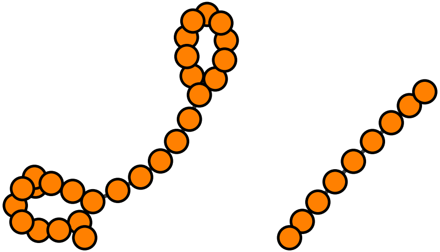
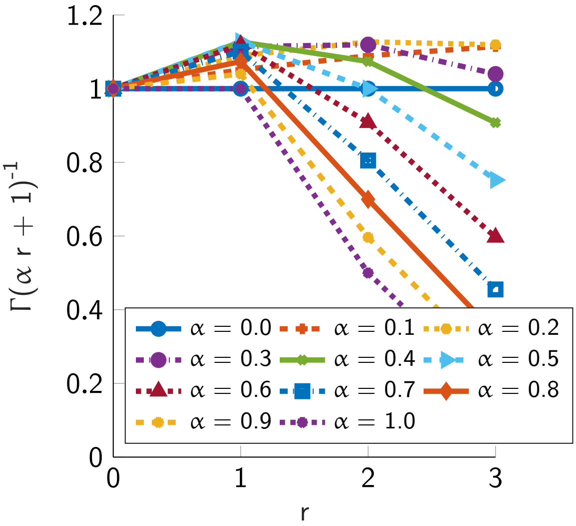


Defining Mittag-Leffler based centralities

For each choice of $\alpha, \beta > 0$ we want to define 🚶 centralities based on

$$E_{\alpha,\beta}(z) = \sum_{r=0}^{\infty} c_r(\alpha,\beta) z^r = \sum_{r=0}^{\infty} \frac{z^r}{\Gamma(\alpha r + \beta)},$$

The idea of a 🚶 centrality relies on the fact that walks of longer lengths are less important, **but** $c(r) := \Gamma(\alpha r + 1)$ is not monotonic for certain values of $\alpha \in (0,1)$!



Enforcing monotonicity

Lemma (Arrigo, D.)

Suppose that $\alpha \in (0,1)$. The coefficients $\widetilde{c}_r(\alpha,\gamma) = \gamma^r c_r(\alpha)$ defining the power series for the entire function $\widetilde{E}_\alpha(z) = E_\alpha(\gamma z)$ are monotonically decreasing as a function of $r = 0, 1, 2, \ldots$ for all $0 < \gamma < \Gamma(\alpha+1)$.

Proof. For each $\alpha \in (0,1)$ we want to determine conditions on $\gamma = \gamma(\alpha)$ that imply that

$$\tilde{c}_r(\alpha,\gamma) \geq \tilde{c}_{r+1}(\alpha,\gamma) \quad \text{for all } r \in \mathbb{N}$$

From the definition of $\tilde{c}_r(\alpha,\gamma)$ we have that the above inequality is equivalent to verifying

$$\gamma \leq \frac{\Gamma(\alpha r + \alpha + 1)}{\Gamma(\alpha r + 1)}, \quad \text{for all } r \geq 0$$

since $\gamma > 0$ and $\Gamma(x) > 0$ for all $x \geq 0$.

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Proof. Since H_x, the *Harmonic number* for $x \in \mathbb{R}$, is an increasing function of x, $\alpha > 0$ by hypothesis, and $\Gamma(x) > 0$ for all $x \geq 0$, it follows that

$$\frac{d}{dx}\left(\frac{\Gamma(\alpha x + \alpha + 1)}{\Gamma(\alpha x + 1)}\right) = \frac{\alpha\left(H_{\alpha(x+1)} - H_{\alpha x}\right)\Gamma(\alpha x + \alpha + 1)}{\Gamma(\alpha x + 1)} \geq 0,$$

and thus the minimum of $\frac{\Gamma(\alpha x+\alpha+1)}{\Gamma(\alpha x+1)}$ is achieved at $x = 0$.

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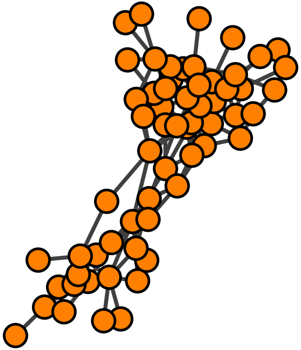
Take-home message

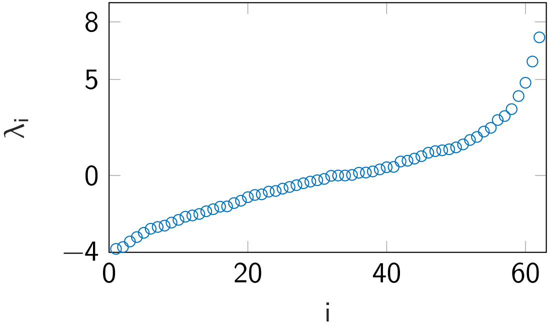
Mittag–Leffler functions with $\alpha \in (0,1)$ can be employed since they have a power series expansion that can be interpreted in terms of walks; however, care should be taken since to enforce monotonic behavior of the coefficients.

A matter of magnitude

Adjacency matrices of simple graphs have **positive** and **negative** eigenvalues ($\mathrm{tr}(A) = 0$)!



Newmann/Dolphins



$$E_{0.4,1}(\rho(A)) = E_{0.4,1}(7.1936\ldots) \approx 10^{60}$$

A matter of magnitude

We know asymptotic expansions for the ML function for $\theta \in (\frac{\pi\alpha}{2}, \min(\pi, \alpha\pi))$ and any $p \in \mathbb{N}$:

Proposition (Gorenflo et al. 2014, Proposition 3.6)

Let $0 < \alpha < 2$ and $\theta \in (\frac{\pi\alpha}{2}, \min(\pi, \alpha\pi))$. Then we have the following asymptotics for the Mittag–Leffler function for any $p \in \mathbb{N}$

$$E_\alpha(z) = \frac{1}{\alpha} e^{z^{\frac{1}{\alpha}}} - \sum_{k=1}^{p} \frac{z^{-k}}{\Gamma(1-\alpha k)} + O(|z|^{-1-p}),\ |z| \to +\infty,\ |\arg(z)| \leq \theta,$$

$$E_\alpha(z) = -\sum_{k=1}^{p} \frac{z^{-k}}{\Gamma(1-\alpha k)} + O(|z|^{-1-p}),\ |z| \to +\infty,\ \theta \leq |\arg(z)| \leq \pi.$$

We need to set the γ to **scale the largest modulus eigenvalue** in the computable range!

A matter of magnitude

Lemma (Arrigo, D.)

Suppose that $\alpha \in (0, 1]$, and $A \in \mathbb{R}^{n\times n}$ is symmetric. Then for all

$$\gamma \leq \frac{1}{\lambda_{\max}(A)} \left(\bar{K}\log(10) + \log(\alpha)\right)^{\alpha}$$

it holds that $\max_{i,j}(|E_\alpha(\gamma A)|)_{i,j} \leq \bar{N}$ where $\bar{N} \approx 10^{\bar{K}}$ for a given $\bar{K} \in \mathbb{N}$ is the largest representable number on a given machine.

Proof. We have $\lambda_{\max}(\gamma A) = \gamma\lambda_{\max}(A) \in \mathbb{R}$, since A is symmetric; then empolying the asymptotic expansion, and using the fact that $\arg(z) = 0$ for $z \in \mathbb{R}$, for $p = 0$ we find

$$\frac{1}{\alpha} e^{(\gamma\lambda_{\max}(A))^{\frac{1}{\alpha}}} \leq \bar{N} \approx 10^{\bar{K}},$$

which immediately yields the conclusion.

Well-posedness and machine representability

Subgraph and total communicability centralities

Let A be the adjacency matrix of a simple graph $G = (V, E)$. Let $\alpha \in [0, 1]$ and let $0 < \gamma \leq \mu(\alpha)$. Then, for all nodes $i \in V = \{1, 2, \ldots, n\}$ we define:

- ML-subgraph centrality:

$$s_i(\widetilde{E}_\alpha) = E_\alpha(\gamma A)_{ii}$$

- ML-total communicability:

$$t_i(\widetilde{E}_\alpha) = (E_\alpha(\gamma A)\mathbf{1})_i$$

Proposition (Arrigo, D.)

Let A be the adjacency matrix of an undirected network with at least one edge and let $\rho(A) > 0$ be its spectral radius. Moreover, let $\bar{N} \approx 10^{\bar{K}}$ be the largest representable number on a given machine. Then the Mittag–Leffler function $\widetilde{E}_\alpha(z) = E_\alpha(\gamma z)$ is representable in the machine, and admits a series expansion with decreasing coefficients when $\alpha \in (0, 1)$ and $0 < \gamma \leq \mu(\alpha)$

$$\mu(\alpha) := \min \begin{cases} \Gamma(\alpha + 1), \\ \dfrac{\left(\bar{K}\log(10) + \log(\alpha)\right)^\alpha}{\rho(A)} \end{cases}$$

The main idea behind ML centralities

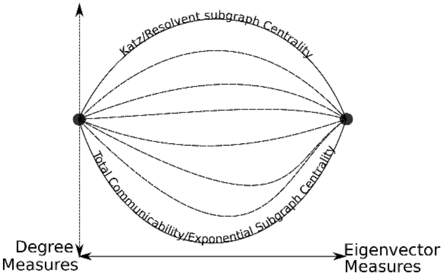
Theorem (Benzi and Klymko 2015)

Let $G = (V, E)$ be a connected, undirected, unweighted network with primitive A, and f an analytic function with strictly positive series expansion defined on the spectrum of A.

- For $\gamma \to 0^+$, the rankings produced by both $\mathbf{s}(\gamma)$ and $\mathbf{t}(\gamma)$ converge to those produced by the vector of degree centralities,
- If in addition f is analytic on the whole real axis or is such that,

$$\sum_{r=0}^{\infty} c_r R_f^r = \lim_{\gamma \to 1^-} \sum_{r=0}^{\infty} c_r t^r R_f^t = +\infty,$$

then, for $t \to R_f/\rho(A)$, the rankings produced by both $\mathbf{s}(\gamma)$ and $\mathbf{t}(\gamma)$ converge to those produced by the eigenvector centrality.



We build measures that "interpolate asymptotically" between four other "central" centralities measures: Degree, Eigenvector, Exponential and Resolvent walk centralities.

ML matrix-function vector products

The tasks of computing ML-subgraph centrality and ML-total communicability relies on the task of computing the ML function "with matrix argument", which is a delicate task

- We can use, e.g., the techniques and the code developed in (Garrappa and Popolizio 2018),
- then for "large networks" we adopt a polynomial Krylov subspace projection technique (Moret and Novati 2011) to handle the computations
  - For V a basis of $\mathcal{K}_m(A, \mathbf{1}) = \operatorname{span}\{\mathbf{v}, A\mathbf{v}, \ldots, A^{m-1}\mathbf{v}\}$

$$\mathbf{t}(\gamma) \approx V E_\alpha(\gamma V^T A V) V^T \mathbf{1},$$

  - For V a basis of $\mathcal{K}_m(A, \mathbf{e}_i) = \operatorname{span}\{\mathbf{e}_i, A\mathbf{e}_i, \ldots, A^{m-1}\mathbf{e}_i\}$,

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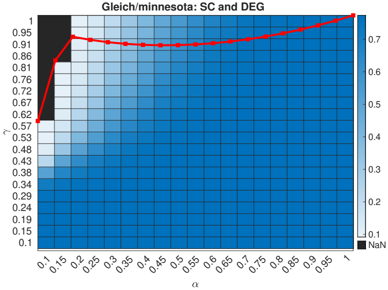
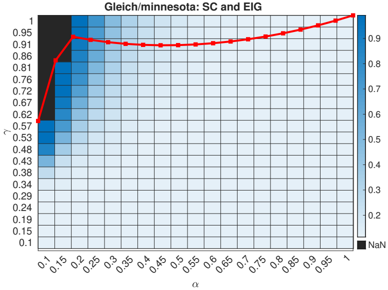
Subgraph centrality is computationally **quite expensive** to derive for all nodes but approximation techniques for few top ranked nodes are available (Fenu et al. 2013).

Numerical Examples

We compare subgraph centrality with **eigenvector centrality** and **degree centrality** as we let α and γ vary on a real-world network



(a)



(b)

Kendall correlation coefficient between the ranking induced by total communicability vectors $\mathbf{s}(\widetilde{E}_\alpha)$ and by (a) degree centrality or (b) eigenvector centrality, the red line displays the value of μ.

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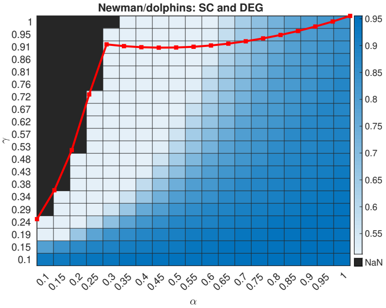

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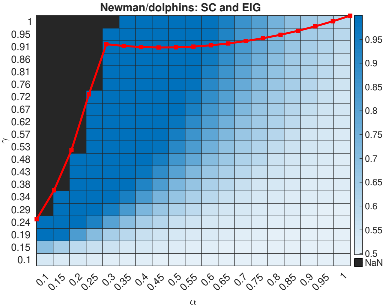

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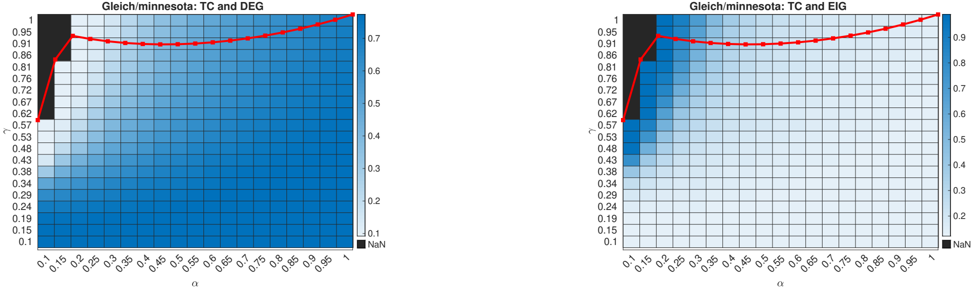

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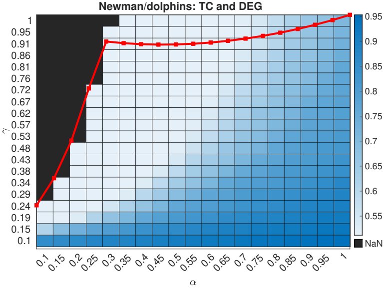

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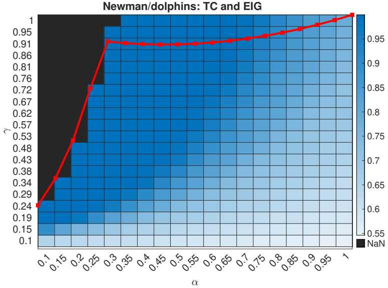

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Kendall correlation coefficient between the ranking induced by total communicability vectors $\mathbf{t}(\widetilde{E}_\alpha)$ and by (a) degree centrality or (b) eigenvector centrality, the red line displays the value of μ.

Time-fractional dynamical models on networks

There are **several generalizations** of ODE-based models on networks:

- Time (and space) generalized diffusion equation on networks (Diaz-Diaz and Estrada 2022)

$$ {}_{CA}D^{\alpha}_{[0,t]}\mathbf{f}(t) = -L\mathbf{f}(t), \quad f(0) = \mathbf{f}_0, $$

  for L the graph Laplacian, i.e., $L = \mathrm{diag}(A\mathbf{1}) - A$, A adjacency matrix of an *undirected graph*,
- Decision-making models (West, Turalska, and Grigolini 2015),
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There are many more models that involve using **fractional derivatives with respect to the "space variables"**, we postpone that discussion after having treated the issue in general for the continuous case.

Other types of fractional derivatives w.r.t. time

Another type of FDE w.r.t. that is gaining traction and interest, they are called **fractional derivatives of distributed order**, i.e.,

$$\int_0^m a(r)\,{}_{CA}D^r_{[0,t]}u(t)\,\mathrm{d}r = f(t), \quad m > 0,$$

and more generally

$$\int_0^m a(r)F\left({}_{CA}D^r_{[0,t]}u(t)\right)\,\mathrm{d}r = f(t,u(t)), \quad m > 0.$$

Applications are, e.g.,

- Dielectric induction and diffusion (Caputo 2001),
- Kinetic models (Sokolov, Chechkin, and Klafter 2004),
- Distributed-order oscillators (Atanackovic, Budincevic, and Pilipovic 2005).

Distributed order FDEs

We can connect them with something we have already seen, consider the **multi-term** differential equation:

$$\begin{cases} \displaystyle\sum_{i=1}^{k} \gamma_i \, {}_{CA}D^{r_i}_{[0,t]} u(t) = f(t, u(t)), & 0 < r_1 < r_2 < \ldots < r_k \\ u^{(\ell)}(0) = \varphi_\ell, & \ell = 0, \ldots, m-1, \;\; m = \left\lceil \max_{i=1,\ldots,k} r_i \right\rceil. \end{cases}$$

- One way of thinking about the distributed-order equation is therefore as the **limiting case** of with a very large number of terms and where the coefficients γ_i take the values from the function a.

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- One way of thinking about the distributed-order equation is therefore as the **limiting case** of with a very large number of terms and where the coefficients γ_i take the values from the function a.
- What can we say about the solutions?

Distributed order FDEs

For the **linear case**

$$\int_0^m a(r) {}_{CA}D^r_{[0,t]} u(t) \,\mathrm{d}r = f(t), \quad m > 0, \qquad \text{(LDFODE)}$$

we can prove existence under some *assumptions*:

(A1) $m \in \mathbb{N}$,

(A2) a is *absolutely integrable* on $[0, m]$ with $\int_0^m a(r) s^r \,\mathrm{d}r \neq 0$ for $\Re(s) > 0$,

(A3) $f \in \mathbb{L}^1([0, \infty)]$,

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We apply Laplace transform

$$\mathcal{L}\left\{\int_0^m a(r)\, {}_{CA}D^r_{[0,t]} u(t)\,\mathrm{d}r\right\}(s) = \mathcal{L}\{f\}(s)$$

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$$\int_0^m a(r)\left(s^r\mathcal{L}\{u\}(s) - u(0)s^{r-1}\right)\,\mathrm{d}r - \sum_{j=1}^{m-1}\int_j^m a(r)u^{(j)}(0)s^{r-j-1}\,\mathrm{d}r = \mathcal{L}\{f\}(s)$$

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We apply Laplace transform, then use (A4) and exchange the transform and the integral. After rearranging and inverting using (A1)–(A3)

$$u(t) = u(0) + \left(f * \mathcal{L}^{-1}\left\{ \frac{1}{\int_0^m a(z)(s)^z\,\mathrm{d}z} \right\} \right)(t) + \sum_{j=1}^{m-1} u^{(j)}(0)\mathcal{L}^{-1}\left\{ \frac{\int_j^m a(r)s^{r-j-1}\,\mathrm{d}r}{\int_0^m s^r a(r)\,\mathrm{d}r} \right\}(t).$$

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Theorem (Diethelm and Ford 2009, Theorem 3.1)

Under assumptions (A1)–(A4) on a, f and u, (LDFODE) has a unique solution.

Properties of the (LDFODE) solution

Proposition (Diethelm and Ford 2009)

1. Under assumptions (A1)–(A4) and for fixed $T > 0$ the solution to (LDFODE) satisfies $u^{(m)}(t)$ is bounded and measurable in $[0, T]$.
2. Let $u \in \mathcal{C}^p([O, T])$ with some $p \in \mathbb{N}$ and $T > 0$. For every fixed $t \in [0, T]$, consider ${}_{CA}D^r_{[0,t]} u(t) = z(r)$ as a function of r. Then,
   - At the integer argument $j = 1, 2, \ldots, p-1$ the function z has a *jump discontinuity* that can be described as

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❓ How can we discretize and solve this type of equations?

Discretization strategies

1. We discretize the **integral term** in the **distributed-order** equation

2. We solve the multi-term equation

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   - Fix $\phi(z) = a(z)\,{}_{CA}D^{z}_{[0,t]}u(t)$ and use a quadrature formula

$$\int_0^m \phi(z)\,\mathrm{d}z \approx \sum_{j=0}^{n} w_j \phi(z_j)$$

   - Every integer value in the interval $[0, m]$ is a z_j, in general every $z_j \in \mathbb{Q}$.

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   - With the choice we have made we now have a multiterm equation of the form

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   - We apply the reformulation as a system of equations of order q being the **g**reatest **c**ommon **d**ivisor of the derivative orders.

Error analysis

To select the **quadrature formula** we have to take into account the **jumps in the integrand**

$$\int_0^m a(r)\,{}_{CA}D^r_{[0,t]}u(t)\,\mathrm{d}r = \sum_{i=0}^{m-1}\int_i^{i+1} a(r)\,{}_{CA}D^r_{[0,t]}u(t)\,\mathrm{d}r = \sum_{i=0}^{m-1}\sum_{j=0}^{n_i} w_{ij}a(z_{ij})\,{}_{CA}D^{z_{ij}}_{[0,t]}u(t)$$

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- The sequence $\{z_j\} = \{z_0 = z_{00}, z_1 = z_{01}, \ldots, z_{n_0} = z_{0n_0} = z_{10} = 1, \ldots\}$.

Error analysis

To proceed further we also need to require further regularity on the a function.
We assume

(Q1) We use a convergent quadrature rule of order $p > 0$,

(Q2) For all i, the weights of the quadrature rule are bounded by

$$C_1 n_i^{-1} \leq \min_{j=0,1,\dots,n_i} |w_{ij}| \leq \max_{j=0,1,\dots,n_i} |w_{ij}| \leq C_2 n_i^{-1},$$

with some constants C_1 and C_2.

(Q3) The function a is p-times continuously differentiable on $[0, m]$.

Proposition (Diethelm and Ford 2009)

If $\tilde{u}$ is the solution of (LDFODE) obtained using a quadrature formula satistying (Q1)–(Q4), then

$$u(t) = \tilde{u}(t) + O(\max_i \{n_i^{-p}\}), \qquad \text{for } n_i \to +\infty \; \forall\, i.$$

Error analysis

Thus, if we assume that we apply a numerical method for the multi-term equation which has order of convergence $O(\tau^q)$ we have then

Theorem (Diethelm and Ford 2009, Theorem 4.1)

Under the conditions (A1)–(A4), (Q1)–(Q3), the overall error of the proposed algorithm for (LDFODE) satisfies for $j\tau \in [0, T]$:

$$\max\{|u_j - u(j\tau)| \;:\; j \geq 0,\, j\tau \leq T\} = O(\tau^q) + O(\max_i\{n_i^{-p}\}) \qquad \text{for } n_i \to +\infty \;\forall\, i,\; \tau \to 0.$$

- To reduce the number of terms and the regularity requirements on a one could use a Gauss-type quadrature built explicitely for the given function $a(z)$ (that now needs to be only continuous) (Durastante 2019).

Variable order FDEs

Consider a function $\alpha : [0, T] \subset \mathbb{R}^+ \to (0, 1)$ we can think of generalizing the Riemann-Liouville integral as

$$I^{\alpha(t)}_{[0,t]} = \frac{1}{\Gamma(\alpha(t))} \int_0^t (t - \tau)^{\alpha(t)-1} f(\tau)\, \mathrm{d}\tau,$$

possibly coupled with the Riemann-Liouville variable-order derivative

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Some of this generalizations have found use in physical modeling, but they are *problematic from a rigorous point of view.*

Variable order FDEs a Laplace domain version

Among the first ideas in developing a time-variable time-fractional calculus there are three seminal works by **Giambattista Scarpi**

- G. Scarpi, Sopra il moto laminare di liquidi a viscosist variabile nel tempo. Atti Accademia delle Scienze, Isitituto di Bologna, Rendiconti (Ser XII), 9 (1972), pp. 54-68,
- G. Scarpi, Sulla possibilità di un modello reologico intermedio di tipo evolutivo. Atti Accad Naz Lincei Rend Cl Sci Fis Mat Nat (8), 52 (1972), pp. 912-917;
- G. Scarpi, Sui modelli reologici intermedi per liquidi viscoelastici. Atti Accad Sci Torino: Cl Sci Fis Mat Natur, 107 (1973), pp. 239-243.

Recently, this approach has been taken again into account to overcome the limitation given by the *naive* replacement of the $\alpha(t)$ function in the kernel of Fractional Integrals and Derivatives; (Garrappa, Giusti, and Mainardi 2021).

Scarpi's Derivative (Garrappa, Giusti, and Mainardi 2021)

To introduce this new version we need to use again the **Laplace transform** of the Caputo derivative and Riemann-Liouville integrals

$$\mathcal{L}\{{}_{CA}D^{\alpha}_{[0,t]}f(t)\}(s) = s^{\alpha}F(s) - s^{\alpha-1}f(0), \quad \mathcal{L}\{I^{\alpha}_{[0,t]}f(t)\}(s) = \frac{1}{s^{\alpha}}F(s),$$

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Scarpi's idea

If $\alpha(t) \equiv \alpha$, $t > 0$, $\mathcal{L}\alpha(s) = A(s) = {}^{\alpha}/_{s}$, then

$$\mathcal{L}\left\{\frac{t^{-\alpha}}{\Gamma(1-\alpha)}\right\}(s) = s^{sA(s)-1} = s^{\alpha-1} \qquad \mathcal{L}\left\{\frac{t^{\alpha-1}}{\Gamma(\alpha)}\right\}(s) = s^{-sA(s)} = \frac{1}{s^{\alpha}}.$$

Apply the same relation to any $\alpha(t)$ with $A(s) = \mathcal{L}\{\alpha(t), s\} = \int_0^{+\infty} e^{-st}\alpha(t)\,\mathrm{d}t$.

Scarpi's Derivative (Garrappa, Giusti, and Mainardi 2021)

Scarpi Fractional Derivative

Let $\alpha(t) : [0, T] \longrightarrow (0, 1)$ be a locally integrable function with Laplace transform $A(s)$, and let $f \in \mathbb{L}^1([0, T])$. We define the Scarpi fractional derivative ${}_S D^{\alpha(t)}_{[0,t]}$ of variable order $\alpha(t)$ as

$${}_S D^{\alpha(t)}_{[0,t]} f(t) = \frac{d}{dt} \int_0^t \phi_\alpha(t-\tau) f(\tau)\, \mathrm{d}\tau - \phi_\alpha(t) f(0), \qquad t \in (0, T],$$

where the kernel function $\phi_a(t)$ is the inverse Laplace transform

$$\phi_a(t) = \mathcal{L}^{-1}\left\{\Phi_\alpha(s)\right\}(t), \qquad \Phi_\alpha(s) = s^{sA(s)-1}.$$

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Proposition (Garrappa, Giusti, and Mainardi 2021, Proposition 2.1)

Let $\alpha(t) : [0, T] \to (0,1)$ be a locally integrable function with Laplace transform $A(s)$, let $\phi_\alpha(t)$ be the inverse Laplace transform of $\Phi_\alpha(s) = s^{sA(s)-1}$, if $f \in \mathbb{A}([0, T])$ then

$$ {}_S D^{\alpha(t)}_{[0,t]} f(t) = \int_0^t \phi_\alpha(t-\tau) f'(\tau)\, \mathrm{d}\tau, \qquad t \in [0, T]. $$

Scarpi's Integral (Garrappa, Giusti, and Mainardi 2021)

To "fix" the behavior of the naive definition we need also the related formulation of the fractional integral, that is having an operator for which

$$ {}_S D^{\alpha(t)}_{[0,t]} \, {}_S I^{\alpha(t)}_{[0,t]} f(t) = f(t) \qquad I^{\alpha(t)}_{[0,t]} \, {}_S D^{\alpha(t)}_{[0,t]} f(t) = f(t) - f(0), $$

Going there-and-back the Laplace domain can be rewritten as the **Sonine condition**

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$$ {}_{S}I^{\alpha(t)}_{[0,t]} f(t) = \int_0^t \psi_\alpha(t-\tau) f(\tau)\,\mathrm{d}\tau, $$

with $\psi_\alpha(t) = \mathcal{L}^{-1}\{\Psi_\alpha(s)\}(t)$ for $\Psi_\alpha(s) = s^{-sA(s)}$.

Finding good $\alpha(t)$ (Garrappa, Giusti, and Mainardi 2021)

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$\Rightarrow$ Any function $\alpha(t)$ with LT $A(s)$ is suitable provided tha $\Phi_\alpha(s)$ and $\Psi_\alpha(s)$ are LTs of some functions.

Solving FDEs with Scarpi's Derivative

Consider the case

$$\begin{cases} {}_S D^{\alpha(t)}_{[0,t]} y(t) = -\lambda y(t), \\ y(0) = y_0 \end{cases} \qquad \mathbb{R} \ni \lambda > 0$$

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1. We apply Laplace transform on both sides

$$s^{sA(s)} Y(s) - s^{sA(s)-1} y_0 = -\lambda Y(s)$$

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2. Solve for $Y(s)$

$$Y(s) = \frac{y_0}{s(1 + \lambda \Psi_\alpha(s))},$$

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3. **Numerically invert the Laplace transform** with one of the algorithms we have seen when discussing the computation of the Mittag-Leffler function, e.g., parabolic contour and Trapezoidal quadrature

$$y(t) = \mathcal{L}^{-1}\{Y(s)\}(t).$$

An example

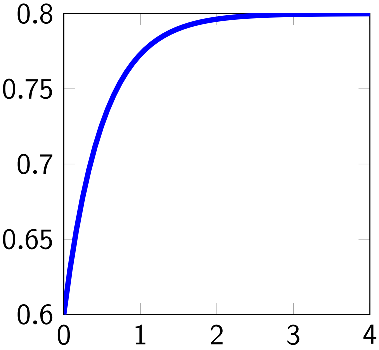
Consider the function

$$\alpha(t) = \alpha_2 + (\alpha_1 - \alpha_2)e^{-ct}$$

together with its Laplace transform

$$A(s) = \int_0^\infty e^{-st}\alpha(t)\,\mathrm{d}t = \frac{\alpha_2 c + \alpha_1 s}{s(c+s)}$$

```
alpha1 = 0.6;
alpha2 = 0.8;
c = 2.0;
a = @(t) alpha2 + (alpha1-alpha2).*exp(-c*t);
A = @(s) (alpha2*c + alpha1*s)./(s.*(c+s));
```



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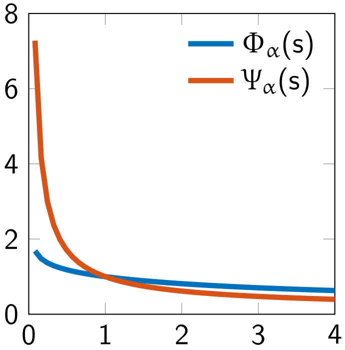
We can easily visualize also the $\Psi_\alpha(s)$ and $\Phi_\alpha(s)$ kernels.

```
plot(t,t.^(t.*A(t)-1),'-',t,t.^(-t.*A(t)),'-
↪  ','LineWidth',2)
legend('\Phi_\alpha(s)','\Psi_\alpha(s)')
```



An example: inverting the Laplace transform

We can then solve

$$\begin{cases} {}_S D_{[0,t]}^{\alpha(t)} y(t) = -0.5 y(t), \\ y(0) = 1 \end{cases}$$

by first setting the various quantities:

```
y0 = 1;
lambda = 0.5;
Psi = @(s) s.^(-s.*A(s));
F = @(s) y0./(s.*(1 + lambda*Psi(s)));
```

An example: inverting the Laplace transform

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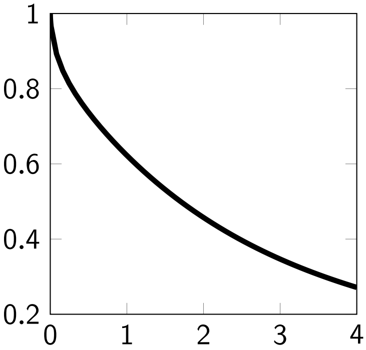
Then inverting the Laplace transform on a **parabolic contour**

```
L = -log(eps); N = ceil(4*L/3/pi);
h = 2*pi/L + L/2/pi/N^2; p = L^3/4/pi^2/N^2;
u = (0:N)*h; f = zeros(size(t));
for n = 1:length(t)
 mu = p/t(n);
 z = mu*(u*1i + 1).^2; z1 = 2*mu*(1i-u);
 G = exp(z.*t(n)).*F(z).*z1;
 f(n) = (imag(G(1))/2+sum(imag(G(2:N+1))))*h/pi;
end
```



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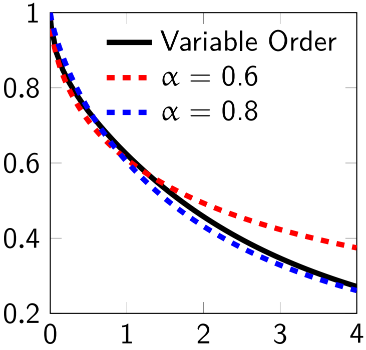
And we can comapre the solution with the one obtained for the two fixed orders, observing that indeed we transition from one behavior to the other:

```
f_fun = @(t,y) -lambda*y;
J_fun = @(t,y) -lambda;
t0 = 0; T = 4; h = 1e-2;
alpha = alpha1;
[t1, y1] = fde_pi2_im(alpha,f_fun,J_fun,t0,T,y0,h);
alpha = alpha2;
[t2, y2] = fde_pi2_im(alpha,f_fun,J_fun,t0,T,y0,h);
```



Possible research directions

- Scarpi FDEs with more difficult dynamics, e.g., the vector case with a non-diagonalizable matrix, non-linear FDEs, *etc.*

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- All-at-once formulations for the *other* FDEs?
- General poles for Rational Krylov methods for the computation of Mittag-Leffler matrix-function times vector algorithms?

Conclusions

In this **first part of the course** we have dealt with

- Defining and analyzing properties of Riemann-Liouville integral and derivatives,
- Defining and analyzing properties of Caputo integral and derivatives,
- Existence, uniqueness and regularity of FDEs with Caputo derivatives,
- Explored the connection between time-fractional derivatives and CTRW,
- FDEs with mulitple, distributed and variable orders.

For what concerns **numerical methods** we have seen

- Product Integral Rules and Fractional Linear Multistep Methods for integrating FDEs,
- An overview of some inversion techniques for the Laplace Transform,
- Computation of the Mittag-Leffler function and its derivative on scalar and matrix arguments,
- Krylov methods for the computation of matrix functions.

Programs for the (*near*) future

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