Electronic Transactions on Numerical Analysis.
Volume 57, pp. 67–79, 2022.

ISSN 1068–9613.
DOI: 10.1553/etna_vol57s67

ETNA
Kent State University and
Johann Radon Institute (RICAM)

THE LEVENBERG–MARQUARDT REGULARIZATION FOR THE BACKWARD HEAT EQUATION WITH FRACTIONAL DERIVATIVE*

PORNSARP PORNSAWAD†¶, CHRISTINE BÖCKMANN‡§, AND WANNAPA PANITSUPAKAMON†¶

Abstract. The backward heat problem with time-fractional derivative in Caputo's sense is studied. The inverse problem is severely ill-posed in the case when the fractional order is close to unity. A Levenberg–Marquardt method with a new a posteriori stopping rule is investigated. We show that optimal order can be obtained for the proposed method under a Hölder-type source condition. Numerical examples for one and two dimensions are provided.

Key words. ill-posed problems, time-fractional derivative, backward heat problem, Levenberg–Marquardt method, a posteriori stopping rule, optimal order

AMS subject classifications. 26A33, 47A52, 65R30, 65M30

1. Introduction.

Differential equations of fractional order have been investigated during the last few decades not only by mathematicians and physicists but also by, for example, biologists and chemists, since such equations are very useful in modeling specific properties. Mathematical models of many real-world phenomena based on the definition of fractional-order derivatives are more appropriate than those depending on integer order. We are interested here in the backward heat equation with fractional derivative.

A backward heat problem consists in determining the initial temperature distribution $x(s),\ 0 \leq s \leq \pi$. The temperature $u(s,\tau)$ of a uniform bar of length π that is insulated on its lateral surface satisfies the partial differential equation

$$u_\tau = u_{ss}, \quad 0 < s < \pi.$$

The temperature distribution at the ends of the bar is fixed at 0 and at time $\tau = 1$ is given by $u(s,1) = y(s)$. It is well known that solving the heat equation backward in time is an inverse ill-posed problem [3].

After the fractional calculus was analyzed in science and engineering, the time derivative or space derivative in Caputo's sense was investigated by many researchers [8, 10, 15, 16]. Liu and Yamamoto [10] considered a backward problem in time for a time-fractional partial differential equation in the one-dimensional (1D) case. The property of the initial status of the medium was recovered by using a regularizing scheme based on eigenfunction expansions. Numerical experiments show that the fractional-derivative model equation reconstructs the initial data better than the classical backward heat problem. The methods suggested in [11, 16, 17] deal with the two-dimensional (2D) case. In [16] Tikhonov regularization is suggested to solve the backward problem for the time-fractional diffusion equation. An inverse source problem using boundary Cauchy data is investigated in [17] using Tikhonov regularization too; however, a conjugate gradient method is proposed to find an approximation to the minimizer of the Tikhonov functional. In [11] a modified kernel method is presented for the sideways heat equation with time-fractional order.

*Received February 24, 2022. Accepted March 31, 2022. Published online on June 3, 2022. Recommended by Stefan Kindermann. Corresponding author: Wannapa Panitsupakamon.

†Department of Mathematics, Faculty of Science, Silpakorn University, 6 Rachamakka Nai Road, 73000 Nakhon Pathom, Thailand (pornsawad_p@silpakorn.edu, panitsupakamon_w@su.ac.th).

‡Institute of Mathematics, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam OT Golm, Germany (bockmann@uni-potsdam.de).

§Helmholtz Centre for Polar and Marine Research, Alfred Wegener Institute, Telegrafenberg A45, 14473 Potsdam, Germany.

¶Centre of Excellence in Mathematics, Mahidol University, Rama 6 Road, 10400 Bangkok, Thailand.

The heat equation with the time derivative in Caputo's sense is written as

$$\frac{\partial^\beta u}{\partial \tau^\beta} = u_{ss}, \tag{1.1}$$

where $\beta \in (0,1)$ is a fractional order of the derivative and

$$\frac{\partial^\beta u}{\partial \tau^\beta} = \frac{1}{\Gamma(1-\beta)} \int_0^\tau (\tau - t)^{-\beta} u_t(s,t)\,\mathrm{d}t,$$

where $\Gamma(\cdot)$ is the standard Γ-function. Nearby, if $\beta = 1$, then the problem (1.1) is the classical heat equation. Choosing the orthogonal basis $\{\sin(ns)\}_{n=1}^{\infty}$, the Fredholm integral equation for the backward heat equation [15] is

$$\int_0^\pi k(s,t)x(t)\,\mathrm{d}t = y(s), \tag{1.2}$$

where $k(s,t) = (2/\pi)\sum_{n=1}^{\infty} e^{-n^2/\beta} \sin(nt)\sin(ns)$. It is noted that the weight $e^{-n^2/\beta}$ in the kernel function causes the instability of the problem. High-frequency components in x are severely damped by the very small factor $e^{-n^2/\beta}$. Therefore, one needs a regularization to recover a stable solution.

In the present work, the problem (1.2) is written as

$$Ax^\delta = y^\delta, \tag{1.3}$$

where the noisy data y^δ satisfy

$$\|y - y^\delta\| \le \delta, \tag{1.4}$$

and $A \in L(X,Y)$ is a linear operator between Hilbert spaces X and Y.

The Levenberg–Marquardt method is a well-known iterative regularization scheme. In the linear setting, it is given by [14]

$$x_{k+1}^\delta = x_k^\delta - (\alpha_k I + A^*A)^{-1}A^*(Ax_k^\delta - y^\delta),$$

where $\alpha_k \in \mathbb{R}_+$ has to be chosen appropriately. Recently Hanke [4] and Jin [7] have proved the order optimality of the regularizing Levenberg–Marquardt scheme for nonlinear ill-posed problems under a Hölder-type source condition and when the stopping index is chosen according to the discrepancy principle, which is given by

$$\|y^\delta - Ax_{k_*}^\delta\| \le \lambda\delta < \|y^\delta - Ax_k^\delta\|, \quad 0 \le k < k_*,$$

where λ is an appropriately chosen positive number. In [13] the Levenberg–Marquardt method is known as the implicit Euler method. For a linear operator, Rieder [14] proved that Runge–Kutta integrators applied to asymptotic regularization and stopped by the discrepancy principle are regularization schemes, where the Hölder-type source set

$$X_{\nu,\rho} := \{(A^*A)^\nu z : z \in N(A)^\perp,\ \|z\| \le \rho\}$$

is used. It is known that the implicit Euler method is A-stable, i.e., the step size can be large. Therefore, the Levenberg–Marquardt method is attractive for solving inverse ill-posed problems. Recently in Zhao et al. [19], a wide class of spectral regularization methods under

ETNA
Kent State University and
Johann Radon Institute (RICAM)

variational source conditions was investigated. It is shown that appropriate general assumptions yield convergence rates under variational source conditions. Furthermore, asymptotic regularization and Runge–Kutta integrators satisfy those assumptions.

For the implicit Euler method or the nonstationary iterated Tikhonov–Phillips regularization [5], a geometrically growing sequence of step sizes is used, which cause an oversatisfaction in the case of noisy data. However, the quotient q between the residual norm and $\lambda\delta$ is used to control this difficulty. The reconstructed solution is accepted if $q \approx 1$ [2, 14]. Note that, for the iterative method, the step size is not a regularization parameter. Here it is the number of iteration steps. In many regularization methods, the discrepancy principle is used as a parameter choice rule. However, the discrepancy principle may terminate the iteration too early [1, 2]. Thus, in Jin [6], the modified discrepancy principle accompanied by Tikhonov regularization for the nonlinear ill-posed problem has been proposed.

It is worth mentioning that the calculus of fractional derivatives may also help to develop new accelerated regularization methods for ill-posed problems. Recently, Zhang and Hofmann [18] investigated the fractional asymptotic regularization for linear problems in a Hilbert space setting using the left-side Caputo fractional derivative under Hölder-type and logarithmic source conditions. It is shown that fractional asymptotic regularization with a fractional order $\beta \in (0, 2)$ exhibits an optimal regularization method, and, moreover, for $\beta \in (1, 2)$, it yields an accelerated method.

Let the singular system of $A : X \to Y$ be given by $\{\sigma_j : v_j, u_j\}$, $j \in N$, where $\sigma_1 > \sigma_2 > \cdots > 0$ is the ordered sequence of singular values of A. The singular functions are orthonormal and satisfy the following properties:

$$Av_j = \sigma_j u_j \quad \text{and} \quad A^* u_j = \sigma_j v_j, \quad j \in N,$$

where $A^* : Y \to X$ is the adjoint operator of A. In this work, the regularized solution by the Levenberg–Marquardt method for the linear ill-posed problem (1.3) is written in a filter representation:

$$x_k^\delta = Ry^\delta = \sum_{n=1}^{\infty} \frac{1}{\sigma_n} \left(1 - \prod_{i=1}^{k} (1 + w_i \sigma_n^2)^{-1}\right) \langle y^\delta, u_n \rangle v_n, \tag{1.5}$$

where w_i is the step size; see [9, 14]. In this work, for simplicity, we set $w_i = w_0 i^2$, with $i \in \mathbb{N}$, although more general choices are possible for the convergence results. An a priori choice of w_i in [7] is $w_i = 1/\alpha_i = r^{-i}/\alpha_0$, $\alpha_0 > 0$, $0 < r < 1$, which is a strongly increasing function.

The aim of this work is to propose an a posteriori parameter choice rule based on the discrepancy principle for the Levenberg–Marquardt method and to retrieve the initial temperature of the backward heat equation with the fractional derivative in time. Our parameter choice rule is different from the one that is proposed in [6]. The convergence rate analysis of the Levenberg–Marquardt method under the Hölder-type source condition is presented in Section 2. Applications of the Levenberg–Marquardt method to the backward heat equation in 1D and 2D are presented in Section 3 and Section 4, respectively.

2. Convergence rate analysis. In this section, we will prove the convergence rate of the Levenberg–Marquardt method (1.5) under Hölder source conditions. We propose the a posteriori parameter choice rule based on the discrepancy principle as presented in the following equation:

$$\|(I + w_k AA^*)^{-1}(y^\delta - Ax_k^\delta)\| = \lambda\delta, \tag{2.1}$$

where $\lambda > 1$ is a constant.

THEOREM 2.1. *Let $x^+ = (A^*A)^\nu z,\ z \in N(A)^\perp,\ 0 < \nu \le 1/2$ be the solution of $Ax = y$ with $\|z\| \le E$ and $\|y^\delta\| \le \tau\delta$, $\tau > 0$. Using the a posteriori stopping rule (2.1), a constant $\tilde{c} > 0$ exists such that the method is of order optimal with*

$$\|x_k^\delta - x^+\| \le \tilde{c}\, E^{1/(2\nu+1)}\, \delta^{2\nu/(2\nu+1)}.$$

Proof. By the triangle inequality, we have

$$\|x_k^\delta - x^+\| \le \|x_k - x^+\| + \|x_k^\delta - x_k\|. \tag{2.2}$$

Using (1.5) with $\delta = 0$ and the Hölder inequality with $p = (2\nu+1)/(2\nu)$ and $q = 2\nu+1$, we obtain

$$\begin{aligned}
&\|x_k - x^+\|^2 \\
&= \left\| \sum_{n=1}^{\infty} \frac{1}{\sigma_n}\left(1 - \prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right)\langle y, u_n\rangle v_n - \sum_{n=1}^{\infty}\frac{1}{\sigma_n}\langle y, u_n\rangle v_n \right\|^2 \\
&= \left\| -\sum_{n=1}^{\infty}\frac{1}{\sigma_n}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y, u_n\rangle v_n \right\|^2 = \sum_{n=1}^{\infty}\frac{1}{\sigma_n^2}\left(\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right)^2\langle y, u_n\rangle^2 \\
&= \sum_{n=1}^{\infty}\left(\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y, u_n\rangle\right)^{4\nu/(2\nu+1)}\frac{1}{\sigma_n^2}\left(\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y, u_n\rangle\right)^{2/(2\nu+1)} \\
&\le \left(\sum_{n=1}^{\infty}\left[\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y, u_n\rangle\right]^{(4\nu/(2\nu+1))(2\nu+1)/(2\nu)}\right)^{2\nu/(2\nu+1)} \\
&\quad\times\left(\frac{\sum_{n=1}^{\infty}[\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y, u_n\rangle]^{(2/(2\nu+1))(2\nu+1)}}{(\sigma_n^2)^{2\nu+1}}\right)^{1/(2\nu+1)} \\
&= \left(\sum_{n=1}^{\infty}\left[\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right]^2\langle y, u_n\rangle^2\right)^{2\nu/(2\nu+1)} \\
&\quad\times\left(\frac{\sum_{n=1}^{\infty}[\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}]^2\langle y, u_n\rangle^2}{\sigma_n^{4\nu+2}}\right)^{1/(2\nu+1)}.
\end{aligned} \tag{2.3}$$

Using $x^+ = (A^*A)^\nu z$, we have

$$\begin{aligned}
\langle y, u_n\rangle^2 &= \langle Ax^+, u_n\rangle^2 = \langle A(A^*A)^\nu z, u_n\rangle^2 = \langle (A^*A)^\nu z, A^*u_n\rangle^2 = \langle (A^*A)^\nu z, \sigma_n v_n\rangle^2 \\
&= \sigma_n^2\langle (A^*A)^\nu z, v_n\rangle^2 = \sigma_n^2\left(\sum_{j=1}^{\infty}\sigma_j^{2\nu}\langle z, v_j\rangle\langle v_j, v_n\rangle\right)^2 = \sigma_n^{4\nu+2}\langle z, v_n\rangle^2.
\end{aligned} \tag{2.4}$$

The second term of (2.3) becomes

$$\begin{aligned}
\sum_{n=1}^{\infty}\frac{[\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}]^2\langle y, u_n\rangle^2}{\sigma_n^{4\nu+2}} &= \sum_{n=1}^{\infty}\left(\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right)^2\langle z, v_n\rangle^2 \\
&\le \sum_{n=1}^{\infty}\langle z, v_n\rangle^2 \le E^2.
\end{aligned} \tag{2.5}$$

Using (1.4) and the orthonormality of u_n, the first term of (2.3) becomes

$$\begin{aligned}
&\left(\sum_{n=1}^{\infty}\left[\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right]^2\langle y,u_n\rangle^2\right)^{1/2}\\
&\quad=\left\|\sum_{n=1}^{\infty}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y,u_n\rangle u_n\right\|\\
&\quad\le\left\|\sum_{n=1}^{\infty}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y-y^\delta,u_n\rangle u_n\right\|+\left\|\sum_{n=1}^{\infty}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y^\delta,u_n\rangle u_n\right\|\\
&\quad\le\left\|\sum_{n=1}^{\infty}\langle y-y^\delta,u_n\rangle u_n\right\|+\tilde{A}\\
&\quad=\|y-y^\delta\|+\tilde{A}\le\delta+\tilde{A}, \qquad (2.6)
\end{aligned}$$

with

$$\tilde{A}=\left\|\sum_{n=1}^{\infty}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y^\delta,u_n\rangle u_n\right\|.$$

Using (1.5) we get

$$Ax_k^\delta=\sum_{n=1}^{\infty}\frac{1}{\sigma_n}\left(1-\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right)\langle y^\delta,u_n\rangle Av_n.$$

Then,

$$\begin{aligned}
\langle Ax_k^\delta,u_n\rangle&=\left\langle\sum_{j=1}^{\infty}\frac{1}{\sigma_j}\left[1-\prod_{i=1}^{k}(1+w_i\sigma_j^2)^{-1}\right]\langle y^\delta,u_j\rangle Av_j,u_n\right\rangle\\
&=\sum_{j=1}^{\infty}\frac{1}{\sigma_j}\left(1-\prod_{i=1}^{k}(1+w_i\sigma_j^2)^{-1}\right)\langle y^\delta,u_j\rangle\langle Av_j,u_n\rangle\\
&=\sum_{j=1}^{\infty}\frac{1}{\sigma_j}\left(1-\prod_{i=1}^{k}(1+w_i\sigma_j^2)^{-1}\right)\langle y^\delta,u_j\rangle\sigma_j\langle u_j,u_n\rangle\\
&=\left(1-\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right)\langle y^\delta,u_n\rangle. \qquad (2.7)
\end{aligned}$$

By (2.7) we have[1]

$$\begin{aligned}
&(w_kAA^*+I)^{-1}(Ax_k^\delta-y^\delta)\\
&\quad=\sum_{n=1}^{\infty}\frac{1}{w_k\sigma_n^2+1}\langle Ax_k^\delta-y^\delta,u_n\rangle u_n\\
&\quad=\sum_{n=1}^{\infty}\frac{1}{w_k\sigma_n^2+1}\langle Ax_k^\delta,u_n\rangle u_n-\sum_{n=1}^{\infty}\frac{1}{w_k\sigma_n^2+1}\langle y^\delta,u_n\rangle u_n
\end{aligned}$$

[1] From spectral theory, we have $f(AA^*)y=\sum_{i=1}^{\infty}f(\sigma_i^2)\langle y,u_i\rangle u_i$, so we obtain $(I+w_kAA^*)^{-1}y=\sum_{i=1}^{\infty}(1/(1+w_k\sigma_i^2))\langle y,u_i\rangle u_i$.

ETNA
Kent State University and
Johann Radon Institute (RICAM)

$$= \sum_{n=1}^{\infty} \frac{1}{w_k\sigma_n^2+1}\left(1-\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right)\langle y^\delta, u_n\rangle u_n - \sum_{n=1}^{\infty}\frac{1}{w_k\sigma_n^2+1}\langle y^\delta, u_n\rangle u_n$$
$$= -\sum_{n=1}^{\infty}\frac{1}{w_k\sigma_n^2+1}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y^\delta, u_n\rangle u_n.$$

Consequently

$$\|(w_kAA^*+I)^{-1}(Ax_k^\delta-y^\delta)\| = \left\|\sum_{n=1}^{\infty}\frac{1}{w_k\sigma_n^2+1}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y^\delta, u_n\rangle u_n\right\|. \tag{2.8}$$

Using (2.1), (2.8), and $\|y^\delta\| \le \tau\delta$, we get

$$\begin{aligned}\tilde{A} &= \left\|\sum_{n=1}^{\infty}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y^\delta, u_n\rangle u_n\right\| \\ &\le \left\|\sum_{n=1}^{\infty}\frac{1}{w_k\sigma_n^2+1}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y^\delta, u_n\rangle u_n\right\| \\ &\quad + \left\|\sum_{n=1}^{\infty}\frac{w_k\sigma_n^2}{w_k\sigma_n^2+1}\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\langle y^\delta, u_n\rangle u_n\right\| \\ &\le \|(w_kAA^*+I)^{-1}(Ax_k^\delta-y^\delta)\| + \left\|\sum_{n=1}^{\infty}\langle y^\delta, u_n\rangle u_n\right\| \le \lambda\delta+\tau\delta. \end{aligned} \tag{2.9}$$

Substituting (2.9) into (2.6) yields

$$\begin{aligned}\left(\sum_{n=1}^{\infty}\left[\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right]^2\langle y, u_n\rangle^2\right)^{1/2} &\le \delta+\tilde{A} \\ &\le \delta+\lambda\delta+\tau\delta = (1+\lambda+\tau)\delta. \end{aligned} \tag{2.10}$$

Now we substitute (2.10) and (2.5) into (2.3) and we get

$$\begin{aligned}\|x_k-x^+\|^2 &\le \{[(1+\lambda+\tau)\delta]^2\}^{2\nu/(2\nu+1)}(E^2)^{1/(2\nu+1)} \\ &= (1+\lambda+\tau)^{4\nu/(2\nu+1)}\delta^{4\nu/(2\nu+1)}E^{2/(2\nu+1)}. \end{aligned} \tag{2.11}$$

Using the fact that

$$|1-\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}| \le 1$$

and [5, equation (15), page 45][2] we have

$$\begin{aligned}&\left|1-\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right| \frac{\left|1-\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right|}{\sigma_n^2} \\ &\qquad \le \frac{\left|1-\prod_{i=1}^{k}(1+w_i\sigma_n^2)^{-1}\right|}{\sigma_n^2} \le c_1\sum_{j=1}^{k}w_j \end{aligned} \tag{2.12}$$

[2]From [5], for some positive α_j, let $\sigma_m := \sum_{j=1}^{m} 1/\alpha_j$, $r_n(\lambda) = \prod_{i=1}^{n}\alpha_i/(\lambda+\alpha_i)$, and $q_n(\lambda) = (1-r_n(\lambda))/\lambda$. Then we have $\max_{\lambda\in[0,\infty)} q_n(\lambda) = \sigma_n$.

ETNA
Kent State University and
Johann Radon Institute (RICAM)

for some $c_1 > 0$. Using (1.4), (1.5), and (2.12) for the second term of (2.2), we have

$$\begin{aligned}
\|x_k^\delta - x_k\| &= \left\| \sum_{n=1}^{\infty} \frac{1}{\sigma_n} \left(1 - \prod_{i=1}^{k} (1 + w_i\sigma_n^2)^{-1}\right) \langle y^\delta - y, u_n\rangle v_n \right\| \\
&= \left(\sum_{n=1}^{\infty} \frac{1}{\sigma_n^2} \left[1 - \prod_{i=1}^{k} (1 + w_i\sigma_n^2)^{-1}\right]^2 \langle y^\delta - y, u_n\rangle^2 \right)^{1/2} \\
&\le \left(\sup_{0<\sigma_n\le\|A\|} \frac{[1 - \prod_{i=1}^{k}(1 + w_i\sigma_n^2)^{-1}]^2}{\sigma_n^2} \right)^{1/2} \left(\sum_{n=1}^{\infty} \langle y^\delta - y, u_n\rangle^2 \right)^{1/2} \\
&\le \hat{C} \left(\sum_{j=1}^{k} w_j \right)^{1/2} \delta. \qquad (2.13)
\end{aligned}$$

Let

$$J = \left\| \sum_{n=1}^{\infty} \frac{1}{w_k\sigma_n^2 + 1} \prod_{i=1}^{k} (1 + w_i\sigma_n^2)^{-1} \langle y, u_n\rangle u_n \right\|.$$

By [5, Lemma 2.2, page 41] we have

$$\sigma_n^{2(\nu+1/2)} \prod_{i=1}^{k} (1 + w_i\sigma_n^2)^{-1} \le c_2 \left(\sum_{j=1}^{k} w_j \right)^{-(\nu+1/2)}, \quad 0 < \nu \le 1/2, \qquad (2.14)$$

for some $c_2 > 0$. By (2.4) and (2.14), we can show that

$$\begin{aligned}
J^2 &= \left\| \sum_{n=1}^{\infty} \frac{1}{1 + w_k\sigma_n^2} \prod_{i=1}^{k} (1 + w_i\sigma_n^2)^{-1} \langle y, u_n\rangle u_n \right\|^2 \\
&= \sum_{n=1}^{\infty} \frac{1}{(1 + w_k\sigma_n^2)^2} \left(\prod_{i=1}^{k} (1 + w_i\sigma_n^2)^{-1} \right)^2 \langle y, u_n\rangle^2 \\
&= \sum_{n=1}^{\infty} \frac{\sigma_n^{4\nu+2}}{(1 + w_k\sigma_n^2)^2} \left(\prod_{i=1}^{k} (1 + w_i\sigma_n^2)^{-1} \right)^2 \langle z, v_n\rangle^2 \\
&\le \sup_{0<\sigma_n\le\|A\|} \left\{ \frac{\sigma_n^{4\nu+2}}{(1 + w_k\sigma_n^2)^2} \left(\prod_{i=1}^{k} (1 + w_i\sigma_n^2)^{-1} \right)^2 \right\} \sum_{n=1}^{\infty} \langle z, v_n\rangle^2 \\
&\le \sup_{0<\sigma_n\le\|A\|} \left(\frac{(\sigma_n^2)^{\nu+1/2}}{1 + w_k\sigma_n^2} \prod_{i=1}^{k} (1 + w_i\sigma_n^2)^{-1} \right)^2 \|z\|^2 \\
&\le C_1 \left(\sum_{j=1}^{k} w_j \right)^{-2(\nu+1/2)} E^2. \qquad (2.15)
\end{aligned}$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

From (2.1), (2.8), and (2.15), we get

$$\begin{aligned}
\lambda\delta &= \|(w_k AA^* + I)^{-1}(Ax_k^\delta - y^\delta)\| = \left\| \sum_{n=1}^{\infty} \frac{1}{w_k\sigma_n^2+1} \prod_{i=1}^{k} (1+w_i\sigma_n^2)^{-1} \langle y^\delta, u_n\rangle u_n \right\| \\
&\le \left\| \sum_{n=1}^{\infty} \frac{1}{w_k\sigma_n^2+1} \prod_{i=1}^{k} (1+w_i\sigma_n^2)^{-1} \langle y^\delta - y, u_n\rangle u_n \right\| \\
&\quad + \left\| \sum_{n=1}^{\infty} \frac{1}{w_k\sigma_n^2+1} \prod_{i=1}^{k} (1+w_i\sigma_n^2)^{-1} \langle y, u_n\rangle u_n \right\| \\
&\le \left\| \sum_{n=1}^{\infty} \langle y^\delta - y, u_n\rangle u_n \right\| + J \le \delta + \sqrt{C_1}\, E \left(\sum_{j=1}^{k} w_j \right)^{-(\nu+1/2)}.
\end{aligned}$$

We thus obtain

$$\sum_{j=1}^{k} w_j \le \left(\frac{\sqrt{C_1}E}{(\lambda-1)\delta} \right)^{2/(2\nu+1)}.$$

From (2.13) we get

$$\|x_k^\delta - x_k\| \le \hat{C} \left(\sum_{j=1}^{k} w_j \right)^{1/2} \delta \le \hat{C} \left(\frac{\sqrt{C_1}E}{(\lambda-1)\delta} \right)^{1/(2\nu+1)} \delta \le C E^{1/(2\nu+1)} \delta^{2\nu/(2\nu+1)}. \tag{2.16}$$

Using (2.11) and (2.16), we find

$$\begin{aligned}
\|x_k^\delta - x^+\| &\le \|x_k^\delta - x_k\| + \|x_k - x^+\| \\
&\le C E^{1/(2\nu+1)} \delta^{2\nu/(2\nu+1)} + (1+\lambda+\tau)^{2\nu/(2\nu+1)} \delta^{2\nu/(2\nu+1)} E^{1/(2\nu+1)} \\
&\le \tilde{c} E^{1/(2\nu+1)} \delta^{2\nu/(2\nu+1)}. \qquad \square
\end{aligned}$$

3. Regularized solution of backward heat equation in 1D. We consider the following backward heat equation with the fractional derivative in time:

$$\begin{aligned}
\frac{\partial^\beta u}{\partial \tau^\beta} &= u_{ss}, \qquad && (s,\tau) \in (0,\pi) \times (0,1], \\
u(0,\tau) &= u(\pi,\tau) = 0, && \tau \in [0,1], \\
u(s,1) &= y(s).
\end{aligned} \tag{3.1}$$

A solution of the problem (3.1) [15] is

$$u(s,\tau) = \sum_{n=1}^{\infty} a_n e^{n^2(1-\tau^\beta)/\beta} \sin(ns).$$

If the distribution temperature at $\tau = 0$ is $x(s)$, then

$$x(s) = \sum_{n=1}^{\infty} a_n e^{n^2/\beta} \sin(ns).$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

TABLE 3.1
Comparison of the a posteriori stopping rule and the discrepancy principle with respect to the absolute Euclidean error and the number of iterations k_* for $\lambda = 1.5$, $\delta = 10^{-2}$, and $w_k = 5k^2$ with different β.

	A posteriori stopping rule (2.1)		Discrepancy principle	
β	Error	k_*	Error	k_*
1	0.88272	4	0.88187	5
0.8	0.88194	5	0.88188	6
0.6	0.88217	6	0.88187	7
0.4	0.88469	9	0.88196	10
0.2	0.93812	39	0.91228	40

TABLE 3.2
Comparison of the a posteriori stopping rule and the discrepancy principle with respect to the absolute Euclidean error and the number of iterations k_* for $\lambda = 1.5$, $\delta = 10^{-3}$, and $w_k = 5k^2$ with different β.

	A posteriori stopping rule (2.1)		Discrepancy principle	
β	Error	k_*	Error	k_*
1	0.88187	5	0.88188	6
0.8	0.88194	5	0.88188	6
0.6	0.88187	7	0.88187	7
0.4	0.88196	10	0.88187	11
0.2	0.88570	43	0.88363	44

Hence,

$$a_n = \frac{2}{\pi} e^{-n^2/\beta} \int_0^\pi x(s) \sin(ns)\, \mathrm{d}s.$$

Using the boundary condition, we obtain

$$y(s) = \int_0^\pi k(s,t) x(t)\, \mathrm{d}t, \tag{3.2}$$

where the kernel function is given by

$$k(s,t) = \frac{2}{\pi} \sum_{n=1}^{\infty} e^{-n^2/\beta} \sin(nt) \sin(ns).$$

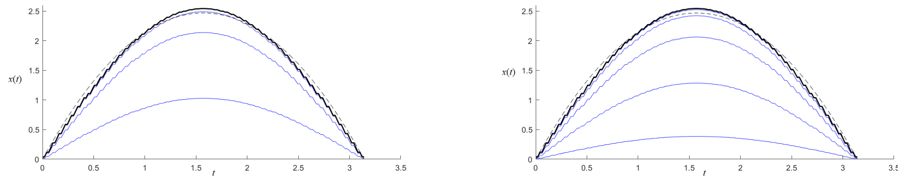
Define $\{s_j\}_{j=1,2,\dots,n+1}$ to be a set of grid points for the interval $[0,\pi]$ and $\{t_j\}_{j=1,2,\dots,n+1}$ for $[0,1]$. Let

$$x(t) = \sum_{j=1}^{m} c_j \varphi_j^{(m)}(t),$$

where $\varphi_j^{(m)} = 1$ for $t \in [t_j, t_{j+1}]$, and $\varphi_j^{(m)} = 0$ for $t \notin [t_j, t_{j+1}]$. Let $y_i = y(s_i)$, $i = 1, 2, \dots, m+1$. Then, the Fredholm integral equation (3.2) is transformed into the following vector form:

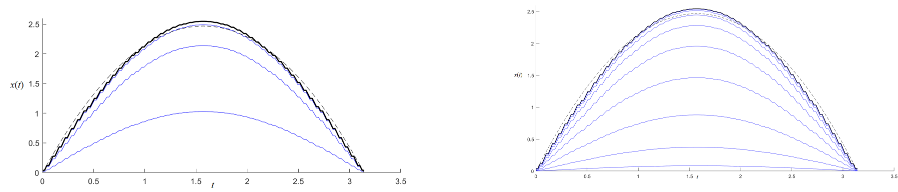
$$Kf = g,$$

where K is the $(m+1) \times m$ matrix, $f = [c_1, c_2, \dots, c_m]^{\mathrm{T}}$, and $g = [y_1, y_2, \dots, y_{m+1}]^{\mathrm{T}}$.



(a) (b)

FIG. 3.1. *Reconstruction result for the experiments as in Table 3.1 with (a) $\beta = 1$ and (b) $\beta = 0.6$ compared with the exact solution (dashed curve) where the stopping rule (2.1) is used.*



(a) (b)

FIG. 3.2. *Reconstruction result for the experiments as in Table 3.2 with (a) $\beta = 1$ and (b) $\beta = 0.4$ compared with the exact solution (dashed curve) where the stopping rule (2.1) is used.*

In the following results, we compare two stopping rules, our a posteriori parameter choice rule (2.1) and the discrepancy principle, for two different noise levels ($\delta = 10^{-2}$ and $\delta = 10^{-3}$), as shown in Table 3.1 and Table 3.2, respectively. We use zero as the initial guess. The exact solution is assumed to be $x(s) = s(\pi - s),\ s \in [0, \pi]$, and we choose $w_k = 5k^2$. The infinite summation in the kernel function is truncated after three terms.

Moreover, we show the approximate solution (solid curve) using a posteriori parameter choice rule (2.1), which is compared with the exact solution (dashed curve) for $\delta = 10^{-2}$ in Figure 3.1 and for $\delta = 10^{-3}$ in Figure 3.2. In both figures the approximate solutions are comparable to the exact solution.

4. Regularized solution of backward heat equation in 2D. In this section, we extend the domain of the heat equation to two dimensions. The backward heat problem for a time-fractional diffusion equation with a bounded domain Ω in $\mathbb{R}^2$ and sufficiently smooth boundary $\partial\Omega$ is written as

$$
\begin{aligned}
\frac{\partial^\beta}{\partial \tau^\beta} u(s,\tau) &= \Delta u(s,\tau), && s \in \Omega \subseteq \mathbb{R}^2,\ \tau \in (0,T),\ 0 < \beta \leq 1,\\
u(s,\tau) &= 0, && s \in \partial\Omega,\ \tau \in (0,T),\\
u(s,T) &= y(s), && s \in \bar{\Omega},
\end{aligned}
$$

with $T = 1$. A similar time-fractional diffusion equation with a smooth star-shaped domain in 2D can be found in [16]. In this section we are interested in finding the initial temperature distribution $x(s) = u(s,0)$ by solving the integral equation

$$
\int_\Omega k(s,t)x(t)\,\mathrm{d}t = y(s), \tag{4.1}
$$

ETNA
Kent State University and
Johann Radon Institute (RICAM)

where the kernel is

$$k(s,t) = \sum_{n=1}^{\infty} E_{\beta,1}(-\lambda_n T^{\beta})\varphi_n(s)\varphi_n(t) \tag{4.2}$$

with the eigenvalues λ_n of the operator $-\Delta$ and the associated orthogonal eigenfunctions $\varphi_n \in H^2(\Omega) \cap H_0^1(\Omega)$. In (4.2), the Mittag–Leffler function is defined by

$$E_{a,b}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(ak+b)}, \quad z \in \mathbb{C},$$

where $a > 0$ and $b \in \mathbb{R}$ are arbitrary constants. For the domain Ω defined by

$$\Omega = \{(s_1, s_2) \in \mathbb{R}^2 \mid s_1 = r\cos\theta,\ s_2 = r\sin\theta,\ 0 \le r \le 1,\ 0 \le \theta \le 2\pi\},$$

the eigenvalues are $\lambda_{mn} = (m^2 + n^2)\pi^2$, for $m, n = 0, 1, \ldots$, and the corresponding orthonormal eigenfunctions are $\varphi_{mn}(s) = \sin(m\pi s_1)\sin(n\pi s_2)$, with $s = (s_1, s_2) \in \mathbb{R}^2$.

In the following proposition we discretize $r \in [0,1]$ and $\theta \in [0, 2\pi]$ by equally spaced grid points:

$$\begin{aligned} r_i &= (i-1)\Delta r = \frac{i-1}{n-1}, & i &= 1, 2, \ldots, n, \\ \theta_j &= (j-1)\Delta\theta = \frac{2\pi(j-1)}{m-1}, & j &= 1, 2, \ldots, m. \end{aligned}$$

PROPOSITION 4.1. *Let Y_j be an $(n \times 1)$ vector $[y_{1j}\ y_{2j}\ \ldots\ y_{nj}]^{\mathrm{T}}$ for $y_{ij} = y(r_i, \theta_j)$ with $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, m$. For $l = 1, 2, \ldots, m$, the $(1 \times n)$ vector $K^l(s)$ is given by*

$$p\left[r_1 k(s, r_1, \theta_l) \quad 2r_2 k(s, r_2, \theta_l) \quad \cdots \quad 2r_{n-1} k(s, r_{n-1}, \theta_l) \quad r_n k(s, r_n, \theta_l)\right],$$

where $p = 1$ if $l = 1$ or m, and $p = 2$ otherwise. Moreover,

$$K_{ij}^l = K^l(r_i, \theta_j) \quad \text{for } l, j = 1, 2, \ldots, m \text{ and } i = 1, 2, \ldots, n.$$

We define the $(n \times mn)$ matrix A_j as follows:

$$A_j = \begin{bmatrix} K_{1j}^1 & K_{1j}^2 & \cdots & K_{1j}^m \\ K_{2j}^1 & K_{2j}^2 & \cdots & K_{2j}^m \\ \vdots & \vdots & \ddots & \vdots \\ K_{nj}^1 & K_{nj}^2 & \cdots & K_{nj}^m \end{bmatrix},$$

with $j = 1, 2, \ldots, m$. Then the regularized solution of (4.1) is given by

$$X_{k+1} = X_k - w_k \left(I + w_k \sum_{j=1}^{m} A_j^{\mathrm{T}} A_j \right)^{-1} \sum_{j=1}^{m} A_j^{\mathrm{T}} (A_j X_k - Y_j)$$

for $k = 0, 1, \ldots, k_*$, where k_* is a regularization parameter.

Next we compare two stopping rules, our a posteriori parameter choice rule (2.1) and the discrepancy principle, for a noise level $\delta = 10^{-2}$ and $\lambda = 8$ with different β as shown in Table 4.1. We choose $w_k = 0.1k^2$. The numerical solution for $\beta = 0.8$ with the a posteriori

ETNA
Kent State University and
Johann Radon Institute (RICAM)

TABLE 4.1
Comparison of the a posteriori stopping rule (2.1) and the discrepancy principle with respect to the absolute Euclidean error and the number of iterations k_* for $\lambda = 8$, $\delta = 10^{-2}$, and $w_k = 0.1k^2$ with different β.

	A posteriori stopping rule (2.1)		Discrepancy principle	
β	Error	k_*	Error	k_*
1.0	0.2046333	3	0.2046333	1
0.8	0.2046340	3	0.2046338	1
0.6	0.2046285	3	0.2046298	1
0.4	0.2046079	3	0.2046145	1
0.2	0.2045625	3	0.2045805	1

stopping rule (2.1) is shown in Figure 4.1(a). The difference between the numerical and the exact solution for $\beta = 0.8$ with stopping rule (2.1) is shown in Figure 4.1(b). Figures 4.1(c) and 4.1(d) show the same but for $\beta = 0.2$ and displayed in three dimensions (3D).

In this 2D example, our proposed a posteriori parameter choice rule needs more iteration steps than the discrepancy principle. This may be useful for certain examples since it was observed and remarked upon in the introduction that the discrepancy principle often stops too early [1, 2].

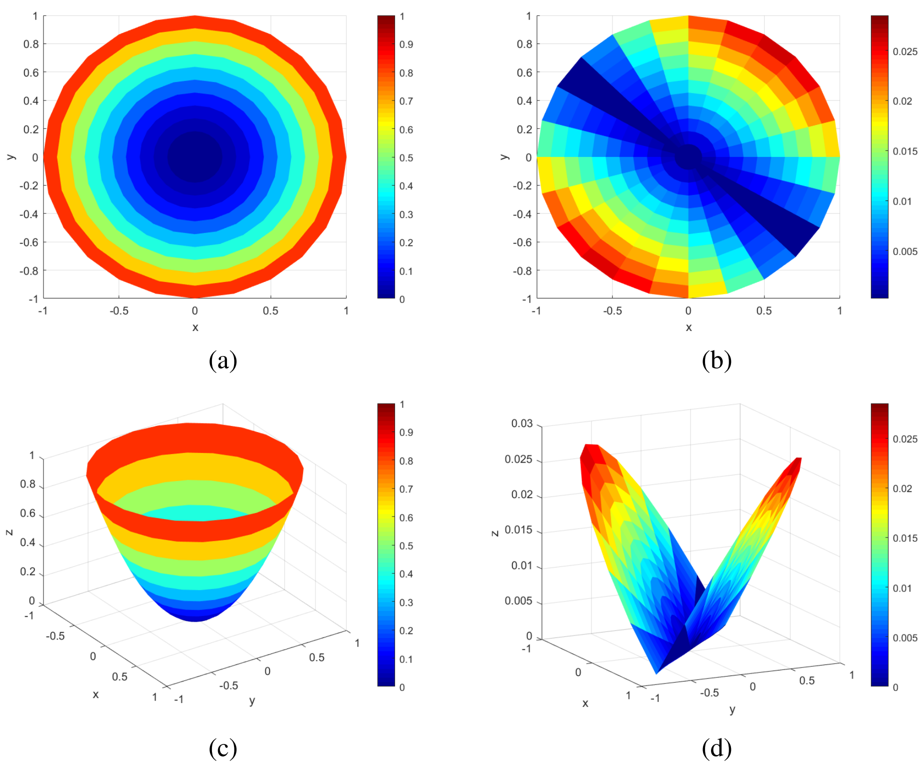


FIG. 4.1. *Reconstruction results for the experiments as in Table 4.1, where $w_k = 0.1k^2$ and $\delta = 10^{-2}$ are used. (a) The numerical solution for $\beta = 0.8$ with the stopping rule (2.1) in 2D. (b) The difference from the exact solution for $\beta = 0.8$ with the stopping rule (2.1) in 2D. (c) The numerical solution for $\beta = 0.2$ with the stopping rule (2.1) in 3D. (d) The difference from the exact solution for $\beta = 0.2$ with the stopping rule (2.1) in 3D.*

5. Conclusion. In this paper, we show that the optimal order of the Levenberg–Marquardt method (1.5) is obtained if the a posteriori stopping rule (2.1) is used. The regularized solutions of the backward heat problem in 1D and 2D are computed for different values of the fractional order β. In 1D, the reconstructed solutions with the stopping rule (2.1) and the discrepancy principle are comparable. Advantageously, the reconstructed solutions in 2D take a few more iteration steps. In the cases $\beta = 0.6$, 0.4, and 0.2, the reconstruction errors are somewhat less. For both examples the Levenberg–Marquardt method provides good results although the fractional order β of the derivative in time is close to unity. It is known that, if β is increasing and close to unity, then the inverse problem is severely ill-posed. A proper regularization scheme can alleviate this problem [10, 12]. In summary, the numerical examples show that the iterative regularization method with our new a posteriori stopping rule (2.1) is stable and not very sensitive with respect to the fractional order β.

Acknowledgments. The authors sincerely thank two anonymous referees for their careful reading of the manuscript. Their valuable comments and suggestions allowed us to eliminate weak points of the manuscript and thus to improve the paper. This work was supported by the Faculty of Science, Silpakorn University, Thailand, under Grant No. SRIF-JRG-2563-01.

REFERENCES

[1] F. BAUER AND T. HOHAGE, *A Lepskij-type stopping rule for regularized Newton methods*, Inverse Problems, 21 (2005), pp. 1975–1991.
[2] C. BÖCKMANN AND P. PORNSAWAD, *Iterative Runge–Kutta-type methods for nonlinear ill-posed problems*, Inverse Problems, 24 (2008), Art. 025002, 17 pages.
[3] C. W. GROETSCH, *Inverse Problems in the Mathematical Sciences*, Vieweg, Braunschweig, 1993.
[4] M. HANKE, *The regularizing Levenberg–Marquardt scheme is of optimal order*, J. Integral Equations Appl., 22 (2010), pp. 259–283.
[5] M. HANKE AND C. W. GROETSCH, *Nonstationary iterated Tikhonov regularization*, J. Optim. Theory Appl., 98 (1998), pp. 37–53.
[6] Q. JIN, *Applications of the modified discrepancy principle to Tikhonov regularization of nonlinear ill-posed problems*, SIAM J. Numer. Anal., 36 (1999), pp. 475–490.
[7] ———, *On a regularized Levenberg–Marquardt method for solving nonlinear inverse problems*, Numer. Math., 115 (2010), pp. 229–259.
[8] B. KALTENBACHER AND W. RUNDELL, *Regularization of a backward parabolic equation by fractional operators*, Inverse Probl. Imaging, 13 (2019), pp. 401–430.
[9] A. KIRSCH, *An Introduction to the Mathematical Theory of Inverse Problems*, Springer, New York, 2011.
[10] J. J. LIU AND M. YAMAMOTO, *A backward problem for the time-fractional diffusion equation*, Appl. Anal., 89 (2010), pp. 1769–1788.
[11] S. LIU AND L. FENG, *An inverse problem for a two-dimensional time-fractional sideways heat equation*, Math. Probl. Eng., 2020, Art. 5865971, 13 pages.
[12] D. A. MURIO, *Time fractional IHCP with Caputo fractional derivatives*, Comput. Math. Appl., 56 (2008), pp. 2371–2381.
[13] P. PORNSAWAD AND C. BÖCKMANN, *Convergence rate analysis of the first-stage Runge–Kutta-type regularizations*, Inverse Problems, 26 (2010), Art. 035005, 12 pages.
[14] A. RIEDER, *Runge–Kutta integrators yield optimal regularization schemes*, Inverse Problems, 21 (2005), pp. 453–471.
[15] H. VU, D. O'REGAN, AND N. V. HOA, *Regularization and error estimates for an inverse heat problem under the conformable derivative*, Open Math., 16 (2018), pp. 999–1011.
[16] J.-G. WANG, T. WEI, AND Y.-B. ZHOU, *Tikhonov regularization method for a backward problem for the time-fractional diffusion equation*, Appl. Math. Model., 37 (2013), pp. 8518–8532.
[17] T. WEI, X.-L. LI, AND Y.-S. LI, *An inverse time-dependent source problem for a time-fractional diffusion equation*, Inverse Problems, 32 (2016), Art. 085003, 24 pages.
[18] Y. ZHANG AND B. HOFMANN, *On fractional asymptotical regularization of linear ill-posed problems in Hilbert spaces*, Fract. Calc. Appl. Anal., 22 (2019), pp. 699–721.
[19] Y. ZHAO, P. MATHÉ, AND S. LU, *Convergence analysis of asymptotical regularization and Runge–Kutta integrators for linear inverse problems under variational source conditions*, CSIAM Trans. Appl. Math., 1 (2020), pp. 693–714.