Mathematics and Computers in Simulation 223 (2024) 394–404

Contents lists available at ScienceDirect

Mathematics and Computers in Simulation

journal homepage: www.elsevier.com/locate/matcom

Original articles

Solving direct and inverse problems for Fredholm-type integro-differential equations with application to pollution diffusion modeling

M.I. Berenguer [a,*], D. Gámez [a], H. Kunze [b], D. La Torre [c], M. Ruiz Galán [a]

[a] Department of Applied Mathematics and Institute of Mathematics (IMAG), University of Granada, Granada, Spain
[b] Department of Mathematics and Statistics, University of Guelph, Guelph, Canada
[c] SKEMA Business School, Université Côte d'Azur, France

ARTICLE INFO

Keywords:
Fredholm-type integro-differential equations
Direct problem
Inverse problem
Pollution diffusion modeling

ABSTRACT

We analyze a particular Fredholm-type partial integro-differential equation. We study the direct problem and prove existence and uniqueness of the solution via a fixed-point argument for generalized contractive maps. This approach also allows us to formulate a collage-type result that can be used to solve inverse problems. We provide numerical examples and we also show how these equations can be used to model pollution diffusion of heavy pollutants and non-volatile substances such as heavy metals, chemical spills, radioactive isotopes, and others.

1. Introduction

Integro-differential equations are expressions that involve the derivative of an unknown function, which also appears under an integral sign. They have been used for several applications in numerous real-world problems (see [1,2] and the references therein). Fredholm integro-differential equations are usually defined in such a way that the integration limits are constant. They arise in various areas of science and engineering, including physics, biology, and finance and they are particularly useful in modeling phenomena with non-local interactions where the behavior of the system at a point depends on the behavior of the system over an interval [16,20,32,36].

In this paper we focus on the analysis of the following problem, which belongs to the family of Fredholm-type integro-differential equations:

$$\begin{cases} u_t(x,t) = g(x,t)u(x,t) + \int_a^b f(x,s,u(s,t))\,d\mu(s), & (x,t) \in [a,b]\times[0,T] \\ u(x,0) = u_0(x), & x \in [a,b] \end{cases} \quad (1)$$

where $u_t(x,t)$ denote the partial derivative of u with respect to t, the functions f and g are given and u_0 is the initial condition and we also suppose that μ is a generic probability measure with compact support over an interval $[a,b]$.

Our interest for this type of equations is motivated by the extensive use of them in pollution diffusion modeling. In that setting, the probability measure μ describes the uncertainty due to unexpected emissions of pollutant or it describes the relative importance and effect of a certain pollutant in a specific location. This family of equations is of particular importance when modeling heavy pollutants or non-volatile substances (heavy metals, non-volatile organic compounds, oil spills, chemical spills, radioactive isotopes

* Corresponding author.
E-mail address: maribel@ugr.es (M.I. Berenguer).

https://doi.org/10.1016/j.matcom.2024.04.021
Received 24 November 2023; Received in revised form 10 April 2024; Accepted 19 April 2024
Available online 22 April 2024
0378-4754/

such as uranium, thorium, radium, and radon) that tend to remain localized in their original states or forms, rather than dispersing into the surrounding atmosphere [35,47].

These pollutants can pose significant environmental and health risks, particularly if they contaminate soil, water bodies, or ecosystems, necessitating careful management and remediation efforts. Such pollutants are often associated with industrial processes, and the contamination process is quite slow and it cannot be described by a classical diffusion term. One can refer to [38] to understand various aspects of atmospheric chemistry and physics of heavy pollutants. In [33,45] the authors provide an overview of environmental modeling techniques, including diffusion modeling, for the fate and transport of pollutants in different environmental media while [6] covers the fundamental principles of fluid flow and transport in porous media, which are relevant to modeling the movement of pollutants in groundwater and soil (see also [15]).

We will show how the previous integro-differential problem (1) can be stated in terms of a fixed-point equation and, for this abstract problem, we will discuss both the direct and the inverse problems.

The *direct problem* for a certain equation consists in proving the existence and uniqueness of a solution as well as the stability of its solution. It starts with the causes and then calculates the effects. Solving a direct problem involves the following steps: Formulation of the problem, selection of a solution technique, solution process, and verification and interpretation.

The *inverse problem*, instead, is the inverse of a direct problem [5,22,23,34,44,46] and it focuses on the estimation of the values of unknown parameters from a set of observations. That is, an inverse problem's solution starts from the effects to calculate (or, more likely, to estimate) the causes. This is usually done by estimating the parameters from observed data or numerical approximations of the solution. Solving inverse problems often requires sophisticated mathematical techniques, optimization algorithms, and numerical simulations. Regularization methods and Bayesian approaches are commonly used to address the challenges associated with ill-posedness and uncertainties in the data. Inverse problems have wide applications in a variety of different fields, ranging from system identification to optics, from acoustics to communication theory, from signal processing to medical imaging, and many others.

In order to analyze the direct and inverse problems for problem (1), we will reformulate the equation using a fixed-point framework. This approach has been used in several previous papers in the literature of differential, integral and integro-differential equations for dealing with both direct and inverse problems (see [7,8,19,26–28]). In this context the direct problem is normally studied by means of Banach's fixed point Theorem (or its extensions), and it is based on a generalized contractivity property of the map and the completeness of the underlying space. The inverse problem, instead, relies on a consequence of Banach's Theorem known as Collage Theorem. Thanks to this result, the inverse problem boils down to a finite dimensional optimization problem over the space of unknown parameters. This optimization is, most of the time, a non-convex problem and it requires the implementation of deterministic or stochastic global optimization algorithms.

The paper proceeds as follows. In Section 2, we recall some well known facts on fixed point theory and we reformulate Problem (1) as a fixed point equation. Under certain hypotheses, an extended fixed-point result allows us to prove existence and uniqueness of the solution. In the same section we also present an algorithm to approximate the solution using the notion of a Schauder basis. We conduct some numerical experiments to test our results and show how the approximation method works in practical contexts. In Section 3, we make use of a generalization of the Collage Theorem to state the inverse problem in terms of an abstract optimization model. By means of practical examples and when specific families of functions are considered, we show how to solve it to estimate the unknown parameters of the model. In Section 4, we present an application of problem (1) to modeling pollution diffusion when heavy pollutants are considered. Finally, in Section 5 we present some conclusions and future research avenues.

2. The direct problem: Model analysis and numerical approximation

In this section we deal with existence and uniqueness of the solution to problem (1). We also derive a numerical algorithm to approximate it and we illustrate this approach by means of numerical experiments.

2.1. Fixed point formulation

In this subsection we provide the theoretical foundations and the fixed-point argument that allow to establish existence and uniqueness of a solution to the above problem (1).

The Banach Fixed-Point Theorem is a well known result and it is the basis for proving existence and uniqueness of fixed-point solutions. We are going to use a more general although well-known version known as Caccioppoli-Banach Fixed Point Theorem (see [3, Theorem 2.3]).

Theorem 1. *Let $(X, \|\cdot\|)$ be a Banach space and let $\mathbf{T} : X \longrightarrow X$ be an operator such that there exits a sequence of nonnegative real numbers $\{\rho_n\}_{n\geq 1}$ satisfying $\|\mathbf{T}^n u_1 - \mathbf{T}^n u_2\| \leq \rho_n \|u_1 - u_2\|$ $\forall u_1, u_2 \in X$ and the serie $\sum_{n\geq 1} \rho_n$ is convergent. Then $\mathbf{T}$ has a unique fixed point $\bar{u} \in X$ and for all $n \in \mathbb{N}$ and $u \in X$,*

$$\|\mathbf{T}^n u - \bar{u}\| \leq \left(\sum_{i=n}^{\infty} \rho_i\right) \|\mathbf{T}u - u\| \tag{2}$$

and in particular,

$$\bar{u} = \lim_n \mathbf{T}^n(u). \tag{3}$$

We study the nonlinear problem presented below: given $g \in C([a,b]\times[0,T])$, $f \in C([a,b]^2\times\mathbb{R})$ and $u_0 \in C([a,b])$, find $u \in C([a,b]\times[0,T])$ with $u_t \in C([a,b]\times[0,T])$ such that:

$$\begin{cases} u_t(x,t) = g(x,t)u(x,t) + \displaystyle\int_a^b f(x,s,u(s,t))d\mu(s) \\ u(x,0) = u_0(x) \end{cases} . \tag{4}$$

We consider that f is Lipschitz in the third variable, and M is the Lipschitz constant. Regarding this equation, we define the integral operator $\mathbf{T}: C([a,b]\times[0,T]) \longrightarrow C([a,b]\times[0,T])$ defined for $(x,t)\in[a,b]\times[0,T]$ and $u \in C([a,b]\times[0,T])$ as

$$(\mathbf{T}u)(x,t) := u_0(x) + \int_0^t g(x,r)u(x,r)dr + \int_0^t \int_a^b f(x,s,u(s,r))d\mu(s)dr, \tag{5}$$

where "dr" denotes Lebesgue measure.

Theorem 2. *Let be $g \in C([a,b]\times[0,T])$, $u_0 \in C([a,b])$ and $f \in C([a,b]^2\times\mathbb{R})$ satisfying a Lipschitz condition with respect to the last variable, with Lipschitz constant M. Then, problem (4) admits a unique solution.*

Proof. Let $\mathbf{T}: C([a,b]\times[0,T]) \longrightarrow C([a,b]\times[0,T])$ be the operator defined by (5). We first proof that $\bar{u}$ is solution of problem (4) if, and only if $\mathbf{T}\bar{u} = \bar{u}$.

If $\bar{u}$ is solution of (4) taking into account that $\bar{u}$ is continuous, by the Fundamental Theorem of Calculus we have that $\bar{u}$ is a fixed point of the operator $\mathbf{T}$. And conversely, if $\mathbf{T}\bar{u} = \bar{u}$, as g, $\bar{u}$ are continuous, then the Fundamental Theorem of Calculus yields

$$\bar{u}_t(x,t) = g(x,t)\bar{u}(x,t) + \int_a^b f(x,s,\bar{u}(s,t))d\mu(s),$$

and since $\bar{u}(x,0) = u_0(x)$, $\bar{u}$ is solution of (4).

Therefore, to conclude the proof we will show that $\mathbf{T}$ has a unique fixed point. To this end, if $u_1, u_2 \in C([a,b]\times[0,T])$, $(x,t)\in[a,b]\times[0,T]$ then, taking $N = \max_{(x,t)\in[a,b]\times[0,T]} |g(x,t)|$, we have by induction that for $n \geq 1$

$$|\mathbf{T}^n u_1(x,t) - \mathbf{T}^n u_2(x,t)| \leq \frac{(t(N+M))^n}{n!}\|u_1 - u_2\|.$$

More specifically, for $n = 1$,

$$|\mathbf{T}u_1(x,t) - \mathbf{T}u_2(x,t)| \leq \int_0^t |g(x,r)|\cdot|u_1(x,r) - u_2(x,r)|dr + \int_0^t\int_a^b |f(x,s,u_1(s,r)) - f(x,s,u_2(s,r))|d\mu(s)dr \leq$$
$$N\|u_1 - u_2\|t + M\|u_1-u_2\|\mu([a,b])t = \frac{t(N+M)}{1!}\|u_1 - u_2\|,$$

and if we suppose that $|\mathbf{T}^n u_1(x,t) - \mathbf{T}^n u_2(x,t)| \leq \dfrac{t^n(N+M)^n}{n!}\|u_1-u_2\|$, then

$$|\mathbf{T}^{n+1}u_1(x,t) - \mathbf{T}^{n+1}u_2(x,t)| \leq$$
$$\int_0^t |g(x,r)|\cdot|\mathbf{T}^n u_1(x,r) - \mathbf{T}^n u_2(x,r)|dr + \int_0^t\int_a^b |f(x,s,\mathbf{T}^n u_1(s,r)) - f(x,s,\mathbf{T}^n u_2(s,r))|d\mu(s)dr \leq$$
$$\leq N\int_0^t \frac{r^n(N+M)^n}{n!}\|u_1-u_2\|dr + M\int_0^t\int_a^b \frac{r^n(N+M)^n}{n!}\|u_1-u_2\|d\mu(s)dr =$$
$$\frac{t^{n+1}}{(n+1)!}N(N+M)^n\|u_1-u_2\| + \frac{t^{n+1}}{(n+1)!}M(N+M)^n\|u_1-u_2\|\mu([a,b]) =$$
$$\frac{t^{n+1}(N+M)^{n+1}}{(n+1)!}\|u_1-u_2\|.$$

As consequence, for $n \geq 1$,

$$\|\mathbf{T}^n u_1 - \mathbf{T}^n u_2\| \leq \rho_n\|u_1 - u_2\| \tag{6}$$

where

$$\rho_n = \frac{(T(N+M))^n}{n!}. \tag{7}$$

Since the series $\sum_{n\geq 1}\rho_n$ is convergent, by Theorem 1, there exists a unique $\bar{u} \in C([a,b]\times[0,T])$ such that $\mathbf{T}(\bar{u}) = \bar{u}$, and for each $u \in C([a,b]\times[0,T])$ and $n \geq 1$,

$$\|\mathbf{T}^n u - \bar{u}\| \leq \left(\sum_{i=n}^{\infty}\rho_i\right)\|\mathbf{T}u - u\|, \tag{8}$$

and thus $\lim_{n\to\infty}\|\mathbf{T}^n u - \bar{u}\| = 0$. □

In view of the above, the solution can be determined as the limit of the iterates of operator $\mathbf{T}$. Since the calculations of such iterates from a practical point of view are not always feasible, in the next section we propose a method to approximate the solution.

2.2. Numerical method

For our purposes, let us recall that a *Schauder basis* of a Banach space X is a sequence $\{\gamma_n\}_{n\geq 1} \subset X$ such that $\forall \gamma \in X$ there is a unique sequence $\{\lambda_n\}_{n\geq 1}$ of real numbers satisfying $\gamma = \sum_{n\geq 1} \lambda_n \gamma_n$.

The sequences of *projections* $P_n : X \to X$ and *coordinate functionals* $\{\gamma_n^*\}_{n\geq 1}$ in X^*, are defined, respectively, as follows:

$$P_n\left(\sum_{n\geq 1} \lambda_n \gamma_n\right) = \sum_{k=1}^{n} \lambda_k \gamma_k \text{ and } \gamma_n^*\left(\sum_{n\geq 1} \lambda_n \gamma_n\right) = \lambda_n$$

and it is verified that

$$\lim_n \|P_n(\gamma) - \gamma\| = 0 \text{ for all } \gamma \in X. \tag{9}$$

Let $\{A_n\}_{n\geq 1}$ be a Schauder basis in $C([a,b]\times[0,T])$ with $\{Q_n\}_{n\geq 1}$ as their associated projections and $\{B_n\}_{n\geq 1}$ a Schauder basis in $C([a,b]^2\times[0,T])$, with its associated projections $\{R_n\}_{n\geq 1}$. For $p \in \mathbb{N}$, we define $\mathbf{G}_p : C([a,b]\times[0,T]) \longrightarrow C([a,b]\times[0,T])$:

$$(\mathbf{G}_p v)(x,t) := u_0(x) + \int_0^t Q_{n_p}(g\cdot v)(x,r)dr + \int_0^t \int_a^b R_{n_p^*}(L_0(v))(x,s,r)d\mu(s)dr \tag{10}$$

where $n_p \in \mathbb{N}$, $n_p^* \in \mathbb{N}$, $v \in C([a,b]\times[0,T])$ and $L_0 : C([a,b]\times[0,T]) \to C([a,b]^2\times[0,T])$,

$$L_0(v)(x,s,t) := f(x,s,v(s,t)), \qquad (x,s,t) \in [a,b]^2\times[0,T]. \tag{11}$$

Let $\widetilde{u} \in C([a,b]\times[0,T])$, and we define:

$$z_0(x,t) := \widetilde{u}(x,t) \tag{12}$$

and for $m \in \mathbb{N}$,

$$z_m(x,t) := \mathbf{G}_m \circ \ldots \circ \mathbf{G}_1(\widetilde{u})(x,t). \tag{13}$$

The following result allows us to choose $n_1,\ldots,n_m,n_1^*,\ldots,n_m^* \in \mathbb{N}$ so that z_m approximates the unique solution of (4).

Theorem 3. *Let $\widetilde{u} \in C([a,b]\times[0,T])$ and let $\bar{u}$ be the unique solution of problem (1), then for each $\varepsilon > 0$ there exist $m \geq 1$ and $n_1,\ldots,n_m,n_1^*,\ldots,n_m^* \geq 1$ such that $\|\bar{u} - z_m\| < \varepsilon$ with z_0 and z_m defined by (12) and (13).*

Proof. If we consider $\rho_0 = 1$ and for all $n \geq 1$, ρ_n is given by (7), then we have that for all $m \geq 0$,

$$\begin{aligned}
&\|\mathbf{T}^m\widetilde{u} - z_m\| \leq \\
&\|\mathbf{T}^m\widetilde{u} - \mathbf{T}^{m-1}z_1\| + \|\mathbf{T}^{m-1}z_1 - \mathbf{T}^{m-2}z_2\| + \cdots + \|\mathbf{T}^2 z_{m-2} - \mathbf{T}z_{m-1}\| + \|\mathbf{T}z_{m-1} - z_m\| \leq \\
&\left(\sum_{p=1}^{m-1} \|\mathbf{T}^{m-p+1}z_{p-1} - \mathbf{T}^{m-p}z_p\|\right) + \|\mathbf{T}z_{m-1} - z_m\| \leq \\
&\left(\sum_{p=1}^{m-1} \|\mathbf{T}^{m-p}\mathbf{T}z_{p-1} - \mathbf{T}^{m-p}z_p\|\right) + \rho_0\|\mathbf{T}z_{m-1} - z_m\| \leq \\
&\left(\sum_{p=1}^{m-1} \mu_{m-p}\|\mathbf{T}z_{p-1} - z_p\|\right) + \rho_0\|\mathbf{T}z_{m-1} - z_m\| = \sum_{p=1}^{m} \rho_{m-p}\|\mathbf{T}z_{p-1} - z_p\|.
\end{aligned}$$

Therefore,

$$\|\mathbf{T}^m\widetilde{u} - z_m\| \leq \sum_{p=1}^{m} \rho_{m-p}\|\mathbf{T}z_{p-1} - z_p\|.$$

For $p \in \{1,\ldots,m\}$, we define $L_p : C([a,b]\times[0,T]) \to C([a,b]^2\times[0,T])$,

$$L_p(v)(x,s,t) := f(x,s,\mathbf{G}_p \circ \ldots \circ \mathbf{G}_1(v)(x,t)), \qquad (x,s,t) \in [a,b]^2\times[0,T]. \tag{14}$$

Then

$$\begin{aligned}
&|\mathbf{T}z_{p-1}(x,t) - z_p(x,t)| \leq \\
&\int_0^t \left|(g\cdot z_{p-1})(x,r) - Q_{n_p}(g\cdot z_{p-1})(x,r)\right| dr + \int_0^t \int_a^b \left|f(x,s,z_{p-1}(s,r)) - R_{n_p^*}(L_{p-1}(\widetilde{u}))(x,s,r)\right| d\mu(s)dr
\end{aligned}$$

Table 1
Absolute error $|z_7(x,t) - \bar{u}(x,t)|$ for Example 2.1 with $n_i = 9^2$ and $n_i^* = 9^3$.

t, x	0.2	0.4	0.6	0.8	1
0.2	1.03155×10^{-3}	2.52247×10^{-3}	4.62988×10^{-3}	7.65072×10^{-3}	1.18063×10^{-2}
0.4	1.67067×10^{-3}	4.06346×10^{-3}	7.42057×10^{-3}	1.21464×10^{-2}	1.86538×10^{-2}
0.6	1.92418×10^{-3}	4.61077×10^{-3}	8.2941×10^{-3}	1.33447×10^{-2}	2.01397×10^{-2}
0.8	1.77083×10^{-3}	4.12469×10^{-3}	7.21951×10^{-3}	1.13068×10^{-2}	1.66163×10^{-2}
1	1.32592×10^{-3}	2.97533×10^{-3}	5.03546×10^{-3}	7.65843×10^{-3}	1.09648×10^{-2}

Table 2
Absolute error $|z_7(x,t) - \bar{u}(x,t)|$ for Example 2.1 with $n_i = 17^2$ and $n_i^* = 17^3$.

t, x	0.2	0.4	0.6	0.8	1
0.2	4.72292×10^{-4}	1.14505×10^{-3}	2.08206×10^{-3}	3.36593×10^{-3}	5.10239×10^{-3}
0.4	3.68087×10^{-4}	8.85775×10^{-4}	1.59959×10^{-3}	2.57172×10^{-3}	3.88733×10^{-3}
0.6	4.47135×10^{-4}	1.07321×10^{-3}	1.93185×10^{-3}	3.09301×10^{-3}	4.64846×10^{-3}
0.8	1.3224×10^{-3}	3.0642×10^{-3}	5.33105×10^{-3}	8.25494×10^{-3}	1.2×10^{-2}
1	5.04882×10^{-4}	1.14554×10^{-3}	1.95615×10^{-3}	2.9809×10^{-3}	4.27573×10^{-3}

$$\leq T\|g \cdot z_{p-1} - Q_{n_p}(g \cdot z_{p-1})\| + T\mu([a,b])\|L_{p-1}(\widetilde{u}) - R_{n_p^*}(L_{p-1}(\widetilde{u}))\|,$$

therefore,

$$\|\mathbf{T}^m\widetilde{u} - z_m\| \leq \sum_{p=1}^{m} T\rho_{m-p}\left(\|g \cdot z_{p-1} - Q_{n_p}(g \cdot z_{p-1})\| + \|L_{p-1}(\widetilde{u}) - R_{n_p^*}(L_{p-1}(\widetilde{u}))\|\right). \tag{15}$$

For all $\varepsilon > 0$, by (3), there exits $m \in \mathbb{N}$ verifying that $\|\bar{u} - \mathbf{T}^m\widetilde{u}\| < \varepsilon/2$. By (9) and (15), there exist $n_1, \ldots, n_m, n_1^*, \ldots, n_m^* \geq 1$ such that

$$\|\mathbf{T}^m\widetilde{u} - z_m\| < \varepsilon/2.$$

Then, by triangle inequality,

$$\|\bar{u} - z_m\| \leq \|\mathbf{T}^m\widetilde{u} - \bar{u}\| + \|\mathbf{T}^m\widetilde{u} - z_m\| < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} < \varepsilon. \quad \square$$

2.3. Numerical experiments

The presented numerical method has been tested on two numerical examples. Given the dense sequence $\{s_n\}_{n\geq 1}$ (respectively $\{t_n\}_{n\geq 1}$) taken on the diadic partition of the interval $[a,b]$ ($[0,T]$, respectively) with $s_1 = a$ and $s_2 = b$ ($t_1 = 0$ and $t_2 = T$ respectively), we consider the Faber Schauder basis $\{\varphi_n\}_{n\geq 1}$ in $C([a,b])$ and $\{\psi_n\}_{n\geq 1}$ in $C([0,T])$, and we fix the concrete Schauder basis $\{A_n\}_{n\geq 1}$ in $C([a,b]\times[0,T])$ and $\{B_n\}_{n\geq 1}$ in $C([a,b]^2\times[0,T])$ as the tensor product of bases $\{\varphi_n\}_{n\geq 1}$ and $\{\psi_n\}_{n\geq 1}$ [39]. The advantage of introducing these bases is that, via the following change-of-variable, the calculations are feasible (see [25, Section 5]): Let us suppose that μ is a measure defined on the Borel subsets of $\mathbb{R}$ and suppose that $\mathrm{supp}(\mu) = [a,b]$ and that is non-atomic. Let $F : K = \mathrm{supp}(\mu) \to [0,1]$ be the cumulative of μ and $F^{-1} : [0,1] \to K$ be its inverse. Then, given a function $f : K \to \mathbb{R}$, the following change of variable rule holds:

$$\int_K f(x)d\mu(x) = \int_0^1 f(F^{-1}(x))dx \tag{16}$$

where dx is the Lebesgue measure.

The computations to implement the algorithm for the approximate solution have been done using Mathematica.

Example 2.1. Consider the following problem

$$\begin{cases} u_t(x,t) = \dfrac{2 + e^{x-2}x^2 - e^x x^2}{2}u(x,t) + \displaystyle\int_0^1 x^2 e^{-s}u(s,t)ds \\ u(x,0) = e^{-x} \qquad\qquad (x,t) \in [0,1]\times[0,1] \end{cases} . \tag{17}$$

where the exact solution is given by $\bar{u}(x,t) = e^{t-x}$. To compare numerical and exact solutions see Tables 1 and 2 where it is shown the absolute errors $|z_7(x,t) - \bar{u}(x,t)|$ taking, on one hand, $n_i = 9^2$ and $n_i^* = 9^3$, and in other hand $n_i = 17^2$ and $n_i^* = 17^3$ for $i = 1, \ldots, 7$. The sup norm of the error $\|z_7 - \bar{u}\|$ is 2.27689×10^{-2} in the first case and 1.66485×10^{-2} in the second one.

Table 3
Absolute error $|z_3(x,t) - \bar{u}(x,t)|$ for Example 2.2 with $n_i = 9^2$ and $n_i^* = 9^3$.

t, x	0.2	0.4	0.6	0.8	1
0.2	1.51415×10^{-4}	3.01377×10^{-4}	4.43192×10^{-4}	6.06209×10^{-4}	1.61912×10^{-3}
0.4	3.04166×10^{-4}	6.16909×10^{-4}	9.16421×10^{-4}	1.04999×10^{-3}	7.86755×10^{-4}
0.6	4.5769×10^{-4}	9.33775×10^{-4}	1.41162×10^{-3}	1.70325×10^{-3}	1.22657×10^{-3}
0.8	6.4003×10^{4}	1.30108×10^{-3}	1.98926×10^{-3}	2.58337×10^{-3}	2.4922×10^{-3}
1	7.50114×10^{-4}	1.55333×10^{-3}	2.51532×10^{-3}	3.74581×10^{-3}	4.89973×10^{-3}

Example 2.2. Let us suppose that the density ξ of the measure μ over the interval $[0,1]$ is equal to $\xi(x) = \frac{3}{4} + \frac{x}{2}$ and 0 otherwise and consider the problem

$$\begin{cases} u_t(x,t) = g(x,t)u(x,t) + \int_0^1 xu(s,t)d\mu(s) \\ u(x,0) = \cos(x) \quad (x,t) \in [0,1] \times [0,1] \end{cases} . \tag{18}$$

where $g(x,t)$ is such that $\bar{u}(x,t) = \cos(x-t)$ is the solution. The obtained results are presented for $m = 3$ with $n_i = 9^2$ and $n_i^* = 9^3$ for $i = 1,2,3$ can be viewed in Table 3. The sup norm of the error $\|z_3 - \bar{u}\|$ is 4.89973×10^{-3}.

3. The inverse problem

The inverse problem consists in determining an estimation of the unknown parameters of the model starting from data that have been gathered by samples or experiments. In the case of our model Eq. (1), the data could be values of u at particular observation points (x_i, t_i), and the parameters we wish to estimate might be the coefficients in the proposed functional forms of g and f. This problem can be solved by using a Collage-type Theorem. The classical "Collage Theorem" for the standard version of Banach's fixed point theorem has been known for many years, but it was first used in the context of solving an inverse problem in [5] for the analysis of inverse problems in fractal image compression. This classical Collage Theorem states an approximation result between any target object u and the solution $\bar{u}$ of a fixed point equation $T\bar{u} = \bar{u}$. In the fractal imaging context, the action of the fractal transform operator T on an image u produces a new image v that is an assemblage of adjusted subsets of u; it is this action that gives rise to name "Collage". The Collage Theorem is a crucial result for solving inverse problems for fixed point equations and it has been used in a variety of different formulations and frameworks (see [4,9,10,12–14,17,18,37,40,41]).

In the current paper, the next result Theorem 4 allows us to formulate a computable inverse problem approach to problem (1). The proof of this result is similar to that in [24], which is based on the application of the standard Collage Theorem to a contraction map $\mathbf{T}^{n_0}$.

Theorem 4 ([24]). *Let $(X, \|\cdot\|)$ be a Banach space and let $\mathbf{T} : X \longrightarrow X$ be an operator such that there exits a sequence of nonnegative real numbers $\{\rho_n\}_{n\geq 1}$ satisfying $\|\mathbf{T}^n u_1 - \mathbf{T}^n u_2\| \leq \rho_n \|u_1 - u_2\|$ $\forall u_1, u_2 \in X$ and the series $\sum_{n\geq 1} \rho_n$ is convergent. Let $\bar{u}$ be the unique fixed point of $\mathbf{T}$, as guaranteed by Theorem 1, and u be a chosen element of X. Then there exists n_0 such that $\rho_{n_0} < 1$ and this implies*

$$\|u - \bar{u}\| \leq \frac{\sum_{i=0}^{n_0-1} \rho_i}{1 - \rho_{n_0}} \|\mathbf{T}u - u\|. \tag{19}$$

When we label the observational data or their interpolant as u, we can identify the right-hand side of (19) as the error in approximating u by the fixed point $\bar{u}$ of $\mathbf{T}$. If $\rho_{n_0} \ll 1$, then the magnitude of the error can be controlled by minimizing $\|\mathbf{T}u - u\|$. If, as usually happens in this context, the operator $\mathbf{T}$ belongs to a fixed family of functions and it is parametrized by a vector $\lambda \in \Lambda \subset \mathbb{R}^p$ (in the inverse problem framework the target element $u \in X$ is fixed and known), the minimization of the term $\Delta(\lambda) := \|\mathbf{T}_\lambda u - u\|$ boils down to solving the optimization problem:

$$\min_{\lambda \in \Lambda} \|\mathbf{T}_\lambda u - u\| \tag{20}$$

which has at least one solution whenever Δ is continuous and Λ is a compact subset of $\mathbb{R}^p$.

Now let us apply the previous abstract inverse problem approach to our specific model. We suppose we know or have an estimate of the target solution u to the model and we want to determine an estimation of g and f. Using the Collage Theorem, this can be stated in terms of the minimization of the Collage distance:

$$\min_{f,g} \|u - \mathbf{T}u\| = \left\| u(x,t) - u_0(x) - \int_0^t g(x,r)u(x,r)dr - \int_0^t \int_a^b f(x,s,u(s,r))d\mu(s)dr \right\|, \tag{21}$$

where the minimization is done over all Lipschitz functions f and g.

The complexity of this optimization problem depends on the assumptions of f and g. A regularization term [42,43], expressed in terms of the zero-norm of f and g, can also be added to reduce the dimensionality.

Table 4
Results from Example 3.1.

N_x	N_t	D	ε	Δ	True values			
					1.0000000	−0.4323324	−0.4323324	−0.2161662
					g_0	g_2	g_3	g_4
20	10	6	0.00	0.0000000	0.9996606	−0.5236164	−0.1846185	−0.4777624
20	10	10	0.00	0.0000000	0.9996503	−0.5218805	−0.1879165	−0.4759510
100	50	6	0.00	0.0000000	0.9996606	−0.5236164	−0.1846185	−0.4777624
100	50	10	0.00	0.0000000	0.9996503	−0.5218805	−0.1879165	−0.4759510
20	10	6	0.01	0.0000037	1.0009614	−0.5334301	−0.3618969	−0.3097484
20	10	10	0.01	0.0000078	1.0037317	−0.2392890	−0.6389388	−0.2441403
100	50	6	0.01	0.0000037	1.0009614	−0.5334301	−0.3618969	−0.3097484
100	50	10	0.01	0.0000078	1.0037317	−0.2392890	−0.6389388	−0.2441403
20	10	6	0.05	0.0000619	0.9953297	−1.3535893	0.8862019	−0.7843862
20	10	10	0.05	0.0001412	1.0012706	−0.5801000	−1.1627976	0.3364531
100	50	6	0.05	0.0000619	0.9953297	−1.3535893	0.8862019	−0.7843862
100	50	10	0.05	0.0001411	1.0012706	−0.5801000	−1.1627976	0.3364531

As mentioned above, in a practical inverse problem, both functions f and g may be assumed to take specific forms. Therefore, the essence of the inverse problem lies in estimating the unknown coefficients within these predefined forms, namely g_i, $i = 1, \dots, n_g$, and f_j, $j = 1, \dots, n_f$. The inverse problem boils down to the following form:

$$\min_{g_i, f_j} \|u - \mathbf{T}u\| . \tag{22}$$

The following examples show a practical implementations of the Collage Theorem.

Example 3.1. We return to (17) considered in Example 2.1. We sample the solution e^{t-x} on $[0,1]^2$ on a uniform grid with N_x (N_t) nodes in the x- (t-) direction, add Gaussian noise with amplitude ε to the sample values, and then fit a polynomial $u(x,t)$ of degree D to the noised data. We seek an equation of the form

$$u_t(x,t) = g(x)u(x,t) + \int_0^1 x^2 e^{-s} u(s,t)ds, \tag{23}$$

supposing that g has the form

$$g(x) = g_0 + g_2 x^2 + g_3 x^3 + g_4 x^4.$$

The resulting collage distance $\|u - \mathbf{T}u\|$, with $\mathbf{T}$ the associated integral operator and u our fitted target, is a function of the g_i. The results of minimizing the collage distance in various scenarios are presented in Table 4. Writing the first terms of the Taylor expansion of the true function $g_{true}(x)$ about $x = 0$, we note that near $x = 0$,

$$g_{true}(x) \approx 1.0000000 - 0.4323324x^2 - 0.4323324x^3 - 0.2161662x^4,$$

with coefficients to 7 decimal places. We see that the quality of the results is alright when there is no noise or very low noise, but the worsens as the noise level grows to 5%.

Example 3.2. Let us suppose that $[a,b] = [-1,1]$, $g(x,t)$ is linear and takes the form

$$g(x,t) = g_0 + g_1 x + g_2 t \tag{24}$$

and the function f, instead, can be written as

$$f(x,s,u(x,t)) = \phi(x,s)u(s,t) \tag{25}$$

where ϕ is a normal kernel taking the form

$$\phi(x,s) = \bar{\phi}(x) e^{-\frac{1}{1-s^2}} . \tag{26}$$

Let us suppose that the density ξ of the measure μ over the interval $[-1,1]$ is equal to $\xi(x) = x + \frac{1}{2}$ and 0 otherwise. Then the cumulative $F(x) = \mu([-1,x])$ is equal to $\frac{x^2}{4} + \frac{x}{2} + \frac{1}{4}$ over $[-1,1]$, 0 when $x \le -1$ and 1 when $x \ge 1$. The inverse of the cumulative $x = F^{-1}(y) = \sqrt{4y} - 1$ and then the operator $\mathbf{T}u$ can be written as

$$\begin{aligned}(\mathbf{T}u)(x,t) &= u_0(x) + \int_0^t g(x,r)u(x,r)dr + \int_0^t \int_{-1}^1 \phi(x,s)u(s,t)d\mu(s)dr \\ &= u_0(x) + \int_0^t (g_0 + g_1 x + g_2 r)u(x,r)dr + \bar{\phi}(x) \int_0^t \int_{-1}^1 e^{-\frac{1}{1-s^2}} u(s,r)d\mu(s)dr\end{aligned}$$

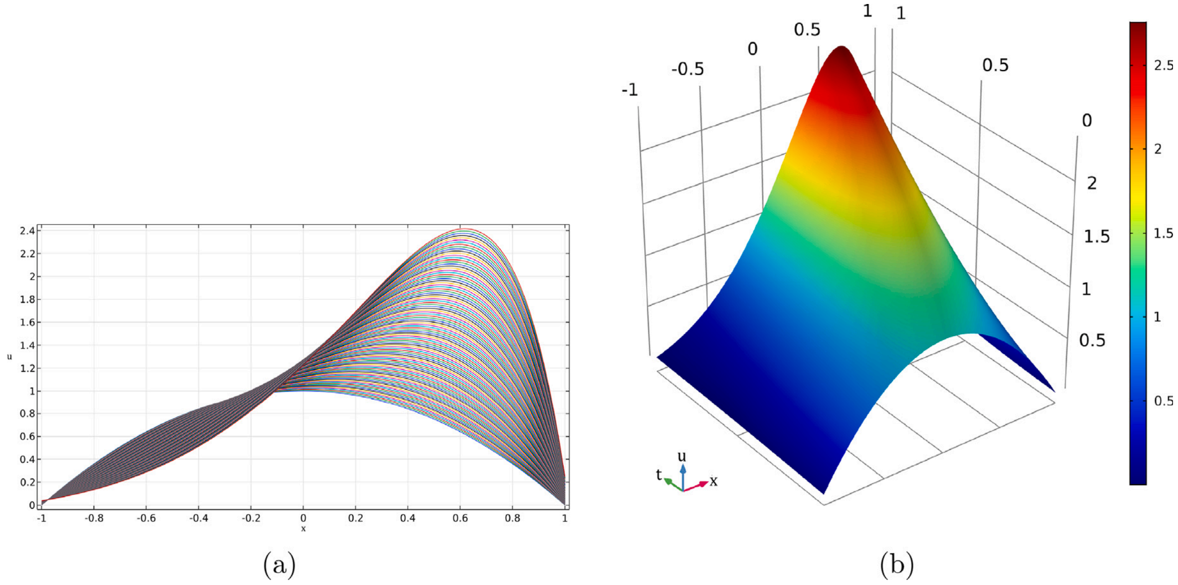

Fig. 1. Solution for Example 3.2, (a) profiles and (b) solution surface for $0 \le t \le 1$.

Table 5
Results for Example 3.2. True values are $(g_0, g_1, g_2) = (0.5, 2, -1)$.

N_x	N_t	ε	Δ	g_0	g_1	g_2
20	10	0.00	0.0001917	0.4950936	2.0116270	−1.0357785
50	25	0.00	0.0001518	0.4948047	2.0129139	−1.0356112
100	50	0.00	0.0001435	0.4946804	2.0133074	−1.0354633
20	10	0.01	0.0002193	0.4938846	2.0039143	−1.0298406
50	25	0.01	0.0001650	0.4869434	2.0167247	−1.0247163
100	50	0.01	0.0001622	0.5015758	2.0094539	−1.0446763
20	10	0.05	0.0009047	0.5205707	1.9106357	−1.0320081
50	25	0.05	0.0002995	0.5208807	2.0356040	−1.0885161
100	50	0.05	0.0002057	0.4713763	2.0317943	−1.0070384
20	10	0.10	0.0021695	0.4923433	1.9702788	−1.0065235
50	25	0.10	0.0009982	0.4551648	2.0330032	−0.9799383
100	50	0.10	0.0002851	0.4853762	2.0299821	−1.0296401

$$= u_0(x) + \int_0^t (g_0 + g_1 x + g_2 r) u(x,r)dr + \bar{\phi}(x) \int_0^t \int_0^1 e^{-\frac{1}{1-(\sqrt{4y}-1)^2}} u(\sqrt{4y}-1, r) dy dr \tag{27}$$

Taking $\bar{\phi}(x) = e^{-x^2}$, $u_0(x) = 1 - x^2$, and, temporarily, $(g_0, g_1, g_2) = (0.5, 2, -1)$, we solve (1) numerically and the solution surface is illustrated in Fig. 1. We display the solution on a uniform grid with N_x (N_t) nodes in the x- (t-) direction, add Gaussian noise with amplitude ε to the sample values, and then fit a polynomial $u(x,t)$ of degree 6 to the noised data. This u plays the role of the target in the Collage Theorem, as described above, with $(\mathbf{T}u)(x,t)$ given in (27). The inverse problem we seek to solve is

$$\min_{g_0, g_1, g_2} \Delta := \left\| u - (\mathbf{T}_{g_0, g_1, g_2} u) \right\|$$

Results are presented in Table 5. We see that the recovered values are reasonable; that improving the target by increasing N_x and N_t improves the results; and that the results are negatively, but not severely, impacted by the addition of noise.

4. An application to pollution diffusion modeling

The control of pollution emissions is probably one of the most challenging issue to guarantee the long-run sustainability and growth. There is a broad research interest in modeling pollution diffusion and determine which actions can be put in place to control the emissions and implement abatement activities and optimal policies. In general, in a one-dimensional environment $[a, b]$, the level of pollution $P(x,t)$ at the time $t \in [0, T]$ and location x can be model through a reaction–diffusion equation taking the form $(x,t) \in [a, b] \times [0, T]$:

$$\begin{cases} P_t(x,t) = c P_{xx}(x,t) + S(x,t)P(x,t) - \delta_P P(x,t) + \int_a^b \phi(s,x) P(s,t) d\mu(s) \\ P(x,0) = P_0(x) \end{cases} \tag{28}$$

Table 6
Numerical results $z_8(x,t)$ obtained in Example 4.1.

$t,\ x$	0.2	0.4	0.6	0.8	1
0.2	0.256062	0.293058	0.30049	0.276818	0.229786
0.4	0.56453	0.712074	0.803802	0.813097	0.738161
0.6	0.932108	1.28944	1.58932	1.74599	1.71097
0.8	1.36636	2.0656	2.76622	3.28263	3.45529
1	1.8741	3.08456	4.46908	5.70699	6.43501

subject to an initial condition at $t = 0$ where $P_t(x,t)$ denote the partial derivative of P with respect to t. Here P_{xx} is the second-order spatial derivative of $P(x,t)$, c is the diffusion coefficient, $S(x,t)$ is the growth rate of pollution and it depends on the level of emissions determined by the production output, $-\delta_P P$ takes into account the natural environmental cleaning, and the integral term models the contribution of the level of pollution at each location s to the accumulation of pollution at x and the probability measure μ describes the relative importance and effect of certain pollutant in a specific location (see [11,21,29–31]). The kernel ϕ weights the contribution of each location in terms of total emissions.

When heavy pollutants or non-volatile substances such as heavy metals, non-volatile organic compounds, oil spills, chemical spills, radioactive isotopes such as uranium, thorium, radium, and radon are considered, the diffusion coefficient can be neglected and the equation boils down to

$$\begin{cases} P_t(x,t) = S(x,t)P(x,t) - \delta_P P(x,t) + \displaystyle\int_a^b \phi(s,x)P(s,t)d\mu(s) \\ P(x,0) = P_0(x) \end{cases} . \tag{29}$$

In fact, heavy pollutants tend to remain localized in their original states or forms, rather than dispersing into the surrounding atmosphere. In this case there is no flow of material associated with pollution diffusion but, instead, the level of pollution increases as a consequence of pollution stocks and water or soil contamination.

We apply the numerical method described in Section 2 for the following pollution model in $[0,1]\times[0,1]$.

Example 4.1. Let us suppose that the density ξ of the measure μ over the interval $[0,1]$ is equal to $\xi(x) = 2x$ and 0 otherwise and consider the problem with $S(x,t) = 2 + 2x - 3t$, $\delta_P = 1$, $\phi(s,x) = x^2\cos(s)$ and $P_0(x) = x$.

The obtained results are presented for $m = 8$ with $n_i = 9^2$ and $n_i^* = 9^3$ for $i = 1,\dots,8$ can be viewed in Table 6. That m has been chosen in such away that

$$\|z_m - z_{m-1}\| \le 10^{-3}.$$

An interesting inverse problem for the above problem (29) is the following: *Given gathered data of P and suppose we know both δ_P and ϕ, let us determine an estimation of the growth rate S*. The following example shows a numerical implementation of the inverse problem with simulated data.

Example 4.2. As an example inverse problem, we proceed similar to Example 3.2, choosing the same measure μ, and again taking $\bar{\phi}(x) = e^{-x^2}$ and $\phi(x,s) = \bar{\phi}(x)e^{-\frac{1}{1-s^2}}$. Here we set, $u_0(x) = 2x^6 + x^5 - 4x^4 - 2x^3 + \frac{3}{2}x^2 + x + \frac{1}{2}$, with its graph identifying two peak pollution levels on $[-1,1]$. We suppose that $S(x,t) = S_0 + S_1x + S_2t$, using the values $(S_0,S_1,S_2) = (1,-2,0.8)$ to generate a target P, in the manner of Example 3.2. For each (N_x,N_t,ε) triplet, we construct two targets, one of degree 8 and the other of degree 10. The numerical solution (with no noise added) is presented in Fig. 2 We now seek to solve the corresponding inverse problem for (S_0,S_1,S_2). The results are presented in Table 7. The recovered values are close to the true values, and they hold up when a low level of noise is added. It is helpful to look again at the solution surface in Fig. 2 to recognize the challenges of using a polynomial basis for the target function. In the third- and second-last rows of the table, for example, we see that increasing the degree of the fitted polynomial reduces the accuracy of the recovered parameter values.

5. Conclusion

In this paper we have analyzed a particular Fredholm-type integro-differential equation. In the first part we have considered the direct problem and proved existence and uniqueness of the solution via a fixed-point argument. In the second part, instead, we have formulated a collage-type result that can be used to solve inverse problems. Numerical examples as well as a potential application to modeling of pollution diffusion conclude the paper. Future avenues include the analysis of more general models of macroeconomic geography in which demography and pollution dynamics affect each other. These problems are modeled with systems of two partial differential equations, one describing the evolution of pollution over time and space and the other describing the evolution of the human population.

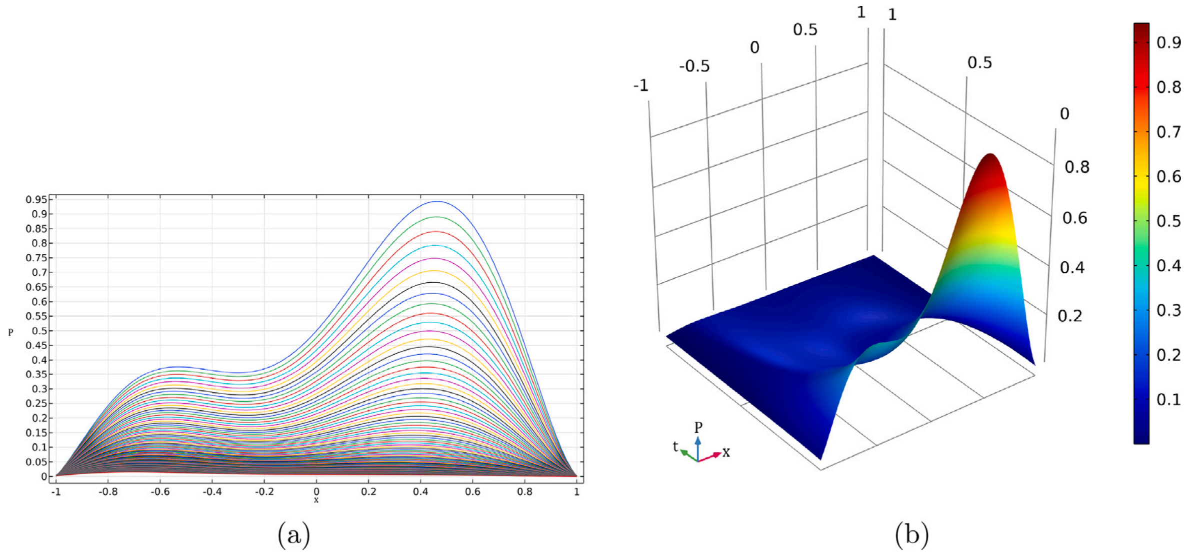

Fig. 2. Solution for Example 4.2, (a) profiles and (b) solution surface for $0 \le t \le 1$.

Table 7
Results for Example 4.2. True values are $(S_0, S_1, S_2) = (1, -2, 0.8)$.

N_x	N_t	u_{deg}	ϵ	Δ	S_0	S_1	S_2
20	10	8	0.00	0.0068456	0.9617454	−2.0042190	0.8510397
20	10	10	0.00	0.0012286	0.9586120	−2.0105501	0.8804124
50	25	8	0.00	0.0045729	0.9530788	−2.0088078	0.8881269
50	25	10	0.00	0.0008383	0.9482695	−2.0115794	0.9097584
100	50	8	0.00	0.0041239	0.9510689	−2.0100785	0.8973780
100	50	10	0.00	0.0007860	0.9483386	−2.0116352	0.9096776
20	10	8	0.01	0.0079357	1.0039053	−2.0249152	0.7235289
20	10	10	0.01	0.0031682	0.9457433	−2.0137754	0.9298703
50	25	8	0.01	0.0054294	0.9686385	−1.9884721	0.8390496
50	25	10	0.01	0.0022734	0.9423102	−1.9752634	0.9260981
100	50	8	0.01	0.0045695	0.9812885	−1.9972603	0.8085704
100	50	10	0.01	0.0021155	0.9745145	−1.9891479	0.8272391
100	50	8	0.10	0.0150653	1.0456401	−1.9884490	0.6865258

CRediT authorship contribution statement

M.I. Berenguer: Conceptualization, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **D. Gámez:** Conceptualization, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **H. Kunze:** Conceptualization, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **D. La Torre:** Conceptualization, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **M. Ruiz Galán:** Conceptualization, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

Research partially supported by Junta de Andalucía, Spain, Project FQM359 "Convex and Numerical Analysis" and by "María de Maeztu, Spain" Excellence Unit IMAG, reference CEX2020-001105-M, funded by MCIN/AEI/10.13039/501100011033/. Funding for open access charge: Universidad de Granada / CBUA.

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