

Numerical algorithms to solve inverse problems for parabolic equations

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Abstract. This paper presents and analyzes robust numerical algorithms for solving inverse problems for parabolic equations, specifically focusing on the determination of an unknown time-dependent source function from an integral flux condition. The study is motivated by mathematical models based on Navier-Stokes equations, particularly those exhibiting Poiseuille-type solutions. We employ a variational approach, formulating the inverse problem as the minimization of a Tikhonov regularization cost functional. Discrete approximation schemes are rigorously derived using finite volume methods in space and both backward Euler and Crank-Nicolson schemes in time. A key contribution of this work is the strict justification of the gradient formula for the cost functional by deriving the adjoint problem directly from the fully discrete scheme, rather than discretizing the continuous adjoint problem. This methodology is extended to problems involving fractional powers of elliptic operators and two-dimensional domains. Numerical experiments are conducted to compare the efficiency of Gradient Descent and Conjugate Gradient methods. The results demonstrate that the Conjugate Gradient method significantly outperforms standard gradient descent, maintaining high accuracy and convergence rates even with the inclusion of regularization terms and complex diffusion operators.

Keywords: inverse problems; parabolic partial differential equations; Tikhonov regularization; adjoint problem; gradient-based optimization.

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1 Problem formulation

Inverse problems for parabolic partial differential equations arise in numerous scientific and engineering applications, including heat conduction, contaminant transport, groundwater flow, and cardiovascular modeling. Such problems are often ill-posed in the sense of Hadamard, meaning that small perturbations in measured data can lead to large deviations in the recovered parameters. Consequently, the development of stable, efficient, and accurate numerical algorithms is essential for reliable solutions in practice.

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This work is motivated by inverse problems emerging from fluid dynamics, particularly those derived from the Navier–Stokes equations. In many practical scenarios, such as flow in pipes, channels, or porous media, the velocity field admits a Poiseuille-type structure [16], which simplifies the governing system to a parabolic equation with an unknown time-dependent source term. Recovering this source from indirect measurements, such as integrated flux, constitutes a classical but challenging inverse problem.

Following [14], we begin by considering an initial-boundary value problem for the incompressible Navier–Stokes equations in an infinite straight pipe $\Pi = \{\vec{x} = (x_1, x_2) \in \mathbb{R}^2 : 0 \leq x_1 \leq 1, -\infty < x_2 < \infty\}$:

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} - \nu \sum_{j=1}^2 \frac{\partial^2 \mathbf{u}}{\partial x_j^2} + (\mathbf{u}(\vec{x}, t) \cdot \nabla) \mathbf{u}(\vec{x}, t) + \nabla p(\vec{x}, t) &= 0, \\ \nabla \cdot \mathbf{u}(\vec{x}, t) &= 0, \end{aligned} \quad (1.1)$$

with no-slip boundary conditions $\mathbf{u}(\vec{x}, t)|_{\Pi} = 0$ and initial condition $\mathbf{u}(\vec{x}, 0) = \mathbf{u}_0(\vec{x})$. For Poiseuille-type solutions of the form

$$\mathbf{u}(\vec{x}, t) = (0, U_2(x_1, t)), \quad p(\vec{x}, t) = -q(t)x_2 + p_0(t),$$

with an arbitrary function $p_0(t)$, the system (1.1) reduces to a one-dimensional parabolic equation for $U_2(x_1, t)$:

$$\frac{\partial U_2}{\partial t} - \nu \frac{\partial^2 U_2}{\partial x_1^2} = -q(t),$$

where $q(t)$ represents an unknown pressure gradient.

Motivated by this setting, we study a more general inverse parabolic problem. Let $\Omega = (0, l)$ be a bounded interval, $T > 0$ be a final time, and define $Q = \Omega \times (0, T]$, $S = \partial\Omega \times (0, T]$. We seek a function $u(x, t)$ satisfying the 1D nonstationary diffusion equation:

$$\begin{aligned} \frac{\partial u}{\partial t} - \nu \frac{\partial^2 u}{\partial x^2} &= g_0(x, t) + f(t)g_1(x), \quad (x, t) \in Q, \\ u|_S &= u_S, \\ u(x, 0) &= u_0(x), \quad x \in \bar{\Omega}, \end{aligned} \quad (1.2)$$

with given boundary and initial conditions, where g_0, g_1 are known functions, ν is a given diffusion coefficient, and $f(t)$ is an unknown time-dependent source term to be determined from the additional integral flux condition

$$Lu := \int_{\Omega} \omega(x)u(x, t)dx = \tilde{h}(t), \quad (1.3)$$

where ω is a prescribed weight function and \tilde{h} is given measurement data.

Thus, we solve an inverse problem: for given initial and boundary conditions u_0, u_S and functions $g_0, g_1, \tilde{h}(t), \omega$ we must find a pair of functions

$(u(x, t), f(t))$ by solving the parabolic problem (1.2) and additional conjugation condition (1.3).

In this paper, we also consider a modified problem, where the classical diffusion operator is replaced by the fractional power elliptic operator [2]

$$\begin{aligned} \frac{\partial u}{\partial t} + \nu \mathcal{A}^p u &= g_0(x, t) + f(t)g_1(x), \quad (x, t) \in Q, \\ \mathcal{A}^p u &:= \left(-\frac{\partial^2 u}{\partial x^2} \right)^p, \quad 0 < p < 1. \end{aligned} \quad (1.4)$$

This extension is motivated by models of anomalous diffusion in heterogeneous or porous media [13].

There are different definitions of the fractional powers \mathcal{A}^p . We use the spectral definition. Let us denote the eigenpairs of the elliptic operator $\mathcal{A}u$ by (φ_j, λ_j) . Eigenvectors φ_j provide an orthonormal basis for $L_2([0, l])$:

$$v(x) = \sum_{j=1}^{\infty} c_j \varphi_j(x), \quad -\frac{\partial^2 \varphi_j}{\partial x^2} = \lambda_j \varphi_j.$$

Then, the spectral fractional powers \mathcal{A}^p for $0 < p < 1$ are defined by eigenvectors expansions:

$$\mathcal{A}^p v = \sum_{j=1}^{\infty} c_j \lambda_j^p \varphi_j(x).$$

There are two popular approaches how to solve such inverse parabolic problems. The first is to derive an equivalent integral equation for the unknown source. For example, one can eliminate the state u to obtain a Volterra integral equation of the first kind for $f(t)$. This approach was investigated in detail in [1]. Numerical schemes for the Volterra integral equations are also investigated in many papers and books, see e.g. [7]. Such equations are typically ill-posed. The standard method for regularization of the ill-posed first kind integral Volterra equations is based on a reduction (approximation) of this equation by the well-posed second kind integral Volterra equation [15, 16].

The second approach treats the problem in a variational PDE framework. In this approach, one defines a Tikhonov regularization functional measuring the discrepancy between the computed flux and the data, and minimizes it with respect to f :

$$J_{\alpha}(f) := \frac{1}{2} \int_0^T (Lu(f) - \tilde{h}(t))^2 dt + \frac{\alpha}{2} \int_0^T f^2(t) dt, \quad (1.5)$$

where $u(f)$ denotes the solution of the direct problem corresponding to a given source $f(t)$ and $\alpha \geq 0$ is the regularization parameter. The minimizing source f balances the fit to measurement data \tilde{h} with the penalty $\alpha \|f\|_{L^2(0, T)}^2$ (see [8] for an introduction to Tikhonov regularization, and [10, 11] for applications to inverse source problems).

We also briefly note here another highly promising general approach that has gained significant popularity in recent years for solving inverse problems. It is based on applications of artificial neural networks, particularly Physics-Informed Neural Networks, which excel at solving inverse problems involving nonlinear partial differential equations [3, 4]. A key advantage of this method lies in its inherent structure, which naturally incorporates variational formulations and minimization algorithms directly into the computational schemes [17].

While Volterra integral equation methods are a standard approach for 1D problems, they do not easily generalize to multidimensional or non-local problems. Therefore, this paper utilizes a variational PDE formulation based on Tikhonov regularization. A key contribution of this work is the rigorous derivation of the discrete adjoint problem. Unlike approaches that discretize the continuous adjoint, we derive the adjoint directly from the fully discrete scheme (using backward Euler and Crank-Nicolson), ensuring the gradient computed is exact for the discrete optimization process.

In this work, we develop and analyze robust and efficient numerical schemes for solving the inverse problem (1.2)–(1.3) (and its fractional variant) in one and two spatial dimensions. In particular, we discretize the state equation and the Tikhonov functional to derive gradient-based optimization algorithms for the source term $f(t)$. We compare the computational cost of different time-stepping and optimization schemes. We emphasize the theoretical formulation and computational methodology; rigorous error estimates and real-world applications are beyond the scope of this paper and will be addressed in future work.

The rest of the paper is organized in the following way. In Section 2, the discretization of the space operators is done. The standard finite volume approximation is used on the uniform space mesh. As a result a semidiscrete model of the inverse parabolic problem is defined. The Tikhonov regularization cost functional (1.5) is also discretized by using the trapezoidal summation formula. In Section 3, a general technique for derivation of the gradient formula for the cost functional $J_{\alpha,h}(f)$ is presented. This information makes a basis for variational minimization algorithms. Inverse problem for ODE is solved in Section 4. The main aim is to show how the general template with an important definition of the adjoint problem arises in the analysis of the direct gradient calculation algorithm. In Section 5, a fully discrete backward Euler scheme is constructed and analyzed. Its main purpose is to strictly justify the definition of the adjoint problem in this algorithm for an inverse discrete parabolic problem. A similar analysis is done for the Crank-Nicolson discrete scheme in Section 6. In Section 7, the fully discrete Crank-Nicolson scheme is constructed and the gradient formula is derived for the fractional power discrete elliptic operator. These schemes can be generalized also for two-dimensional inverse parabolic problems. This analysis is done in Section 8. In order to solve variational minimization problems for determination of unknown source function gradient descent type algorithms are used. In Section 9, first a simple gradient descent method is applied and next the Conjugate Gradient Method is used to solve the formulated minimization problems. A comparison of both techniques is

done. Results of numerical experiments are presented in Section 10. Some final conclusions are done in Section 11.

2 Discrete approximation

In this section we construct discrete in space operators. A uniform discrete grid in space is defined (here $l = 1$):

$$\omega_h = \{x_j : x_j = jh, j = 1, \dots, J-1\}, \quad x_J = 1, \quad \bar{\omega}_h = \omega_h \cup \{0, 1\}.$$

Semi-discrete functions $V(x_j, t) = (v_0, v_1, \dots, v_J)$ are approximations of $u(x_j, t)$, where $v_j = V(x_j, t)$, $j = 0, \dots, J$.

In the following analysis it is sufficient to take homogeneous boundary conditions $v_0 = 0$, $v_J = 0$. For any V we define the discrete diffusion operator

$$A_h V = -\frac{v_{j+1} - 2v_j + v_{j-1}}{h^2}, \quad j = 1, \dots, J-1.$$

The eigenvectors $V_k = (v_{k1}, \dots, v_{k, J-1})$ and eigenvalues λ_k of A_h are well known [12]:

$$A_h V_k = \lambda_k V_k, \quad k = 1, \dots, J-1.$$

$$v_{kj} = \sqrt{2} \sin(\pi k x_j), \quad \lambda_k = \frac{4}{h^2} \sin^2\left(\frac{\pi k h}{2}\right).$$

Let us define a scalar product and L_2 norm for the discrete functions, which satisfy homogeneous boundary conditions

$$(V, W)_h = \sum_{j=1}^{J-1} v_j w_j h, \quad \|V\| = (V, V)_h^{1/2}.$$

The set of eigenvectors $\{V_k\}$, $k = 1, \dots, J-1$ make an orthonormal and complete basis in L_2 space.

The semi-discrete approximation of problem (1.2)–(1.3) is given by

$$\begin{aligned} \frac{\partial V}{\partial t} + \nu A_h V &= g_0(x_j, t) + f(t)g_1(x_j), \quad x_j \in \omega_h, \\ v_0(t) &= 0, \quad v_J(t) = 0, \\ v(x_j, 0) &= u_0(x_j), \quad j = 0, \dots, J, \end{aligned} \tag{2.1}$$

and the discrete flux condition is defined as

$$L_h V := \sum_{j=1}^{J-1} \omega_j v_j h = \tilde{h}(t).$$

We obtain the one-dimensional semi-discrete nonstationary parabolic PDE problem (2.1). It is an inverse problem and we are interested to analyze the conditioning of this formulation. This aim is based on the well known fact, that

inverse problems can be ill-posed. In the case of ill-posed problems the main aim is to apply the efficient and accurate regularization techniques in order to construct efficient and robust discrete schemes.

We define the discrete regularization Tikhonov functional

$$J_{\alpha,h}(f) := \frac{1}{2} \int_0^T (L_h V(f) - \tilde{h}(t))^2 dt + \frac{\alpha}{2} \int_0^T f^2(t) dt.$$

We solve the following discrete least square problem

$$J_{\alpha,h}(f_*) = \min_{f \in F} J_{\alpha,h}(f),$$

where F is a set of admissible time-dependent sources.

3 Gradient formula for the cost functional $J_{\alpha,h}(f)$

Next we present a short (and quite standard) derivation of the gradient formula. Consider the first variations

$$\delta J_{\alpha,h}(f) := J_{\alpha,h}(f + \delta f) - J_{\alpha,h}(f), \quad \delta V(t; \delta f) := V(t; f + \delta f) - V(t; f), \quad \delta f \in F.$$

We get

$$\begin{aligned} \delta J_{\alpha,h}(f) &= \frac{1}{2} \int_0^T \left[\left(L_h V(t; f + \delta f) - \tilde{h}(t) \right)^2 - \left(L_h V(t; f) - \tilde{h}(t) \right)^2 \right] dt \\ &\quad + \frac{\alpha}{2} \int_0^T \left[(f(t) + \delta f(t))^2 - f(t)^2 \right] dt \\ &= \int_0^T \left(L_h V(t; f) - \tilde{h}(t) \right) L_h \delta V(t; \delta f) dt + \int_0^T (L_h \delta V(t; \delta f))^2 dt \\ &\quad + \alpha \int_0^T f(t) \delta f(t) dt + \alpha \int_0^T (\delta f(t))^2 dt. \end{aligned}$$

We write the first variation of Equation (2.1) as

$$\frac{\partial \delta V}{\partial t} + \nu A_h \delta V = \delta f(t) g_1(x_j), \quad x_j \in \omega_h. \quad (3.1)$$

We multiply (3.1) by function $\Phi(t)$ and integrate the obtained equation:

$$\begin{aligned} I &= \int_0^T \left([\delta V_t(t; \delta f) + A_h \delta V(t; \delta f)], \Phi(t) \right)_h dt \\ &= \int_0^T (g_1 \delta f(t), \Phi(t))_h dt. \end{aligned} \quad (3.2)$$

Integrating and summing by parts and taking into account initial and boundary conditions

$$\begin{aligned} \delta V(x, 0; \delta f) &= 0, \quad \delta V(0, t; \delta f) = 0, \quad \delta V(1, t; \delta f) = 0, \\ \Phi(x, T) &= 0, \quad \Phi(0, t) = 0, \quad \Phi(1, t) = 0, \end{aligned}$$

we obtain the left-side part of Equation (3.2) in the form

$$I = \int_0^T (-\Phi_t(t) + A_h \Phi(t), \delta V(t; \delta f))_h dt.$$

Neglecting terms of order $\mathcal{O}(\|\delta f\|^2)$, the first variation of the functional is given by

$$\begin{aligned} \delta J_{\alpha,h}(f) &= \int_0^T \left(L_h V(t; f) - \tilde{h}(t) \right) L_h \delta V(t; \delta f) dt + \alpha \int_0^T f(t) \delta f(t) dt \\ &= \int_0^T \sum_{j=1}^{J-1} \omega_j \left(L_h V(t; f) - \tilde{h}(t) \right) \delta v_j(t; \delta f) h dt + \alpha \int_0^T f(t) \delta f(t) dt. \end{aligned}$$

Then, we solve the following adjoint problem

$$\begin{cases} -\varphi_{jt}(t) + A_h \Phi(t) = \omega_j \left(L_h V(t; f) - \tilde{h}(t) \right), & j = 1, \dots, J-1, \\ \varphi_j(T) = 0, \\ \varphi_0(t) = 0, \quad \varphi_J(t) = 0, \quad 0 \leq t \leq T \end{cases}$$

and get that

$$\int_0^T \sum_{j=1}^{J-1} \omega_j \left(L_h V(t; f) - \tilde{h}(t) \right) \delta v_j(t; \delta f) h dt = \int_0^T (g_1, \Phi(t))_h \delta f(t) dt. \quad (3.3)$$

It follows from (3.2) and (3.3) that the gradient of the functional $J_\alpha(f)$ can be calculated as

$$J'_{\alpha,h}(f) = (g_1, \Phi(t))_h + \alpha f(t).$$

4 Inverse problem for ODE

We restrict to the uniform discrete grid in time

$$\omega_\tau = \{t^n : t^n = n\tau, n = 0, \dots, N\}, \quad t^N = T.$$

In this section, our aim is to construct gradient formula for the minimization algorithm based on the cost functional in the case of discrete approximation of the inverse ODE problem

$$\frac{U^n - U^{n-1}}{\tau} = g_0^n + f^n g_1, \quad U^0 = 0. \quad (4.1)$$

We find $U = \{U^n\}$, $f = \{f^n\}$, $n = 1, \dots, N$ by minimizing the functional

$$J_{\alpha,\tau}(f) = \frac{1}{2} \sum_{n=1}^N (U^n - H^n)^2 \tau + \frac{\alpha}{2} \sum_{n=1}^N (f^n)^2 \tau.$$

The gradient $J'_{\alpha,\tau}(f)$ is defined as

$$J'_{\alpha,\tau}(f) = \left\{ \frac{\partial J_{\alpha,\tau}(f)}{\partial f^n}, n = 1, \dots, N \right\}$$

and it can be calculated directly if explicit formula of functional $J_{\alpha}(f)$ with respect to f is known. Here we want to compare this result with the approach given above and based on solving adjoint/dual problems.

It is easy to write the solution of (4.1) in the explicit form

$$U^n = U^0 + \tau \sum_{k=1}^n \left(g_0^k + f^k g_1 \right), \quad n = 1, \dots, N.$$

Then, the functional $J_{\alpha,\tau}$ is presented in the following explicit form

$$J_{\alpha,\tau}(f) = \frac{1}{2} \tau \sum_{n=1}^N \left[U^0 + \tau \sum_{k=1}^n \left(g_0^k + f^k g_1 \right) - H^n \right]^2 + \frac{\alpha}{2} \tau \sum_{n=1}^N (f^n)^2.$$

The gradient follows from this equality

$$\frac{\partial J_{\alpha,\tau}(f)}{\partial f^r} = \tau \alpha f^r + \tau \sum_{n=r}^N g_1 \tau (U^n - H^n).$$

We can write it in a form well fitted for generalizations. The following adjoint (backward in time) problem is solved

$$-\frac{V^n - V^{n-1}}{\tau} = \tau (U^n - H^n), \quad V^N = 0, \quad n = N, \dots, 1.$$

Then, we write the gradient in a form analogous to one derived for the semidiscrete parabolic problem

$$\frac{\partial J_{\alpha}(f)}{\partial f^r} = \tau (\alpha f^r + g_1 V^r).$$

Thus, such a technique based on adjoint problems is a very convenient template for computation of the gradient of regularization functional.

5 The backward Euler discrete scheme

The full discrete approximation of problem (1.2)–(1.3) by using the Backward Euler (BE) scheme is defined as

$$\begin{aligned} \frac{V^n - V^{n-1}}{\tau} + \nu A_h V^n &= g_0(x_j, t^n) + f(t^n) g_1(x_j), \quad x_j \in \omega_h, \\ v_0^n &= 0, \quad v_J^n = 0, \\ v^0(x_j) &= u_0(x_j), \quad j = 0, \dots, J, \end{aligned} \tag{5.1}$$

and the discrete flux condition is defined as

$$L_h V^n := \sum_{j=1}^{J-1} \omega_j v_j^n h = \tilde{h}(t^n).$$

Vectors $V^n = (v_1^n, v_2^n, \dots, v_{J-1}^n)$ are approximations of the solution $u(x_j, t^n)$ of the differential problem (1.2)–(1.3).

We find $V = \{V^n\}$, $f = \{f^n\}$, $n = 1, \dots, N$ by minimizing the discrete regularization cost functional

$$J_{\alpha, h}(f) = \frac{1}{2} \sum_{n=1}^N (L_h V^n - \tilde{h}^n)^2 \tau + \frac{\alpha}{2} \sum_{n=1}^N (f^n)^2 \tau.$$

In order to define the gradient of this functional we have two possibilities.

1. The first approach is more general but not fully justified: we discretize the adjoint problem solved for the semidiscrete scheme. The BE scheme can be used to solve the adjoint problem, also.

2. In the second approach the discrete adjoint problem of the BE scheme is derived by using the same technique as applied for the semidiscrete problem. By using this approach we strictly justify the derived gradient formula.

Here we restrict to the second technique. The first order variation of the discrete scheme equation (5.1) and the cost functional are defined as

$$\begin{aligned} \frac{\delta V^n - \delta V^{n-1}}{\tau} + \nu A_h \delta V^n &= g_1(x_j) \delta f^n, \quad x_j \in \omega_h, \\ \delta J_{\alpha, h}(f) &= \sum_{n=1}^N \left[\sum_{j=1}^{J-1} \omega_j (L_h V^n - \tilde{h}^n) \delta v_j^n (\delta f^n) h \right] \tau + \alpha \sum_{n=1}^N (f^n) \delta f^n \tau. \end{aligned} \quad (5.2)$$

Next, we multiply the discrete scheme Equation (5.2) by function φ_j^{n-1} and apply the summation by parts formula:

$$\begin{aligned} &\sum_{n=1}^N \left[\left(\sum_{j=1}^{J-1} \frac{\delta v_j^n - \delta v_j^{n-1}}{\tau} - \nu (\delta V^n (\delta f^n))_{\bar{x}x} \right) \varphi_j^{n-1} h \right] \tau \\ &= \sum_{n=1}^N \left[\left(\sum_{j=1}^{J-1} -\frac{\varphi_j^n - \varphi_j^{n-1}}{\tau} - \nu (\Phi^{n-1})_{\bar{x}x} \right) \delta v_j^n (\delta f^n) h \right] \tau, \end{aligned}$$

here we use a simple equality for any discrete functions u^n, φ^n such that $u^0 = 0$, $\varphi^N = 0$:

$$\sum_{n=1}^N (u^n - u^{n-1}) \varphi^{n-1} = \sum_{n=1}^N [-u^n (\varphi^n - \varphi^{n-1})].$$

Then, we solve the adjoint (backward in time) problem

$$\begin{aligned} -\frac{\varphi_j^n - \varphi_j^{n-1}}{\tau} + \nu A_h \Phi^{n-1} &= \omega_j (L_h V^n - \tilde{h}^n), \quad x_j \in \omega_h, \\ \varphi_0^{n-1} &= 0, \quad \varphi_J^{n-1} = 0, \quad n = 1, \dots, N, \\ \varphi_j^N &= 0, \quad j = 0, \dots, J. \end{aligned} \quad (5.3)$$

It follows from (5.3) that the gradient of the cost functional $J_{\alpha,h}$ can be calculated as

$$J'_{\alpha,h}(f)(t^n) = (g_1, \Phi^n)_h + \alpha f^n.$$

6 The Crank-Nicolson discrete scheme

The fully discrete approximation of problem (1.2)-(1.3) is derived by using the Crank-Nicolson (CN) scheme and is defined as

$$\begin{aligned} \frac{V^n - V^{n-1}}{\tau} + \nu A_h V^{n-\frac{1}{2}} &= g_0(x_j, t^{n-\frac{1}{2}}) + f^{n-\frac{1}{2}} g_1(x_j), \quad x_j \in \omega_h, \\ v_0^n &= 0, \quad v_J^n = 0, \\ v^0(x_j) &= u_0(x_j), \quad j = 0, \dots, J, \end{aligned} \quad (6.1)$$

where we use the notation

$$V^{n-\frac{1}{2}} = \frac{1}{2} (V^n + V^{n-1}), \quad f^{n-\frac{1}{2}} = f(t^{n-\frac{1}{2}}).$$

The discrete flux condition is approximated as

$$L_h V^{n-\frac{1}{2}} := \sum_{j=1}^{J-1} \omega_j v_j^{n-\frac{1}{2}} h = \tilde{h}^{n-\frac{1}{2}}, \quad \tilde{h}^{n-\frac{1}{2}} = \frac{1}{2} (\tilde{h}^n + \tilde{h}^{n-1}).$$

We find $V = \{V^n\}$, $f = \{f^{n-\frac{1}{2}}\}$, $n = 1, \dots, N$ by minimizing the discrete Tikhonov functional

$$J_{\alpha,h}(f) = \frac{1}{2} \sum_{n=1}^N (L_h V^{n-\frac{1}{2}} - \tilde{h}^{n-\frac{1}{2}})^2 \tau + \frac{\alpha}{2} \sum_{n=1}^N (f^{n-\frac{1}{2}})^2 \tau. \quad (6.2)$$

The first order variation of the discrete equation (6.1) and the cost functional (6.2) are defined as

$$\frac{\delta V^n - \delta V^{n-1}}{\tau} + \nu A_h \delta V^{n-\frac{1}{2}} = \delta f^{n-\frac{1}{2}} g_1(x_j), \quad x_j \in \omega_h, \quad (6.3)$$

$$\delta J_{\alpha,h}(f) = \sum_{n=1}^N \left[\sum_{j=1}^{J-1} \omega_j (L_h V^{n-\frac{1}{2}} - \tilde{h}^{n-\frac{1}{2}}) \delta v_j^{n-\frac{1}{2}} h \right] \tau + \alpha \sum_{n=1}^N (f^{n-\frac{1}{2}}) \delta f^{n-\frac{1}{2}} \tau.$$

We multiply the discrete Equation (6.3) by function $\varphi_j^{n-\frac{1}{2}}$ and apply the formula of summation by parts:

$$\begin{aligned} & \sum_{n=1}^N \left[\left(\sum_{j=1}^{J-1} \frac{\delta v_j^n - \delta v_j^{n-1}}{\tau} - \nu (\delta V^{n-\frac{1}{2}} (\delta f^{n-\frac{1}{2}}))_{\bar{x}x} \right) \varphi_j^{n-\frac{1}{2}} h \right] \tau \\ &= \sum_{n=1}^N \left[\left(\sum_{j=1}^{J-1} -\frac{\varphi_j^n - \varphi_j^{n-1}}{\tau} - \nu (\Phi^{n-\frac{1}{2}})_{\bar{x}x} \right) \delta v_j^{n-\frac{1}{2}} (\delta f^{n-\frac{1}{2}}) h \right] \tau. \end{aligned}$$

In order to prove the equality

$$\sum_{n=1}^N (u^n - u^{n-1})(\varphi^n + \varphi^{n-1}) = - \sum_{n=1}^N (u^n + u^{n-1})(\varphi^n - \varphi^{n-1}),$$

we use two simple equalities valid for any discrete functions u^n, φ^n such that $u^0 = 0, \varphi^N = 0$

$$\begin{aligned} \sum_{n=1}^N (u^n - u^{n-1})\varphi^{n-1} &= \sum_{n=1}^N [-u^n(\varphi^n - \varphi^{n-1})], \\ \sum_{n=1}^N (u^n - u^{n-1})\varphi^n &= \sum_{n=1}^N [-u^{n-1}(\varphi^n - \varphi^{n-1})] \end{aligned}$$

and add these two equalities.

Then we solve the adjoint problem

$$\begin{aligned} -\frac{\varphi_j^n - \varphi_j^{n-1}}{\tau} + \nu A_h \Phi^{n-\frac{1}{2}} &= \omega_j (L_h V^{n-\frac{1}{2}} - \tilde{h}^{n-\frac{1}{2}}), \quad x_j \in \omega_h, \\ \varphi_0^{n-1} &= 0, \quad \varphi_J^{n-1} = 0, \quad n = 1, \dots, N, \\ \varphi_j^N &= 0, \quad j = 0, \dots, J. \end{aligned}$$

It follows from (6.3) that the gradient of the regularization cost functional $J_{\alpha, h}$ can be calculated as

$$J'_{\alpha, h}(f) = \left(g_1, \Phi^{n-\frac{1}{2}} \right)_h + \alpha f^{n-\frac{1}{2}}, \quad n = 1, \dots, N.$$

7 The Crank-Nicolson scheme for the fractional elliptic operator

In this section, we apply the results obtained in the previous section also for the inverse parabolic type problem when the diffusion operator is changed by the fractional power Laplace operator. We approximate the problem (1.4) by the fully discrete scheme

$$\begin{aligned} \frac{V^n - V^{n-1}}{\tau} + \nu \mathcal{A}_h^p V^{n-\frac{1}{2}} &= g_0(x_j, t^{n-\frac{1}{2}}) + f^{n-\frac{1}{2}} g_1(x_j), \quad x_j \in \omega_h, \quad (7.1) \\ v_0^n &= 0, \quad v_J^n = 0, \\ v^0(x_j) &= u_0(x_j), \quad j = 0, \dots, J. \end{aligned}$$

This discrete problem is solved efficiently by using the efficient discrete FFT algorithm [6].

A simple analysis shows that \mathcal{A}_h^p is a symmetric operator, therefore the adjoint problem for discrete functions $\phi^{n-\frac{1}{2}}$ is defined as

$$\begin{aligned} -\frac{\varphi_j^n - \varphi_j^{n-1}}{\tau} + \nu \mathcal{A}_h^p \Phi^{n-\frac{1}{2}} &= \omega_j (L_h V^{n-\frac{1}{2}} - \tilde{h}^{n-\frac{1}{2}}), \quad x_j \in \omega_h, \\ \varphi_0^{n-1} &= 0, \quad \varphi_J^{n-1} = 0, \quad n = 1, \dots, N, \\ \varphi_j^N &= 0, \quad j = 0, \dots, J \end{aligned} \quad (7.2)$$

and the gradient of the cost functional $J_{\alpha,h}$ can be computed by the same formula as for the classical Laplace operator

$$J'_{\alpha,h}(f) = \left(g_1, \Phi^{n-\frac{1}{2}} \right)_h + \alpha f^{n-\frac{1}{2}}, \quad n = 1, \dots, N,$$

only function Φ is obtained by solving the modified adjoint problem (7.2).

8 Two dimensional inverse parabolic problem

Let Ω be a bounded domain $(0, 1) \times (0, 1)$ and T be a given positive number. Denote $Q := \Omega \times (0, T]$, and $S := \partial\Omega \times (0, T]$. Let us consider an initial-boundary value problem for 2D parabolic equation

$$\begin{aligned} \frac{\partial u}{\partial t} - \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) &= g_0(x, y, t) + f(t)g_1(x, y), \quad (x, y, t) \in Q, \\ u|_S &= 0, \\ u(x, y, 0) &= u_0(x, y), \quad (x, y) \in \bar{\Omega}, \end{aligned} \quad (8.1)$$

where g_0, g_1 are given functions and ν is a given diffusion coefficient.

The problem consists of determining the solution $u(x, y, t)$ of (8.1) and finding the right hand side source function $f(t)$ from the additional flux condition

$$Lu := \int \int_{\Omega} \omega(x, y) u(x, y, t) dx = \tilde{h}(t).$$

Define the regularization cost functional

$$J_{\alpha}(f) := \frac{1}{2} \int_0^T (Lu(f) - \tilde{h}(t))^2 dt + \frac{\alpha}{2} \int_0^T f^2(t) dt.$$

In the following we restrict to the definition of the Crank-Nicolson discrete scheme. First we approximate the 2D domain Ω by the uniform mesh $\omega_{h,2D}$

$$\omega_{h,2D} = \{(x_i, y_j) : x_i = ih, y_j = jh, 1 \leq i, j \leq J-1\}.$$

The boundary points of $S_h := \partial\omega_{h,2D}$ are defined in a standard way. The discrete functions are denoted as $v_{ij} := v(x_i, y_j)$. Then, the problem (8.1) is

approximated by the Crank-Nicolson scheme as

$$\begin{aligned} \frac{V^n - V^{n-1}}{\tau} + \nu A_{h,2D} V^{n-\frac{1}{2}} &= g_0(x_i, y_j, t^{n-\frac{1}{2}}) + f^{n-\frac{1}{2}} g_1(x_i, y_j), \quad (8.2) \\ (x_i, y_j) &\in \omega_{h,2D}, \\ v_{S_h}^n &= 0, \quad v^0(x_i, y_j) = u_0(x_i, y_j), \quad 0 \leq i, j \leq J, \end{aligned}$$

where the discrete Laplace operator $A_{h,2D}$ is defined as

$$A_{h,2D} V := - \left(\frac{v_{i+1,j} - 2v_{ij} + v_{i-1,j}}{h^2} + \frac{v_{i,j+1} - 2v_{ij} + v_{i,j-1}}{h^2} \right).$$

The discrete flux condition is approximated as

$$L_{h,2D} V^{n-\frac{1}{2}} := \sum_{i=1}^{J-1} \sum_{j=1}^{J-1} \omega_{ij} v_{ij}^{n-\frac{1}{2}} h^2 = \tilde{h}^{n-\frac{1}{2}}, \quad \tilde{h}^{n-\frac{1}{2}} = \frac{1}{2} (\tilde{h}^n + \tilde{h}^{n-1}).$$

The variational problem is defined as a minimization of the cost functional with respect to the source function f :

$$J_{\alpha,h,2D}(f) = \frac{1}{2} \sum_{n=1}^N (L_{h,2D} V^{n-\frac{1}{2}} - \tilde{h}^{n-\frac{1}{2}})^2 \tau + \frac{\alpha}{2} \sum_{n=1}^N (f^{n-\frac{1}{2}})^2 \tau.$$

We solve the adjoint problem, which is derived applying the same technique as for 1D case:

$$\begin{aligned} - \frac{\varphi_{ij}^n - \varphi_{ij}^{n-1}}{\tau} + \nu A_{h,2D} \varPhi^{n-\frac{1}{2}} &= \omega_{ij} (L_h V^{n-\frac{1}{2}} - \tilde{h}^{n-\frac{1}{2}}), \quad x_{ij} \in \omega_h, \quad (8.3) \\ \varphi_{S_h}^{n-1} &= 0, \quad n = 1, \dots, N, \quad \varphi_{ij}^N = 0, \quad 0 \leq i, j \leq J. \end{aligned}$$

The gradient of the cost functional $J_{\alpha,h,2D}$ can be calculated as

$$J'_{\alpha,h,2D}(f) = \left(g_1, \varPhi^{n-\frac{1}{2}} \right)_h + \alpha f^{n-\frac{1}{2}}, \quad n = 1, \dots, N,$$

where the scalar product is defined as

$$(U, V)_h = \sum_{i=1}^{J-1} \sum_{j=1}^{J-1} u_{ij} v_{ij} h^2.$$

Both discrete problems (8.2) and (8.3) are solved efficiently by using discrete FFT algorithm [6].

Remark 1. We note that an interesting algorithm is obtained by using splitting techniques to solve 2D direct and adjoint problems. For example we solve the 2D problems applying the Peaceman–Rachford ADI scheme for the direct parabolic problem and its modification for the dual problem [12]. This method of calculation of the gradient of 2D cost function is based on the second approach suggested in Section 5. Still such minimization algorithm is not strongly justified because it is not shown that the adjoint problem strictly follows from the direct problem. This analysis is not done in the present paper and will be considered in a separate paper.

9 Gradient descent type methods

A general technique to find a minimum point for the cost functional $J_{\alpha,h}$ is based on standard gradient descent method, when a new approximation of the discrete source function f is computed by applying the formula [12]

$$f^{s+1,n} = f^{s,n} - \beta^{(s)} J'(f^s), \quad n = 1, \dots, N,$$

where s is the iteration number and $\beta^{(s)} > 0$ is an adjustable step length of iteration parameter.

In different realizations of this general scheme the negative gradient direction can be changed and modified directions, such as conjugated gradient directions can be used. We will give more information on this topic below.

A template of the Gradient Descent algorithm, which is used in this paper is defined as follows.

1. Initialization. Set the iteration counter $s = 0$ and choose the initial iteration $f^{(0)}$, usually we set $f^{(0)} = 0$.

Compute the initial value of the cost functional $\tilde{J} = J_{\alpha,h}(f^{(0)})$.

2. Descent direction. Calculate the new descent direction $q^{(s)}$. In the simple version of the gradient descent method we use the negative gradient of $J_{\alpha,h}$:

$$q^{(s)} := -J'_{\alpha,h}(f^{(s)}).$$

3. New approximation. The adjustable step length parameter $\beta^{(s)}$ is computed by solving a line search in the direction $q^{(s)}$ until it reaches the local minimum point

$$\beta^{(s)} := \arg \min_{\beta} J_{\alpha,h} \left(f^{(s)} + \beta^{(s)} q^{(s)} \right).$$

We use the following search algorithm:

```

 $ok = 1, \beta = \beta_0$ 
while ( $ok == 1$ ){
   $f = f^{(s)} + \beta q^{(s)}, \tilde{J}_1 = J_{\alpha,h}(f)$ 
  if ( $\tilde{J}_1 < \tilde{J}$ )
     $\tilde{J} = \tilde{J}_1, \beta^{(s)} = \beta$ 
     $\beta = 2\beta$ 
  else
     $ok = 0$ 
}

```

Find a new approximation of the source term

$$f^{(s+1)} = f^{(s)} + \beta^{(s)} q^{(s)}.$$

Change the counter $s := s + 1$.

4. New iteration of the gradient descent method. If the required accuracy is not reached $\tilde{J} > \varepsilon^2$ and the maximum number of iterations is not reached, then go to Step 2. Otherwise Stop the algorithm.

9.1 The Conjugate Gradient Method - Version 1.

Next, we define two modifications of the Gradient descent method, they are based on the Conjugate Gradient (CG) method for nonlinear optimization. It extends the classical and very efficient linear CG algorithm in order to find minima of general non-linear functions. The aim as in linear CG methods is iteratively generate conjugate gradient descent directions. Our analysis is based on Fletcher-Reeves variant to generate adjustable step length parameter $\beta^{(s)}$ [5].

In the first version of the CGM (Step 2 of the general algorithm) a descent direction is defined by taking a linear combination of the previous conjugate vector and the new negative gradient direction of $J_{\alpha,h}$ (see also [10]):

$$\begin{aligned} q^{(s)} &:= -J'_{\alpha,h}(f^{(s)}) + \gamma^{(s)}q^{(s-1)}, \\ \gamma^{(s)} &= \|J'_{\alpha,h}(f^{(s)})\|^2 / \|J'_{\alpha,h}(f^{(s-1)})\|^2. \end{aligned}$$

This selection of $\gamma^{(s)}$ is recommended in [5] and seeks to preserve the orthonormality of system of conjugate vectors. Techniques like restarts are recommended if the loss of conjugacy occurs, and this drawback phenomenon is inherent in nonlinear settings.

9.2 The Conjugate Gradient Method - Version 2.

In the second version of the CGM the descent direction is defined as in the Version 1 algorithm. The changes are introduced in calculation of the length of the search parameter $\beta^{(s)}$. It is defined not by solving a line search for a local minimization problem as in Step 3 but by using a generalized classical formula known for the linear CGM algorithms (see also [9, 10]):

Find a new approximation of the source term

$$f^{(s+1)} = f^{(s)} + \beta^{(s)}q^{(s)},$$

where

$$\beta^{(s)} := - \langle q^{(s)}, J'_{\alpha,h}(f^{(s)}) \rangle / (\|d^{(s)}\|^2 + \alpha\|q^{(s)}\|^2),$$

and

$$d^{(s,n-\frac{1}{2})} = (\omega, \tilde{V}^{(s,n-\frac{1}{2})})_h, \quad n = 1, \dots, N,$$

here $\tilde{V}^{(s)}$ is a solution of the red auxiliary discrete problem

$$\begin{aligned} \frac{\tilde{V}^{s,n} - \tilde{V}^{s,n-1}}{\tau} + \nu A_h \tilde{V}^{s,n-\frac{1}{2}} &= q^{s,n-\frac{1}{2}} g_1(x_j), \quad x_j \in \omega_h, \\ \tilde{v}_0^{s,n} &= 0, \quad \tilde{v}_J^{s,n} = 0, \quad \tilde{v}^{s,0}(x_j) = 0, \quad j = 0, \dots, J. \end{aligned}$$

The new updated residue vector can be computed by the explicit recursion formula

$$\tilde{r}^{(s+1)} = \tilde{r}^{(s)} + \beta^{(s)} L_h \tilde{V}^s.$$

10 Numerical experiments

First, we solve 1D parabolic problem (1.2) with the following coefficients:

$$\nu = 1, \quad g_1(x) = x^2, \quad \omega = 1,$$

where $g_0(x, t)$ and $\tilde{h}(t)$ are selected such that the exact solution is defined as

$$u(x, t) = 4x(1-x)t, \quad f(t) = (t+1)^2.$$

This inverse parabolic problem is approximated by the Crank-Nicolson discrete scheme (6.1). In order to guarantee that the discrete solution (V^n, f^n) is equal the exact solution of the differential problem we modified the definition of discrete flux condition and the function $\tilde{h}(t^n)$ is computed as

$$\tilde{h}^n = L_h u^n,$$

where L_h is the trapezoidal summation formula.

Initial and boundary data are defined according to the exact solution.

10.1 Conjugate Gradient Method without Tikhonov regularization term $\alpha = 0$

Let us fix the space mesh ω_h size $J = 20$ and take a sequence of time meshes with different N .

First we solve this test problem with $N = 8$. Errors of the reconstructed source function

$$e(\tau) = |f(t^{N-\frac{1}{2}}) - f^{N-\frac{1}{2}}|$$

for different iteration numbers s are presented in Tables 1 and 2.

Table 1. Errors $e(\tau)$ of the reconstructed source function for $J = 20$ and $N = 8$.

s	1	3	5	7	8
$e(\tau)$	2.2543	1.1268	0.6707	0.3440	6.417e-12

Table 2. Errors $e(\tau)$ of the reconstructed source function for $J = 20$ and $N = 12$.

s	1	3	5	8	11	12
$e(\tau)$	2.6511	1.5389	0.9789	0.5122	0.2357	1.691e-06

Two conclusions follow from the presented results. First, the error of approximations for different iterations decrease as a geometric progression. Second, we see the well-known property that CGM solves quadratic minimization

problems as a direct solver in N iterations (some influence of the fact that the system of conjugate vectors is not strictly orthonormal can be seen in Table 2). Next, we solve the parabolic equation with the fractional power Laplace operator. The power parameter $p = 0.8$, the space and time meshes are of sizes $J = 20$, $N = 8$. Errors $e(\tau)$ for different iteration numbers s are presented in Table 3. It follows that both previous statements on the accuracy of ob-

Table 3. Errors $e(\tau)$ of the reconstructed source function for the discrete parabolic problem (7.1) with power Laplace operator. The mesh parameters are selected as $J = 20$ and $N = 8$.

s	1	3	5	7	8
$e(\tau)$	2.5809	1.4237	0.7666	0.3640	5.2682e-12

tained approximations are valid for this more complicated non-local diffusion operator, also.

10.2 CG method with Tikhonov regularization term $\alpha > 0$

Errors of the reconstructed source function

$$e(\tau) = |f^* - f^{N-\frac{1}{2}}|$$

for different iteration numbers s are presented in Table 4. Here f^* is the value of the stabilized solution for a sufficiently large number of iterations s . It follows

Table 4. Errors $e(\tau)$ of the reconstructed source function for $J = 20$, $N = 8$ and $\alpha = 0.00001$.

s	1	3	5	7	8
$e(\tau)$	1.6149	0.5617	0.2003	0.0318	2.6734e-13

from the presented results that the convergence rate is not degraded due to the inclusion of regularization term into the cost functional $J_{\alpha,h}$.

10.3 CG method for the 2D parabolic problem

We solve 2D parabolic problem (1.2) with the following coefficients:

$$\nu = 1, \quad g_1(x, y) = x^2 + y^2, \quad \omega = 1,$$

where $g_0(x, t)$ and $\tilde{h}(t)$ are selected such that the exact solution is defined as

$$u(x, y, t) = 16x(1-x)y(1-y)t, \quad f(t) = (t+1)^2.$$

This inverse parabolic problem is approximated by the Crank-Nicolson discrete scheme (6.1). In order to guarantee that the discrete solution (V^n, f^n) is equal the exact solution of the differential problem we modified the definition of discrete flux condition and the function $\tilde{h}(t^n)$ is computed as

$$\tilde{h}^n = L_h u^n,$$

where L_h is the 2D trapezoidal summation formula. Initial and boundary data are defined according to the the exact solution.

The obtained system of linear equations is solved by using the well known FFT solver [6].

The space and time meshes are of sizes 20×20 , $N = 8$. Errors e for different iteration numbers s are presented in Table 5. We note that the convergence

Table 5. Errors $e(\tau)$ of the reconstructed source function for the 2D discrete parabolic problem (6.1). The mesh parameters are selected as 20×20 and $N = 8$.

s	1	3	5	7	8
$e(\tau)$	1.5897	0.5928	0.3402	0.2682	1.7763e-15

behavior of the iterations is very similar to one obtained for the 1D case.

10.4 Gradient descent method for the 2D parabolic problem

For a comparison of convergence of gradient descent and CGM, consider the following versions of minimization algorithms. First, we consider the classical gradient descent algorithm but the descent direction vector is defined by a conjugate gradient.

The space mesh size is taken 20×20 and time mesh size is $N = 8$. A sufficiently large step increasing parameter $d = 2$ in line search algorithm is used to variate the optimization step lengths in the minimization algorithm.

Errors $e(\tau)$ for different iteration numbers s are presented in Table 6. It is

Table 6. Errors $e(\tau)$ of the reconstructed source function for the 2D discrete parabolic problem (6.1). The mesh parameters are selected as 20×20 and $N = 8$.

s	1	4	7	10	15
$e(\tau)$	1.4318	0.3964	0.2839	0.1902	0.02153

clearly seen that such version of the gradient descent method defines the iterative sequence of approximations and does not satisfy the property of becoming a direct solver after N iterations.

Next we reduced the parameter d value till the value $d = 1.05$. Errors $e(\tau)$

Table 7. Errors $e(\tau)$ of the reconstructed source function for the 2D discrete parabolic problem (6.1). The mesh parameters are selected as 20×20 and $N = 8$.

s	1	4	7	9	11
$e(\tau)$	1.6118	0.4281	0.2708	0.0112	0.00458

for different iteration numbers s are presented in Table 7. It follows that after achieving a much better accuracy of local approximations at each iterations this modification of the gradient descent method mimics convergence dynamics of the CGM algorithm.

In the last series of numerical experiments we compared the results in Table 7 with results obtained by taking the plain antigradient direction as the descent direction. The factor d for dynamical changes of the minimization step was fixed to $d = 2$. Errors $e(\tau)$ for different iteration numbers s are presented in Table 8.

Table 8. Errors $e(\tau)$ of the reconstructed source function for the 2D discrete parabolic problem (6.1). The descent direction is defined as the antigradient direction. The mesh parameters are selected as 20×20 and $N = 8$.

s	1	4	7	10	13	16
$e(\tau)$	1.4318	0.5921	0.3194	0.1988	0.1854	0.16768

This comparison of Gradient Descent and CGM algorithms show that CGM algorithms can be recommended for solution of real world applications.

11 Conclusions

In this work, we developed and analyzed a set of robust numerical algorithms for solving one- and two-dimensional inverse parabolic problems. The proposed methodology is based on finite-volume and finite-difference discretizations of the direct and adjoint problems, combined with variational regularization and gradient-based optimization techniques. Both backward Euler and Crank–Nicolson schemes were examined in detail, and their corresponding discrete adjoint formulations were rigorously derived. We also extended the framework to parabolic equations involving fractional powers of elliptic operators, demonstrating that the same optimization structure applies naturally to non-local diffusion models.

The computational experiments confirm that the Conjugate Gradient Method significantly accelerates convergence compared to the classical gradient descent approach. In particular, the CG method exhibits near–direct-solver behavior in the noise-free setting, requiring approximately N iterations to recover the

source term on a mesh with N time levels. These observations remain valid for problems with fractional diffusion and for two-dimensional spatial domains, illustrating the flexibility and efficiency of the proposed approach.

The results presented here form a foundation for tackling more complex inverse parabolic models. Two promising research directions arise. First, the integration of physics-informed neural networks and hybrid PINN–adjoint techniques may provide alternative solvers capable of handling noisy data and irregular geometries. Second, the extension of the methods to multidimensional problems with variable or anisotropic diffusion coefficients would require the development of scalable parallel solvers, since FFT-based methods are no longer applicable in such settings.

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