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On fractional Tikhonov regularization

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Abstract. It is well known that Tikhonov regularization in standard form may determine approximate solutions that are too smooth, i.e., the approximate solution may lack many details that the desired exact solution might possess. Two different approaches, both referred to as fractional Tikhonov methods have been introduced to remedy this shortcoming. This paper investigates the convergence properties of these methods by reviewing results published previously by various authors. We show that both methods are order optimal when the regularization parameter is chosen according to the discrepancy principle. The theory developed suggests situations in which the fractional methods yield approximate solutions of higher quality than Tikhonov regularization in standard form. Computed examples that illustrate the behavior of the methods are presented.

Keywords. ill-posed problem, regularization method, fractional Tikhonov, filter function, discrepancy principle.

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1 Introduction

Let A be a linear compact operator between the Hilbert spaces X and Y, and consider the operator equation

$$Ax = b, \qquad x \in X, \quad b \in Y, \tag{1.1}$$

which we assume to be consistent. We would like to determine the solution of minimal X-norm, which we denote by $x^\dagger$. It can be computed as $x^\dagger = A^\dagger b$, where $A^\dagger$ is the Moore–Penrose pseudoinverse of A. The computation of $x^\dagger$ is an ill-posed problem, because a small perturbation in b may give rise to an arbitrarily large perturbation in $x^\dagger$, or even make the problem unsolvable. Moreover, the right-hand side function that is available in applications represents data that is contaminated by noise. Thus, instead of b, the error-contaminated function b^δ is available. We assume that a bound for the error

$$\|b^\delta - b\|_Y \leq \delta \tag{1.2}$$

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is known. We will implicitly assume that $\epsilon := b^\delta - b$ lies in the appropriate spaces whenever we use it in norms or scalar products.

Straightforward solution of (1.1) with b replaced by b^δ generally does not yield a meaningful approximation of $x^\dagger$ because of severe propagation of the error in b^δ into the computed solution. A common remedy, known as *Tikhonov regularization*, is to replace (1.1) by a penalized least squares problem of the form

$$\min_{x \in X} J_\mu(x) \tag{1.3}$$

with

$$J_\mu(x) := \|Ax - b^\delta\|_Y^2 + \mu \|x\|_X^2; \tag{1.4}$$

see, e.g., [2, 7, 10] for discussions and many details on this solution approach. The parameter $\mu > 0$ is referred to as the regularization parameter and determines how sensitive the minimizer x_μ^δ of J_μ is to the error in b^δ and how close x_μ^δ is to the desired solution $x^\dagger$.

Because the bound (1.2) is known, we may determine a suitable value $\mu > 0$ by the discrepancy principle, i.e., we choose $\mu > 0$ so that

$$\|Ax_\mu^\delta - b^\delta\|_Y = \tau\delta,$$

where $\tau > 1$ is a user-supplied constant that is independent of δ. We refer to x_μ^δ as an *approximate* or *regularized* solution of (1.1).

The Tikhonov regularization problem (1.3)-(1.4) is said to be in *standard form*, because the penalty term is the square of the X-norm of the computed solution. Determining the minimum of (1.4) is equivalent to solving the normal equations

$$(A^*A + \mu I)x = A^* b^\delta, \tag{1.5}$$

where A^* denotes the adjoint of A.

It is well known that Tikhonov regularization in standard form typically determines a regularized solution x_μ^δ that is too smooth, i.e., many details of the desired solution $x^\dagger$ are not represented by x_μ^δ. This shortcoming led Klann and Ramlau [6] to introduce the fractional Tikhonov regularization method. Subsequently another approach, also referred to as fractional Tikhonov regularization, was investigated by Hochstenbach and Reichel [4]. The latter approach fits both into the framework of generalized Tikhonov regularization introduced by Louis [7, Chapter 4] and into the framework presented in [8]. A more detailed comparison of the three approaches is presented in Section 3. Application of the fractional approach in [4] to Lavrentiev regularization is discussed in [5].

The method in [4] can be derived by replacing the Y-norm in the fidelity term in (1.4) by a weighted seminorm

$$\|y\|_W := \|W^{1/2}y\|_Y$$

with

$$W = (AA^*)^{(\alpha-1)/2} \tag{1.6}$$

for some parameter $0 \leq \alpha \leq 1$, where W is defined with the aid of the Moore–Penrose pseudoinverse of AA^* when $\alpha < 1$. We obtain the minimization problem

$$\min_{x\in X} \widetilde{J}_\mu(x) \tag{1.7}$$

with

$$\widetilde{J}_\mu(x) := \|Ax - b^\delta\|_W^2 + \mu\|x\|_X^2 \tag{1.8}$$

and denote its solution by $\widetilde{x}_\mu^\delta$. It can be computed by solving the associated normal equations

$$((A^*A)^{(\alpha+1)/2} + \mu I)x = (A^*A)^{(\alpha-1)/2}A^*b^\delta. \tag{1.9}$$

Oversmoothing in Tikhonov regularization in standard form (which corresponds to $\alpha = 1$) is caused by the fact that b^δ is multiplied by A^*. Letting $0 < \alpha < 1$ reduces oversmoothing. We will show that, by the theory presented in [7, 8], choosing $-1 < \alpha \leq 1$ is possible.

Klann and Ramlau [6] propose another approach to reduce oversmoothing. They advocate that an approximation of $x^\dagger$ be computed by solving

$$(A^*A + \mu I)^\alpha x = (A^*A)^{\alpha-1}A^*b^\delta \tag{1.10}$$

for some $0 < \alpha \leq 1$, where $(A^*A)^{\alpha-1}$ is defined with the Moore–Penrose pseudoinverse when $\alpha < 1$. This leads to an interpolation between standard Tikhonov regularization and the generalized inverse. We denote the solution by $\widehat{x}_\mu^\delta$. Also this method simplifies to Tikhonov regularization in standard form when $\alpha = 1$.

The present paper is organized as follows. Section 2 introduces necessary notation. We show in Section 3 that the method defined by (1.7)-(1.8) is an order optimal regularization method for suitable parameters α. Moreover, we show that both fractional methods defined by (1.7)-(1.8) and (1.10) are order optimal when used with the discrepancy principle. A discussion on advantages and disadvantages of these fractional methods concludes the section. Section 4 contains a few illustrative numerical examples. Concluding remarks can be found in Section 5.

2 Regularization methods and filter factors

This section reviews definitions and properties of regularization methods; see, e.g., [2,7] for further details. A *regularization method* for $A^\dagger$ is a family of operators

$$\{R_\mu\}_{\mu>0}, \quad R_\mu : Y \to X$$

with the following properties: There is a mapping $\mu : \mathbb{R}_+ \times Y \to \mathbb{R}_+$ such that for all $b \in \mathcal{D}(A^\dagger)$ and all $b^\delta \in Y$ with $\|b - b^\delta\|_Y \leq \delta$, it holds

$$\lim_{\delta \searrow 0} R_{\mu(\delta, b^\delta)} b^\delta = A^\dagger b.$$

Here μ is a regularization parameter.

The quality of a regularization method is determined by the asymptotics of $\|A^\dagger b - R_\mu b^\delta\|_X$ as $\delta \searrow 0$. Convergence rates can only be achieved under additional assumptions on the solution. For our analysis, we assume a Hölder-type smoothness assumption, i.e., that the minimal norm solution $x^\dagger$ of the error-free problem (1.1) satisfies a smoothness condition of the form

$$x^\dagger \in \text{range}\left((A^*A)^{\nu/2}\right) \quad \text{with} \quad \|x^\dagger\|_\nu := \left(\sum_{n\geq 1} \sigma_n^{-2\nu} |\langle x^\dagger, u_n\rangle|^2\right)^{1/2} \leq \rho \tag{2.1}$$

for some constant ρ. Here $(\sigma_n; u_n, v_n)_{n\geq 1}$ is the singular system of the operator A. A regularization method is said to be *order optimal* if there is a constant c independent of δ and ρ such that

$$\|x^\dagger - R_\mu b^\delta\|_X \leq c\, \delta^{\frac{\nu}{\nu+1}} \cdot \rho^{\frac{1}{\nu+1}}.$$

It is well known that Tikhonov regularization in standard form is an order optimal method, see, e.g., [2].

Generalized Tikhonov regularization is obtained by replacing the penalty term in (1.4) by $\|Bx\|_X^2$, where $B : \mathcal{N}(A)^\perp \to X$ is an operator whose domain $\mathcal{D}(B)$ is dense in $\mathcal{N}(A)^\perp$ and $(B^*B)^{-1} : \mathcal{N}(A)^\perp \to X$ is continuous. Here $\mathcal{N}(A)^\perp$ denotes the orthogonal complement of the null space of A. The associated functional is

$$J_{\mu,B}(x) := \|Ax - b^\delta\|_Y^2 + \mu\|Bx\|_X^2. \tag{2.2}$$

Certain conditions on the operator B allow for results on optimality and order optimality of generalized Tikhonov regularization; see Louis [7]. In the next section we show the equivalence of generalized Tikhonov regularization with a special operator B and fractional Tikhonov regularization (1.8).

Filter factors provide insight into the properties of regularization methods. Let the linear compact operator A have the singular system $(\sigma_n; u_n, v_n)_{n\geq 1}$. We replace the Moore–Penrose generalized inverse of A by an operator R_μ defined by

$$R_\mu b^\delta := \sum_{\sigma_n>0} F_\mu(\sigma_n)\sigma_n^{-1}\langle b^\delta, v_n\rangle u_n. \tag{2.3}$$

The real-valued function F_μ is referred to as a filter function and its values $F_\mu(\sigma_n)$ as filter factors; $\mu > 0$ is a regularization parameter. Thus, $R_\mu b^\delta$ furnishes an approximation of $x^\dagger$. For example, Tikhonov regularization in standard form can be characterized by the filter function

$$F_\mu^{\text{Tikh}}(\sigma) = \frac{\sigma^2}{\sigma^2+\mu}. \tag{2.4}$$

That is, the minimizer of (1.4) can also be computed as

$$x_\mu^\delta = \sum_{\sigma_n>0} \frac{\sigma_n}{\sigma_n^2+\mu}\langle b^\delta, v_n\rangle u_n.$$

as well as by (1.5). The filter function associated with the fractional Tikhonov regularization method (1.7)-(1.8) is given by

$$\widetilde{F}_{\mu,\alpha}(\sigma) = \frac{\sigma^{\alpha+1}}{\sigma^{\alpha+1}+\mu} \tag{2.5}$$

and gives the associated approximation

$$\widetilde{x}_\mu^\delta = \sum_{\sigma_n>0} \frac{\sigma_n^\alpha}{\sigma_n^{\alpha+1}+\mu}\langle b^\delta, v_n\rangle u_n \tag{2.6}$$

of $x^\dagger$. This expression is provided in [4] with slightly different notation. There also graphs of the filter functions as functions of σ for different values of α are shown.

The fractional Tikhonov method (1.10) can be written in terms of a filter function in a similar fashion. We have

$$\widehat{F}_{\mu,\alpha}(\sigma) := (F_\mu^{\text{Tikh}}(\sigma))^\alpha = \left(\frac{\sigma^2}{\sigma^2+\mu}\right)^\alpha. \tag{2.7}$$

Graphs of these filter functions can be found in [6]. The corresponding approximation of $x^\dagger$ is given by

$$\widehat{x}_\mu^\delta = \sum_{\sigma_n>0} \left(\frac{\sigma_n^{2-1/\alpha}}{\sigma_n^2+\mu}\right)^\alpha \langle b^\delta, v_n\rangle u_n. \tag{2.8}$$

3 Order optimality of fractional Tikhonov methods

The method (1.7)-(1.8), introduced here as described in [4], can be treated as a special case of the methods proposed by Louis [7] and Mathé and Tautenhahn [8]. Their convergence results apply to the method (1.7)-(1.8). We will show in this section that the results by Louis [7] and Mathé and Tautenhahn [8] coincide for the special case of fractional Tikhonov regularization (1.7)-(1.8). It is worth mentioning that neither in [7] nor [8] the applicability of the methods was discussed; no numerical experiments were shown. One of the major concerns of this paper is to show that fractional Tikhonov methods only in certain situations are preferable to Tikhonov regularization in standard form.

Louis [7] considers a special case of generalized Tikhonov regularization (2.2) and obtains with $B^*B = (A^*A)^{-\eta}$ the normal equations

$$(A^*A + \mu(A^*A)^{-\eta})x_\mu^\delta = A^*b^\delta, \tag{3.1}$$

where $(A^*A)^{-1}$ is replaced by the Moore–Penrose pseudoinverse if A is not invertible. Louis [7, Satz 4.2.3] establishes that this method is order optimal for $\eta \geq -1/2$ under an a priori parameter choice rule if $x^\dagger$ fulfills (2.1) with $\nu \leq 2\eta + 2$. Multiplying (3.1) by $(A^*A)^\eta$ and setting $\eta = \frac{\alpha-1}{2}$ we obtain (1.9). Hence, with this correlation between the parameters, we can immediately conclude that the fractional Tikhonov method (1.8) is order optimal for $\alpha \geq 0$ and $\nu < \alpha + 1$. Results from Louis's book [7] make is possible to extend the range of α to $-1 < \alpha \leq 1$ using the following theorem (given here with slightly different notation).

Theorem 3.1. [7, Theorem 3.4.3] *Let* $b \in \operatorname{range}(A)$ *and* $\|b - b^\delta\|_Y \leq \delta$. *Let* $F_{\mu,\alpha}(\sigma)$ *be a regularizing filter* [1] *and assume that for* $0 \leq \nu \leq \nu^*$,

$$\sup_{0<\sigma\leq\sigma_1} \sigma^{-1}|F_{\mu,\alpha}(\sigma)| \leq c\mu^{-\beta} \quad \text{and} \quad \sup_{0<\sigma\leq\sigma_1} |1 - F_{\mu,\alpha}(\sigma)|\sigma^{\nu^*} \leq c_{\nu^*}\mu^{\beta\nu^*}, \tag{3.2}$$

where $\beta > 0$ *and* c, c_{ν^*} *are constants independent of* δ. *Then with the a priori parameter choice*

$$\mu = C\left(\frac{\delta}{\rho}\right)^{1/\beta(\nu+1)}, \qquad C > 0 \quad \text{fixed},$$

the method induced by the filter $F_{\mu,\alpha}$ *is order optimal for all* $0 \leq \nu \leq \nu^*$.

[1] A filter $F_{\mu,\alpha}$ is said to be regularizing, if $\sup_n |F_{\mu,\alpha}(\sigma_n)\sigma_n^{-1}| = c(\mu) < \infty$, $\lim_{\mu\to 0} F_{\mu,\alpha} = 1$ point wise in σ_n and $|F_{\mu,\alpha}(\sigma_n)| \leq c$ for all μ and σ_n, c.f. [7, Definition 3.3.2]

Lemma 3.2. *The regularizing filter* $\tilde{F}_{\mu,\alpha}(\sigma)$ *from* (2.5) *with* $-1 < \alpha \leq 1$ *fulfills* (3.2) *with* $\beta = \frac{1}{\alpha+1}$ *and* $\nu^* = \alpha + 1$.

Proof. The filter $\tilde{F}_{\mu,\alpha}(\sigma)$ is continuous on $(0, \infty)$. The regularizing properties of the filter $F_{\mu,\alpha}$ are easily verified. One sees that

$$\lim_{\sigma\to 0} \sigma^{-1}|\tilde{F}_{\mu,\alpha}(\sigma)| = \lim_{\sigma\to\infty} \sigma^{-1}|\tilde{F}_{\mu,\alpha}(\sigma)| = 0,$$

$$\lim_{\sigma\to 0} |1 - F_{\mu,\alpha}(\sigma)|\sigma^{\nu} = 0,$$

$$\lim_{\sigma\to\infty} |1 - F_{\mu,\alpha}(\sigma)|\sigma^{\nu} = \begin{cases} \infty & \nu > \alpha + 1, \\ 1 & \nu = \alpha + 1, \\ 0 & \nu < \alpha + 1. \end{cases}$$

Hence, as long as $\nu < \alpha + 1$, the suprema in (3.2) are attained as local maxima, which can be derived by simple calculus. One obtains

$$\sup_{0<\sigma\leq\sigma_1} \sigma^{-1}|F_{\mu,\alpha}(\sigma)| \leq c\mu^{-\frac{1}{\alpha+1}} \quad \text{and} \quad \sup_{0<\sigma\leq\sigma_1} |1 - F_{\mu,\alpha}(\sigma)|\sigma^{\nu^*} \leq c_{\nu^*}\mu^{\frac{1}{\alpha+1}\nu}.$$

□

Consequently, by Theorem 3.1 the fractional method (1.7)-(1.8) is order optimal for $-1 < \alpha \leq 1$ and $0 \leq \nu \leq \alpha + 1$.

Now let us investigate the connection of the fractional Tikhonov regularization (1.7)-(1.8) to [8]. There, without mentioning the previous work by Louis [7], the authors considered the solution of the equation

$$((A^*A)^{s+1} + \mu I)x_\mu^\delta = (A^*A)^s A^* b^\delta, \tag{3.3}$$

for $s > -1$, assuming that

$$||(A^*A)^{q/2}(b - b^\delta)|| \leq \delta \quad \text{and} \quad x^\dagger \in \{x \in X : (A^*A)^{p/2}v, ||v|| \leq E\}. \tag{3.4}$$

Therefore, setting $s = \frac{\alpha-1}{2}$, $q = 0$, $p = \nu$ and $E = \rho$, we arrive exactly at the fractional method (1.7)-(1.8) in the setting introduced in Section 1. The following result is shown in [8].

Theorem 3.3. *Under the assumptions* (3.4) *and with* $\mu = \left(\frac{\delta}{E}\right)^{(2s+2)/(p+q+1)}$, *the method* (3.3) *is of optimal order provided that* $s \geq \max(\frac{p-2}{2}, \frac{q-1}{2})$.

Translating this theorem into our notation for the fractional Tikhonov method (1.7)-(1.8), we obtain order optimality provided that $\alpha \geq \max(\nu - 1, 0)$, i.e., $\nu \leq \alpha + 1$ in case $\nu > 1$. We summarize the results in the following theorem.

Theorem 3.4. *Let $A : X \to Y$ be a linear compact operator between Hilbert spaces X and Y. Let $x^\dagger := A^\dagger b$ satisfy $\|x^\dagger\|_\nu \leq \rho$. Then for all $-1 < \alpha \leq 1$ and $0 \leq \nu \leq \alpha + 1$ the fractional Tikhonov method* (1.7)-(1.8) *is of optimal order under the a-priori parameter choice rule*

$$\mu = C \left(\frac{\delta}{\rho}\right)^{(\alpha+1)/(\nu+1)}.$$

While the method (1.8) is order optimal for all $-1 < \alpha \leq 1$ and appropriate ν, this is not the case for the fractional Tikhonov method (1.10). We have the following result.

Proposition 3.5. [6, Proposition 3.2] *Let $A : X \to Y$ be a compact operator with singular system $(\sigma_n, u_n, v_n)_{n\geq 0}$, and let $x^\dagger := A^\dagger b$ satisfy $\|x^\dagger\|_\nu \leq \rho$ for some constant ρ and the ν-norm defined by* (2.1). *Then for $\alpha \in (1/2, 1]$, the fractional Tikhonov method* (1.10) *is order optimal with the parameter choice rule*

$$\mu = C \left(\frac{\delta}{\rho}\right)^{1/2(\nu+1)}$$

for all $0 < \nu < 2$. Here C is a positive constant independent of δ and ρ.

Klann and Ramlau [6, Theorem 4.4] show that after appropriate presmoothing of the error-contaminated data b^δ, fractional powers $0 < \alpha \leq 1/2$ together with a suitable choice of the regularization parameter μ yield quasi-optimal convergence rates.

The above approaches to determine μ generally are not very useful for the solution of specific problems. When an accurate estimate of the norm of the error in the data $\|b^\delta - b\|_Y$ is known, the *discrepancy principle*, discussed, e.g., in [2, 9], can be applied to determine a suitable value of μ. The idea is to choose the value of μ so that the residual is approximately of the same norm as the error in the data b^δ. There are several slightly different formulations of the discrepancy principle. Here we will choose $\mu = \mu(\delta, b^\delta)$ such that

$$\|Ax_\mu^\delta - b^\delta\|_Y = \tau\delta, \tag{3.5}$$

where $\tau > 1$ is a user-supplied constant independent of δ. This is a nonlinear equation for μ. Its solution can be calculated by finding the positive zero of

$$G_\alpha(\mu) := \sum_{n\in\mathbb{N}} (1 - F_{\mu,\alpha}(\sigma))^2 \langle b^\delta, v_n\rangle^2 - (\tau\delta)^2, \tag{3.6}$$

for example with Newton's method; see, e.g., [4] for further details. This reference discusses linear discrete ill-posed problems, but the results carry over to the setting of the present paper.

Convergence of regularized approximate solutions determined by filtered regularization methods using the discrepancy principle has been analyzed in the works of Louis [7] and Mathé and Tautenhahn [8]. As for the a-priori parameter choice, the order optimality of the fractional Tikhonov method (1.7)-(1.8) is derived immediately from both [7] and [8] by identifying corresponding parameters as done in the first part of this section. Thus without going into detail again, the following theorem follows independently from [7, Theorem 3.5.2] and [8, Theorem 2.4].

Theorem 3.6. *Let $A : X \to Y$ be a linear compact operator between Hilbert spaces X and Y. Let $x^\dagger := A^\dagger b$ satisfy $\|x^\dagger\|_\nu \leq \rho$. Then for all exponents $\alpha > 0$ and $0 < \nu \leq \alpha$, the fractional Tikhonov method* (1.7)-(1.8) *is order optimal with the regularization parameter μ determined by the discrepancy principle* (3.5).

Remark 3.7. It might appear appealing to substitute the standard norm in (3.5) by the weighted norms from (1.8) (or (3.4) for $-1 < q < 0$, respectively). Then with $W = (A^*A)^{(\alpha-1)/2}$,

$$\|A\widetilde{x}_\mu^\delta - b^\delta\|_W^2 = \sum_{\sigma_n > 0} (1 - \widetilde{F}_\mu(\sigma_n))^2 \sigma_n^{\alpha-1} \langle b^\delta, v_n \rangle^2. \tag{3.7}$$

However, since $\lim_{\sigma_n \to 0} \widetilde{F}_\mu(\sigma_n) = 0$, the sum typically will not converge since for large n the inner products $\langle b^\delta, v_n \rangle$ generally are dominated by the error in b^δ and may converge to zero slowly. In a discrete setting, in actual computations using finite-precision arithmetic, the quantities $\langle b^\delta, v_n \rangle$ also are contaminated by propagated round-off errors introduced during the computations. The residual (3.7) therefore will be very large due to error amplification, and the equation

$$\|A\widetilde{x}_\mu^\delta - b^\delta\|_W = \tau\delta$$

is not guaranteed to have a solution. Hence, the weighted residual norm is in general not useful for determining the regularization parameter in actual computations.

Order optimality for the fractional Tikhonov method (1.10) can be shown with the help of the results in [7].

Theorem 3.8. *Let $A : X \to Y$ be a linear compact operator between Hilbert spaces X and Y. Let $x^\dagger := A^\dagger b$ satisfy $\|x^\dagger\|_\nu \leq \rho$. Then for all exponents*

$\alpha \in (1/2, 1]$ *and* $0 < \nu \leq 1$, *the fractional Tikhonov method of* (1.10) *is order optimal with the regularization parameter* μ *given by the discrepancy principle* (3.5).

Proof. Klann and Ramlau showed in [6] that the filter function (2.7) fulfills (3.2) with $\beta = \frac{1}{2}$ and $\nu^* = 2$ for $\alpha > \frac{1}{2}$. Hence, by [7, Theorem 3.5.2], the claim follows. □

Approximations of $x^\dagger$ determined by fractional Tikhonov regularization typically are closer to $x^\dagger$ in the X-norm than approximations obtained with Tikhonov regularization in standard form; see [4] for computed examples. However, a smaller error does not always correspond to a more pleasing approximation of $x^\dagger$, because the fractional Tikhonov approximation may be more oscillatory than the approximation determined by Tikhonov regularization in standard form. We would like to elucidate in which situations fractional methods yield more pleasing approximations. The following lemma is helpful. A similar result has been shown in [4].

Lemma 3.9. *Let the mappings* $\mu \mapsto F_{\mu,\alpha}(\sigma)$ *and* $\alpha \mapsto F_{\mu,\alpha}(\sigma)$ *be continuous and monotonically decreasing for* $\mu > 0$ *and* α *in an interval* $\underline{\alpha} < \alpha < \overline{\alpha}$. *Let* $\mu = \mu(\alpha)$ *be determined by the discrepancy principle* (3.5). *Then* $\frac{d\mu(\alpha)}{d\alpha} < 0$.

Proof. We can write (3.6) in the form $G(\alpha, \mu(\alpha)) = 0$. Since G is differentiable, we have

$$\frac{dG}{d\mu} = \sum_{\sigma_n > 0} 2(1 - F_{\mu,\alpha}(\sigma_n)) \cdot (-1) \cdot \frac{dF_{\mu,\alpha}}{d\mu} \cdot \langle b^\delta, v_n \rangle^2 \quad > 0,$$

because $1 - F_{\mu,\alpha}(\sigma) > 0$ and $\frac{dF_{\mu,\alpha}}{d\mu} < 0$. Analogously, one finds that $\frac{dG}{d\alpha} > 0$. Hence, by the implicit function theorem,

$$\frac{d\mu}{d\alpha} = -\left(\frac{dG}{d\mu}\right)^{-1} \frac{dG}{d\alpha} < 0.$$

□

An immediate consequence of the above lemma is that decreasing α results in an increase of the regularization parameter μ. It is therefore inappropriate to compare fractional methods with the standard Tikhonov filter using the same regularization parameter.

We are now in position to take a closer look at the computed approximations. Again we will make use of the explicit representation of the solution in terms of the singular system of A. Let

$$\epsilon = b^\delta - b.$$

Since

$$\sigma_n \langle x^\dagger, u_n \rangle = \langle x^\dagger, A^* v_n \rangle = \langle b, v_n \rangle,$$

cf. [2], and

$$\langle b^\delta, v_n \rangle = \langle b, v_n \rangle + \langle \epsilon, v_n \rangle,$$

the approximation error $e(\delta, \alpha, \mu) := x^\dagger - R_\mu b^\delta$ is given by

$$e(\delta, \alpha, \mu) = \sum_{\sigma_n > 0} \left(1 - F_{\mu,\alpha}(\sigma_n)\right) \langle x^\dagger, u_n \rangle u_n + \sum_{\sigma_n > 0} F_{\mu,\alpha}(\sigma_n) \frac{1}{\sigma_n} \langle -\epsilon, v_n \rangle u_n. \tag{3.8}$$

Let ϵ be fixed. The quality of the computed solution then is determined by the positive coefficients $1 - F_{\mu,\alpha}(\sigma)$ and $F_{\mu,\alpha}(\sigma)$. One immediately sees that the filter $F_{\mu,\alpha}(\sigma)$ has to achieve two contradicting properties: $F_{\mu,\alpha}(\sigma)$ should be close to one to give a small deviation of the reconstruction from $x^\dagger$, and $F_{\mu,\alpha}(\sigma)$ should be close to zero in order to effectively reducing propagation of the error ϵ into the computed approximation.

It is not obvious from (3.8) in which situations letting $\alpha < 1$ improves the quality of the computed approximation of $x^\dagger$. We can shed some light on this by studying the derivative $\frac{d}{d\alpha} F_{\mu,\alpha}(\sigma)$. We first consider the filter function (2.5). Since μ depends on α (the function (3.6) used to calculate μ depends on α via the filter functions $F_{\mu,\alpha(\sigma)}$), we get

$$\frac{d}{d\alpha} \widetilde{F}_{\mu,\alpha}(\sigma) = -\frac{d}{d\alpha} \left(1 - \widetilde{F}_{\mu,\alpha}(\sigma)\right) = h(\sigma, \alpha, \mu(\alpha)) \left(\ln \sigma - \frac{\mu'(\alpha)}{\mu(\alpha)}\right), \tag{3.9}$$

where $h(\sigma, \alpha, \mu(\alpha))$ is a positive function. The sign of the derivative is determined by the factor $\ln \sigma - \frac{\mu'(\alpha)}{\mu(\alpha)}$. When α and the error norm δ are fixed, so is μ, and the sign only depends on σ. By Lemma 3.9, $\mu'(\alpha) < 0$. Therefore, the derivative (3.9) changes sign at some $0 < \widetilde{\sigma}_0 < 1$. Only for n with $\sigma_n < \widetilde{\sigma}_0$, the coefficient of $\langle x^\dagger, u_n \rangle$ in (3.8) will be reduced by decreasing α, since then $\frac{d}{d\alpha}(1 - \widetilde{F}_{\mu,\alpha}(\sigma_n)) > 0$. Hence, the coefficient of $\langle \epsilon, v_n \rangle$ increases. The opposite holds true for the coefficients of the terms associated with the propagated error. Whereas for large σ_n the propagated error is damped, it is amplified for all $\sigma_n < \widetilde{\sigma}_0$.

The result for the fractional filter (2.7) is analogous. Similarly to (3.9), one has

$$\begin{aligned}\frac{d}{d\alpha}\widehat{F}_{\mu,\alpha}(\sigma) &= -\frac{d}{d\alpha}\left(1-\widehat{F}_{\mu,\alpha}(\sigma)\right)\\ &= \widehat{h}(\sigma,\alpha,\mu(\alpha))\left(-\ln\left(\frac{\sigma^2+\mu(\alpha)}{\sigma^2}\right)-\alpha\frac{\mu'(\alpha)}{\sigma^2+\mu(\alpha)}\right) \qquad (3.10)\end{aligned}$$

with $\widehat{h}(\sigma,\alpha,\mu(\alpha)) > 0$. The logarithm is positive and $\mu'(\alpha) < 0$. Therefore, the sign of (3.10) changes at some $\sigma = \widehat{\sigma}_0 > 0$. Hence, the above discussion also applies to this filter function. However, it is not clear whether the operator A has singular values that satisfy $\sigma_n > \widehat{\sigma}_0$. If this is not the case, then decreasing α will result in error amplification in all components of the computed approximate solution.

Although it is an open problem how to determine a value of α that yields the best approximation of $x^\dagger$, we can identify two situations in which fractional Tikhonov methods outperform standard Tikhonov regularization (1.3)-(1.4):

a) the problem is severely ill-posed, i.e., the singular values of A decrease rapidly to zero, and

b) the error in b^δ is concentrated to low frequencies.

In case the problem is severely ill-posed, $\widetilde{\sigma}_0$ and $\widehat{\sigma}_0$ are likely to be large enough for the propagated error to be damped. A slight loss in accuracy of terms in (2.6) and (2.8) associated with large singular values is typically acceptable, since they are much larger than the error and therefore usually are recovered quite accurately. On the other hand, if there is only little error in the high frequency components in (2.6) and (2.8), the amplification of the error in b^δ is largely avoided, while the reconstruction is improved. In other cases, both fractional methods do not perform significantly better than Tikhonov regularization in standard form. The reason for this can again be found in the dependency of the filter factors $F_{\mu,\alpha}(\sigma)$ on the parameters α and μ. By decreasing α, the filter factors $F_{\mu,\alpha}(\sigma)$ increase. At the same time, decreasing α increases the regularization parameter μ as shown in Lemma 3.9. From the definition of the filter factors (2.5) and (2.7), respectively, one sees that this leads to decreasing values of the filter factors. Hence, both effects cancel each others out to some extend. Although α is decreased below one, the filter factors corresponding to larger singular values stay almost constant. The following section provides some illustrative computed examples.

4 Numerical examples

Several computed examples that show the performance of the fractional Tikhonov regularization methods discussed in this paper are provided in [4, 6]. These examples demonstrate that it may be attractive to use fractional Tikhonov methods instead of standard Tikhonov regularization. In this paper, we present a few examples that show the relative performance of the fractional methods (1.7)-(1.8) and (1.10), and that illustrate the comments in the last paragraph of the previous section.

Our first example is a severely ill-posed Fredholm integral equation of the first kind given by

$$b_1(s) = [A_1 x](s) = \int_0^1 \sqrt{s^2 + t^2} x(t) dt, \quad 0 \le s \le 1, \tag{4.1}$$

with error-free data $b_1(s) = \frac{1}{3}\left((1+s^2)^{3/2} - s^3\right)$ and solution $x_1^\dagger(t) = t$. This equation was first introduced by Fox and Goodwin, cf. [1]. Numerically, the singular values decrease exponentially until they stagnate around attainable computational precision. We used the discretization of (4.1) provided in Regularization Tools [3]. This gave a 1000×1000 matrix.

The second example is the mildly ill-posed Volterra integral equation of the first kind

$$b_2(s) = [A_2 x](s) = \int_0^s x(t) dt, \quad 0 \le s \le 1, \tag{4.2}$$

with error-free data

$$b_2(s) = \begin{cases} -s & 0 \le s \le 0.5, \\ s-1 & 0.5 < s \le 1, \end{cases}$$

and solution

$$x_2^\dagger(t) = \begin{cases} -1 & 0 \le t \le 0.5, \\ 1 & 0.5 < t \le 1. \end{cases}$$

This example has been used in [6]. The coefficients $\langle x_1^\dagger, u_n \rangle$ decrease slowly to zero. The singular system $\{\sigma_n; u_n, v_n\}_{n \ge 1}$ of A_2 (without discretization) is given in [7]. The integration problem (4.2) has been discretized with the Nyström method based on the trapezoidal rule with 1000 equidistant nodes.

In all experiments shown, we equipped both the domain and range of the discretized operators with the Euclidean vector norm. We added noise with prescribed noise level $\eta := \frac{||b - b^\delta||}{||b||}$ to the error-free data b.

We compare approximate solutions obtained by the two fractional methods (1.7)-(1.8) (denoted by $\tilde{x}_{\mu,\alpha}^\delta$) and (1.10) (denoted by $\hat{x}_{\mu,\alpha}^\delta$) with the approximate solution determined by Tikhonov regularization in standard form (1.4) (denoted by $\bar{x}_\mu^\delta$). The key ingredient for this is a comparable choice of the regularization parameter. For all approximate solutions, the regularization parameter is determined by the discrepancy principle (3.5). It turns out, that the relative performance of the fractional methods when compared to Tikhonov regularization in standard form varies significantly with the choice of the free parameter τ in (3.5). We therefore conduct the following experiment. For each $\tau \in \{1, 1.05, 1.1, 1.2, 1.3, 1.4, 1.5\}$, we compute the standard Tikhonov solution $\bar{x}^{\delta}_{\mu(\tau)}$ and solutions for the fractional methods (1.7)-(1.8) and (1.10) for the fractional parameters α from discrete sets $\mathcal{A}_1 := \{-1 + 0.05i, i = 0, 1, 2, \ldots, 40\}$ and $\mathcal{A}_2 := \{0.05i, i = 0, 1, 2, \ldots, 20\}$, respectively. Out of all these solutions, we select for each fractional method and each τ the best approximation. In other words, we choose $\alpha^*(\tau)$ such that it gives the minimum deviation from the true solution $x^\dagger$ over all α-values considered,

$$\tilde{x}^{\delta}_{\mu(\tau),\alpha^*} := \min_{\alpha \in \mathcal{A}_1} ||\tilde{x}^{\delta}_{\mu(\tau),\alpha} - x^\dagger|| \quad \text{and} \quad \hat{x}^{\delta}_{\mu(\tau),\alpha^*} := \min_{\alpha \in \mathcal{A}_2} ||\hat{x}^{\delta}_{\mu(\tau),\alpha} - x^\dagger||.$$

We compute for both fractional methods the relative deviation when compared to Tikhonov regularization in standard form,

$$\widetilde{\mathrm{re}}(\tau) = \frac{\|\tilde{x}^{\delta}_{\mu(\tau),\alpha^*} - x^\dagger\|}{\|\bar{x}^{\delta}_{\mu(\tau)} - x^\dagger\|} \quad \text{and} \quad \widehat{\mathrm{re}}(\tau) = \frac{\|\hat{x}^{\delta}_{\mu(\tau),\alpha^*} - x^\dagger\|}{\|\bar{x}^{\delta}_{\mu(\tau)} - x^\dagger\|}. \tag{4.3}$$

The quantities $\widetilde{\mathrm{re}}(\tau)$, $\widehat{\mathrm{re}}(\tau)$, and the optimal fractional parameters are plotted as functions of τ in Figure 1 for the Fox–Goodwin problem (4.1). Only one realization of perturbed data is used for this experiment. Figure 1 is typical for many experiments. The fractional methods can be seen to yield reconstruction errors that are smaller than those obtained with Tikhonov regularization in standard form. For $\tau \geq 1.05$, the error obtained with the method (1.7)-(1.8) is about half the error obtained with standard Tikhonov regularization. Also direct inspection of the computed solutions, shown in Figure 6, strongly favors this fractional method. However, for $\tau = 1$, the difference in performance is almost negligible. In fact, in a direct comparison of the three approximate solutions computed with the fractional and standard Tikhonov methods, the difference between these solutions is barely visible. Moreover, for some noisy right-hand sides, with the same noise characteristics as in Figure 1 but different realizations of the noise, standard Tikhonov regularization with $\tau = 1$ gives the best reconstruction. The regularization parameters for the fractional methods and Tikhonov regularization in standard form are shown in Figure 2. For all $\tau \geq 1$, the regularization parameter for the latter method is much smaller than for the fractional methods.

We now carry out the same experiment as above with the integration problem (4.2). The result is shown in Figure 3. Observe that for this problem Tikhonov regularization in standard form with the regularization parameter obtained for $\tau = 1$ always gives the best solution. Although for larger τ-values the fractional methods give a slightly smaller error, one would nevertheless typically prefer the solution obtained with Tikhonov regularization in standard form since it is smoother than the fractional solutions. A typical case is shown in Figure 7. The plot of the regularization parameters is similar to the corresponding plot for the Fox–Goodwin problem; see Figure 2. We should mention that the relative performance of the methods in our comparison does not change significantly if a different true solution $x^\dagger$ is chosen. The properties of the operator A are far more important than the choice of true solution for the performance of the methods.

Our experience with the Fox–Goodwin problem leads us to conclude that it is important to carefully chose the parameter τ in a comparison of the methods in order to avoid a bias towards fractional Tikhonov methods. To make this point even more evident, we repeat the above experiment, but now calculate the relative reconstruction errors

$$\widetilde{\mathrm{re}_1}(\tau) = \frac{\|\tilde{x}^\delta_{\mu(\tau),\alpha^*} - x^\dagger\|}{\|\bar{x}^\delta_{\mu(1)} - x^\dagger\|} \quad \text{and} \quad \widehat{\mathrm{re}_1}(\tau) = \frac{\|\hat{x}^\delta_{\mu(\tau),\alpha^*} - x^\dagger\|}{\|\bar{x}^\delta_{\mu(1} - x^\dagger\|}, \tag{4.4}$$

with respect to the solution obtained with Tikhonov regularization in standard form for fixed $\tau = 1$; see Figure 4. For the integration problem the relative reconstruction errors do not change much, but for the Fox–Goodwin problem they increase by a large factor. A comparison with Figure 1 illustrates that, although for each value of τ the fractional methods are better than Tikhonov regularization in standard form, this claim does not hold anymore when $\tau = 1$ is used for Tikhonov regularization in standard form. Hence, it is important to choose τ carefully when comparing methods.

In the above examples the data was perturbed by white Gaussian noise. The observation of Section 3 leads us to repeat the experiments with low-frequency noise. An example of this kind of noise and a comparison with white noise is displayed in Figure 8. Figure 9 shows the fractional methods to give more accurate approximations of $x^\dagger$ than Tikhonov regularization in standard form for low-frequency noise. The improved performance for low-frequency noise becomes even more evident if instead of a one-dimensional signal a two-dimensional image is taken as the true solution. Figure 5 compares the solutions obtained with the methods (1.7)-(1.8), (1.10) and (1.4) for a chessboard-like image $x^\dagger$ of size 75×75 pixels which has been blurred using a blurring matrix that is block Toeplitz with Toeplitz blocks with bandwidth 6 and approximates a Gaussian point-spread function with variance $\sigma = 0.7$. The regularization parameter was determined by the discrepancy principle (3.5) with $\tau = 1$. For this example, the method (1.10) produces the best approximation of the exact image. The reconstruction error is only 36% of the reconstruction error determined by Tikhonov regularization in standard form.

To further illustrate the different behaviors of the methods in our comparison

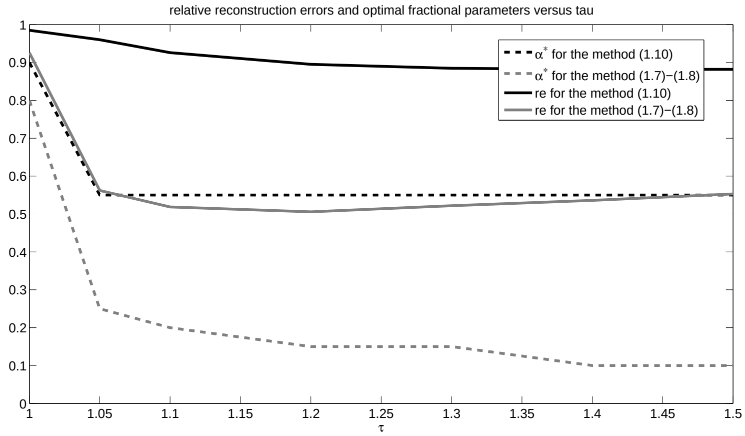

Figure 1. Relative errors from (4.3) and optimal fractional parameters α^* as functions of τ for the Fox–Goodwin problem (4.1) with white noise of level $\eta = 0.05$. The larger τ is chosen, the more favorable in particular the fractional method (1.7)-(1.8) becomes. For $\tau = 1$, the difference is almost negligible.

in the settings introduced above, we include tables in which we give regularization parameters and approximation errors relative to those obtained with Tikhonov regularization in standard form (4.3). All errors are averages over 20 experiments with different error-realizations. Table 1 shows results for the Fox–Goodwin problem (4.1). In agreement with Figure 6, the fractional method (1.7)-(1.8) performs the best. For the problem (4.2) with Gaussian white noise, the error in the approximate solutions determined by the fractional methods is only slightly smaller than the error obtained with Tikhonov regularization in standard form, as shown in Table 2. However, using the same problem with low-frequency error instead of white Gaussian error, the fractional methods yield a much better approximations of $x^\dagger$ than Tikhonov regularization in standard form; see Table 3.

5 Conclusion

We have investigated the fractional Tikhonov method of [4], defined by (1.7)-(1.8), and the fractional Tikhonov method [6], given by (1.10). The method of [4] is shown to be a special case of more general approaches presented in [7, 8], and we used this to establish that the method is of optimal order for a certain interval of parameters α with an appropriate choice of the regularization parameter. Moreover, we demonstrated that both fractional Tikhonov methods are of optimal

α	0.05	0.1	0.3	0.5	0.6	0.7	0.9	1
$\widetilde{\mu}$	6.1e-3	5.9e-3	5.2e-3	4.3e-3	3.8e-3	3.3e-3	2.4e-3	2.0e-3
$\widehat{\mu}$	1.1e-1	3.9e-2	8.2e-3	4.4e-3	3.5e-3	2.9e-3	2.2e-3	2.0e-3
$\widetilde{\mathrm{re}}$	10.3	5.2	1.5	0.60	0.61	0.72	0.92	1
$\widehat{\mathrm{re}}$	2.4e15	4.7e13	1e7	4.2	0.93	0.91	0.97	1

Table 1. Regularization parameter and relative reconstruction error for both fractional filters, tilde standing for (1.7)-(1.8), hat for (2.7); and the Fox–Goodwin problem (4.1). In both cases μ grows monotonically with decreasing α. The reconstruction errors (4.3) are shown in the two bottom rows. For the method (1.7)-(1.8), there is a minimum clearly below one. Hence, the reconstructions are significantly improved. Since for $\alpha < 0.5$ the filter (2.7) is not regularizing anymore, the reconstruction error explodes.

α	0.05	0.1	0.3	0.5	0.6	0.7	0.9	1
$\widetilde{\mu}$	4.7e-3	4.3e-3	2.7e-3	1.6e-3	1.3e-3	1.0e-3	0.6e-3	0.4e-3
$\widehat{\mu}$	3.4e-2	1.1e-2	2.3e-3	1.1e-3	0.8e-3	0.7e-3	0.5e-3	0.4e-3
$\widetilde{\mathrm{re}}$	2.7	2.3	1.4	1.07	1.02	0.991	0.990	1
$\widehat{\mathrm{re}}$	21.8	12.5	2.3	1.13	1.03	1.007	0.998	1

Table 2. Regularization parameter and relative reconstruction error for both fractional filters and the integration problem (4.2). In both cases μ grows monotonically with decreasing α. The reconstruction errors (4.3) grow nearly monotonically, only for α close to one it is slightly below one, i.e., the fractional methods give a slightly lower residual than Tikhonov regularization in standard form.

α	0.05	0.1	0.3	0.5	0.6	0.7	0.9	1
$\widetilde{\mu}$	6.0e-3	5.5e-3	3.8e-3	2.6e-3	2.1e-3	1.7e-3	1.1e-3	0.9e-3
$\widehat{\mu}$	3.9e-2	1.4e-2	3.5e-3	1.9e-3	1.5e-3	1.3e-3	1.0e-3	0.9e-3
$\widetilde{\mathrm{re}}$	0.62	0.65	0.75	0.84	0.88	0.91	0.97	1
$\widehat{\mathrm{re}}$	0.54	0.60	0.81	0.91	0.94	0.96	0.99	1

Table 3. Regularization parameter and relative reconstruction error for both filters and the integration problem (4.2) in presence of low frequency noise (cf. Figure 8). The reconstruction errors (4.3) are shown in the two bottom rows. Both fractional filters give a much better result than Tikhonov regularization in standard form.

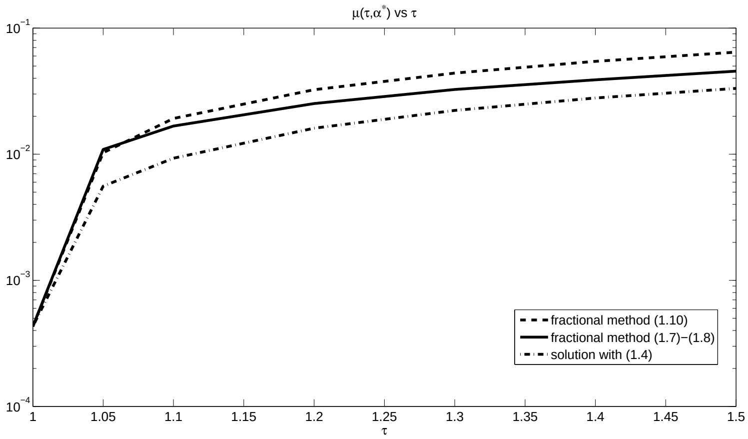

Figure 2. Regularization parameter for the solutions with the methods (1.7)-(1.8), (1.10) and (1.4) for the Fox–Goodwin problem (4.1) with white noise of level $\eta = 0.05$, obtained by the discrepancy principle (3.5). For $\tau = 1$ the regularization parameters almost coincide whereas for larger τ the regularization parameter of Tikhonov regularization in standard form is significantly smaller than for the fractional methods. The same quality of the curves is obtained for the integration problem (4.2).

order with the discrepancy principle. Our analysis suggested two situations in which the fractional methods are significantly better than Tikhonov regularization in standard form. This is confirmed by numerical experiments. We showed that the choice of the parameter $\tau \geq 1$ in (3.5) is important for the comparison.

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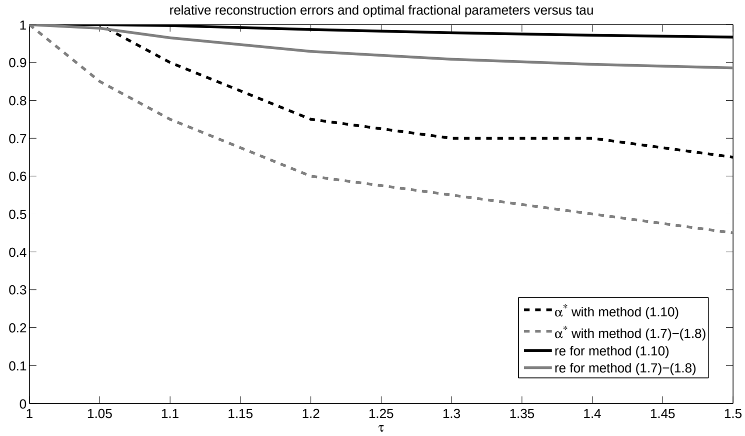

Figure 3. Relative errors from (4.3) and optimal fractional parameters α^* as functions of τ for the integration problem (4.2) with white noise of level $\eta = 0.05$. Even for large values of τ, there is not a big difference between the fractional methods and Tikhonov regularization in standard form.

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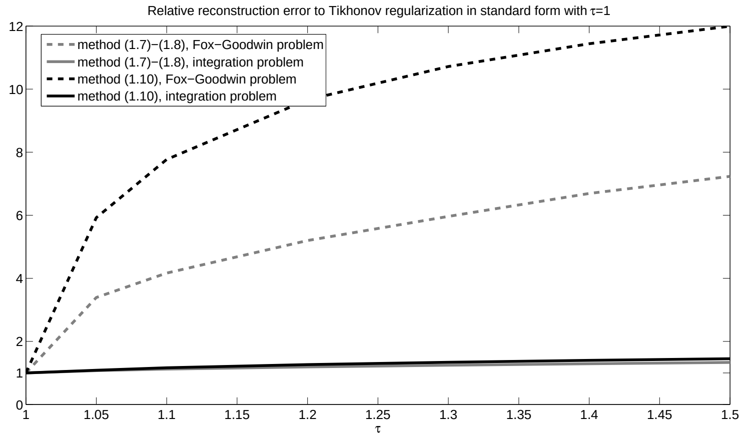

Figure 4. Comparison of relative reconstruction errors (4.4). For the integration problem (4.2), increasing τ does not change the error much. However, for the Fox–Goodwin problem (4.1), the difference becomes much more evident.

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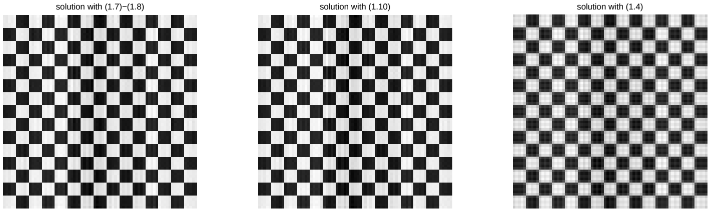

Figure 5. Comparison of fractional Tikhonov methods and Tikhonov regularization in standard form for a two dimensional deblurring problem of size 75×75 with low-frequency noise of noise level $\eta = 0.05$. The solutions obtained with the fractional methods provide much sharper edge recovery. The best fractional parameters were $\alpha^* = 0.05$ for the method (1.10) and $\alpha^* = -1$ for the method (1.7)-(1.8). The relative reconstruction error to Tikhonov solution in standard form (see (4.3)) are $\widehat{\text{re}} = 0.36$ and $\widetilde{\text{re}} = 0.48$, respectively.

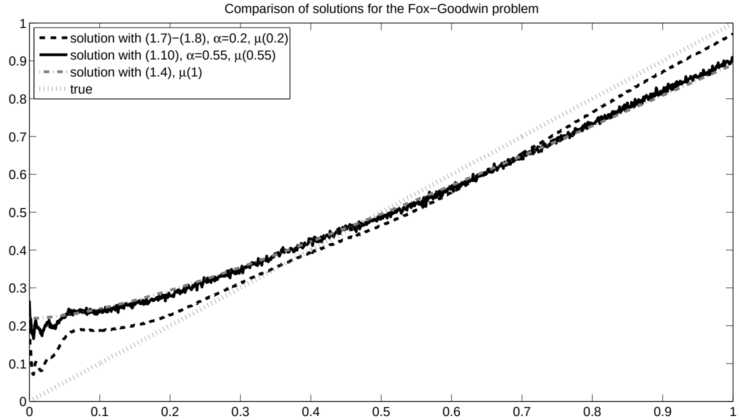

Figure 6. Comparison of solutions for the severely ill-posed Fox–Goodwin problem (4.1) with Gaussian white noise of level $\eta = 0.05$, μ according to (3.5), $\tau = 1.1$. For the fractional methods the solutions with smallest reconstruction error are shown. The solution for the method (1.7)-(1.8) is plotted with the dashed line. For this type of problems it is to be preferred over the other two methods. Those are the method (1.10) (solid) and Tikhonov regularization in standard form (dash-dotted).

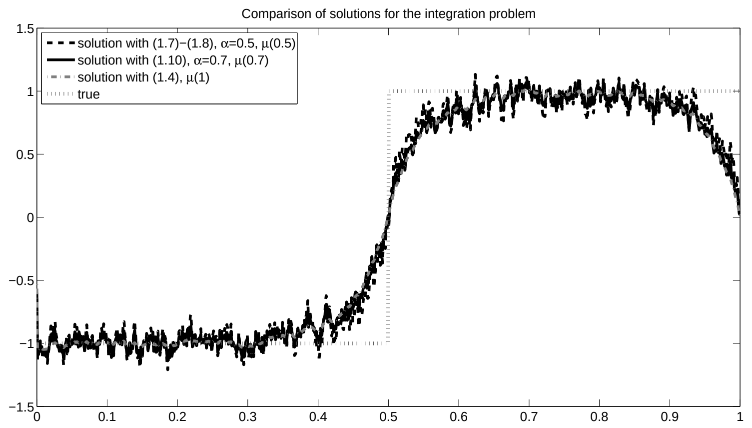

Figure 7. Comparison of solutions for the mildly ill-posed integration problem (4.2) with Gaussian white noise of level $\eta = 0.05$, μ according to (3.5), $\tau = 1.1$. Upper plot: discontinuous solution, lower plot: smooth solution. In this case the fractional methods (1.7)-(1.8) and (1.10) do not perform better than Tikhonov regularization in standard form. On the contrary, the noise is amplified even more.

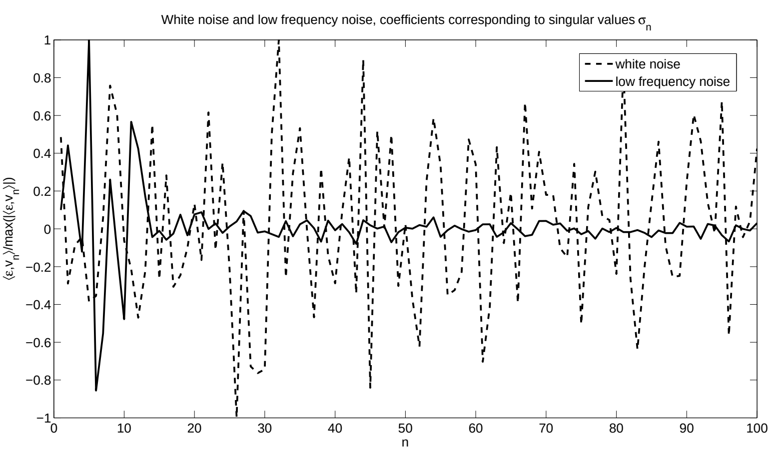

Figure 8. Comparison of typical random draws of white noise and low-frequency noise w.r.t. the singular values. For white noise, the coefficients are equally distributed over all singular values. The low-frequency noise decreases with growing n.

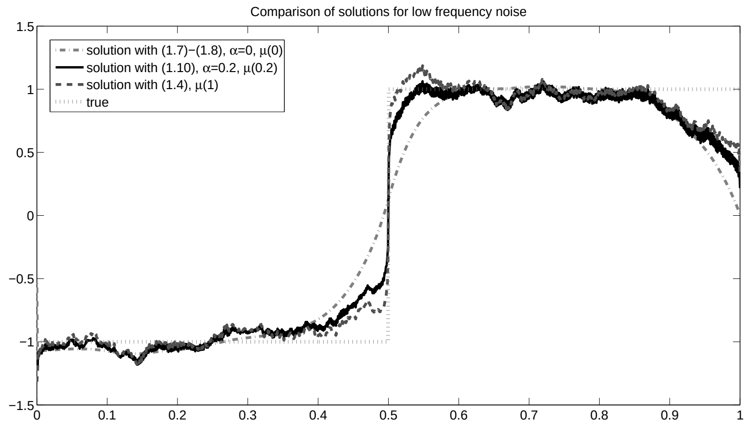

Figure 9. Comparison of solutions for the mildly ill-posed integration problem (4.2) with low-frequency noise (c.f. Figure 8) of level $\eta = 0.05$, μ according to (3.5), $\tau = 1.1$ The solution of the fractional methods (1.7)-(1.8) (dashed) and (1.10) (solid) with appropriate α approximate the discontinuity much better than the results of Tikhonov regularization in standard form (dash-dotted).