An Iterative Tikhonov Method for Large Scale Computations.

E. Loli Piccolomini∗ F. Zama†

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Abstract

In this paper we present an iterative method for the minimization of the Tikhonov regularization functional in the absence of information about noise. Each algorithm iteration updates both the estimate of the regularization parameter and the Tikhonov solution. In order to reduce the number of iterations, an inexact version of the algorithm is also proposed. In this case the inner Conjugate Gradient (CG) iterations are truncated before convergence. In the numerical experiments the methods are tested on inverse ill posed problems arising both in signal and image processing.

Keywords: Regularization methods, Tikhonov method, Truncated Conjugate Gradient method, Ill-posed problems, Integral equations.

1 Introduction

A large variety of applications give raise naturally to ill-posed problems whenever the underlying physical or technical problem is modeled by an integral equation of the first kind with a smooth kernel. These inverse problems are mathematically modeled by

\[ Hx = y \]  

(1)

where \( H \) denotes a compact operator between Hilbert spaces \( \mathcal{X} \) and \( \mathcal{Y} \).

The data \( y \) usually stem from measurements with a limited precision, i.e., only perturbed data \( y^\delta \) with an error bound

\[ ||y - y^\delta|| \leq \delta \]

are available. The inverse problem is ill-posed since \( H \) is not continuously invertible or, equivalently, the set \( \{ x \in \mathcal{X} : ||Hx - y|| \leq \delta \} \) is unbounded. This instability requires regularization methods for treating the inverse problem.

∗Department of Mathematics, University of Bologna, e-mail: piccolom@dm.unibo.it
†Department of Mathematics, University of Bologna, e-mail: zama@dm.unibo.it
One of the most used and well established regularization method is the Tikhonov-Phillips regularization method which finds the solution $x^\delta$ to the following minimization problem:

$$\min_x \|Hx - y^\delta\|^2 + \lambda\|Lx\|^2$$

where $\lambda$ is known as regularization parameter whose value must be determined. The operator $L$ is used to impose some constraints about the smoothness of the solution.

The aim of this paper is to describe an iterative algorithm which computes a good approximate solution of the problem (2) within a practically acceptable number of iterations without any information about noise.

The computation of the regularization parameter is a delicate subject. There exists a significant amount of research in the development of appropriate strategies for selecting regularization parameters (see [5, 2, 1, 3, 6]). Some of these techniques, such as Generalized Cross Validation (GCV) and L-Curve, need to try a large number of regularization parameters in order to find a reasonably good value. This can be very time-consuming. Some other techniques require some additional information about the noise present in the data or about the amount of regularization prescribed by the optimal solution. In this work we assign the value of the ratio between the regularization part $\|Lx\|^2$ and the value of the Tikhonov functional $\|Hx - y^\delta\|^2 + \lambda\|Lx\|^2$, in the hypotheses that the regularization part should somehow preserve the fidelity to the data represented by the residual norm $\|Hx - y^\delta\|^2$. We propose a method for updating the value of the regularization parameter which decreases the Tikhonov functional if the regularization part is too large and increases it otherwise. In order to gain more efficiency by limiting the number of inner CG iterations, we use the properties of the given update method to stop the CG iterations and update the regularization parameter using only the solution and residual vectors computed in the inner CG iterations.

In section 2 we propose a general framework for updating the value of the regularization parameter and we derive the increase/decrease properties of the Tikhonov functional. We obtain an iterative algorithm without truncating the inner CG iterations. In section 3 a an inexact version of the algorithm is proposed by truncating the inner CG iterations. In section 4 we report the numerical examples relative to the methods proposed in sections 2 and 3 and finally the conclusions are given in section 5.

## 2 Tikhonov Iterative Method

The Tikhonov method is based on the property that the functional

$$\Theta(x, \lambda) = \|Hx - y^\delta\|^2 + \lambda\|Lx\|^2$$

has a unique minimizer for any value $\lambda > 0$, provided that

$$\mathcal{N}(H) \cap \mathcal{N}(L) = \{0\}$$
where $\mathcal{N}(\cdot)$ is the null space of a matrix. Denoting $x_\lambda$ such a minimizer, it can be characterized as the solution of the system:

$$(H^*H + \lambda L^*L)x_\lambda = H^*y^\delta$$

(4)

or in variational form:

$$(Hx_\lambda, Hv) + \lambda(Lx_\lambda, Lv) = (y^\delta, Hv) \quad \forall v \in \mathcal{X}$$

(5)

We define an iterative procedure to compute the values $(x_k, \lambda_k)$, where $\lambda_k$ is obtained by means of an additive update method and $x_k$ is computed applying CG iterations to (4) with $\lambda = \lambda_k$.

In the following propositions we state some properties of the Tikhonov functional $\Theta$ (3) as a consequence of the regularization parameter update method.

**Proposition 1.** Let $(x_k, \lambda_k)$ be such that $\lambda_k > 0$ and

$$(Hx_k, Hv) + \lambda_k(Lx_k, Lv) = (y^\delta, Hv) \quad \forall v \in \mathcal{X}.$$  

(6)

By setting $\lambda_{k+1} = \lambda_k + \mu$ with $|\mu| < \lambda_k$

(7)

then the Tikhonov functional $\Theta$ has the following properties:

$$0 < \Theta(x_k, \lambda_{k+1}) < \Theta(x_k, \lambda_k), \quad \text{if } \mu < 0$$

(8)

$$0 < \Theta(x_k, \lambda_k) < \Theta(x_k, \lambda_{k+1}) < \Theta(x_k, 2\lambda_k), \quad \text{if } \mu > 0$$

(9)

**Proof.** Using (7) we have:

$$\Theta(x_k, \lambda_{k+1}) = \|Hx_k - y^\delta\|^2 + (\lambda_k + \mu)\|Lx_k\|^2$$

If $\mu < 0$ then $0 < \lambda_{k+1} < \lambda_k$ and this proves: (8)

$$\Theta(x_k, \lambda_{k+1}) < \Theta(x_k, \lambda_k).$$

If $\mu > 0$ then $0 < \lambda_k < \lambda_{k+1} < 2\lambda_k$ and we have

$$\Theta(x_k, \lambda_k) < \Theta(x_k, \lambda_{k+1}) < \Theta(x_k, 2\lambda_k).$$

**Proposition 2.** Let $\lambda_{k+1} > 0$ as in (7) and $x_{k+1}$ the minimizer of the Tikhonov functional $\Theta(x, \lambda_{k+1})$. Then

$$0 < \Theta(x_{k+1}, \lambda_{k+1}) < \Theta(x_k, \lambda_{k+1}), \quad \text{if } \mu < 0$$

(10)

$$0 < \Theta(x_k, \lambda_k) < \Theta(x_{k+1}, \lambda_{k+1}) < \Theta(x_k, \lambda_{k+1}) \quad \text{if } \mu > 0.$$  

(11)
Proof. The relation (10) and the right inequality of (11) follow immediately by observing that
\[ \Theta(x_{k+1}, \lambda_{k+1}) < \Theta(x, \lambda_{k+1}), \; \forall x \in \mathcal{X}. \]

In order to prove the left inequality in (11) we have:
\begin{align*}
\Theta(x_{k+1}, \lambda_{k+1}) &= \| Hx_{k+1} - y_\delta \|^2 + \lambda_{k+1}\| Lx_{k+1} \|^2 \\
&= \| Hx_{k+1} - y_\delta \|^2 + \lambda_k\| Lx_{k+1} \|^2 + \mu\| Lx_{k+1} \|^2. \quad (12)
\end{align*}

Since \( \mu > 0 \):
\[ \Theta(x_{k+1}, \lambda_{k+1}) > \| Hx_{k+1} - y_\delta \|^2 + \lambda_k\| Lx_{k+1} \|^2 = \Theta(x_{k+1}, \lambda_k) \]

Since \( \Theta(x_k, \lambda_k) \) is the minimum of \( \Theta(x, \lambda_k) \), then \( \Theta(x_{k+1}, \lambda_k) > \Theta(x_k, \lambda_k) \). \qed

In the case \( L = I \) different approaches can be found in the literature to obtain an iterative implementation of the Tikhonov method. In [6] the discrepancy principle is used to compute a solution \( x_\delta \) such that \( \| Hx_\delta - y_\delta \|^2 < \tau \delta \) with \( \tau > 1 \) where \( \lambda_k = 1/2^k, \; k > 0 \). In this case the noise \( \delta \) must be estimated and \( \lambda_k \) is a decreasing sequence with a prescribed behavior which does not depend on the problem. In [8],[7] the Tikhonov problem is seen as a special instance of trust-region subproblem:

\[ \min \| Hx - y_\delta \|^2 : \| x \| < \Delta \]

requiring the value \( \Delta \) which prescribes the regularity of the solution. The computation of the regularization parameter requires the solution of a large scale eigenvalue problem at each outer iteration and does not apply to the case \( L \neq I \).

Aim of this work is to compute a good approximating sequence of regularized solutions \( x_k \) and regularization parameters \( \lambda_k \) in the general case \( L \neq I \). We implement an iterative algorithm to solve the Tikhonov problem (2) with an outer iteration loop to update the regularization parameter \( \lambda \) and an inner iteration loop to solve the equation (4). The inner loop is implemented by CG iterations while the outer loop is performed by using some additional knowledge about the problem.

In order to update the value of \( \lambda \), we consider the Tikhonov functional \( \Theta \) as a weighted sum of the residual norm \( \| Hx - y_\delta \|^2 \) related to the data fidelity and the regularization norm \( \| Lx \|^2 \) which takes into account the required regularity of the solution.

Definition 3. Let \( \hat{\gamma} \) the prescribed weight of regularization part \( \| Lx \|^2 \) with respect to the Tikhonov functional. For each given value of \( \lambda_k \) we compute \( x_k \) by solving (2) and \( \gamma_k \) as:
\[ \gamma_k = \frac{\| Lx_k \|^2}{\Theta(x_k, \lambda_k)}. \]

Using the following rule to update the regularization parameter:
\[ \mu = \lambda_k/2, \; \lambda_{k+1} = \lambda_k + \text{sign}(\hat{\gamma} - \gamma_k)\mu, \]

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we define the Tikhonov CG Algorithm (TKCG) for obtaining a suitable regularized solution of (2).

Algorithm 1 (TKCG Algorithm).
Choose $\lambda_0 > 0$ and set $\mu = \lambda_0$.
Choose $\hat{\gamma} > 0$

for $k = 0, 1, 2, \ldots$

1. Computation of the approximate solution $x_k$
   Compute $x_k$ by applying the CG method to (4) setting $\lambda = \lambda_k$;

2. Computation of the weight factor $\gamma_k$
   $\gamma_k = \|Lx_k\|^2/\Theta(x_k, \lambda_k)$;

3. Update the regularization parameter
   Set $\mu = \mu/2$;
   Set $\lambda_{k+1} = \lambda_k + \text{sign}(\hat{\gamma} - \gamma_k)\mu$;

4. Set $k = k + 1$;

The TKCG method represents an extension to the method presented in [9] where the Tikhonov functional $\Theta(x_k, \lambda_k)$ has a decreasing behavior. In algorithm 1 the value of the Tikhonov functional decreases when $\gamma_k > \hat{\gamma}$ and increases otherwise. Indeed using the propositions 1 and 2 we obtain that:

- if $\gamma_k > \hat{\gamma}$ then $\Theta(x_{k+1}, \lambda_{k+1}) < \Theta(x_k, \lambda_k)$
- if $\gamma_k < \hat{\gamma}$ then $\Theta(x_k, \lambda_k) < \Theta(x_{k+1}, \lambda_{k+1}) < \Theta(x_k, 2\lambda_k)$.

The complexity of this procedure is given by the number of CG iterations required in the solution of the system $(H^*H + \lambda_kL^*L)x_k = H^*y_\delta$, $k = 0, 1, \ldots$.

The number of CG iterations can become quite large as the value of $\lambda$ decreases, hence the idea of truncating the iterations of the Conjugate Gradient method is quite common in the literature. As observed by some authors ([6], [3]), it is not necessary to search for an accurate solution $x_k$ when $\lambda_k$ is far from being accurate.

3 Inexact Tikhonov Iterations

In this section we define an inexact version of the method presented in the previous section, where the CG iterations are stopped as soon as a suitable value for the update $\mu$ is computed.
We remind that the regularization parameter is computed by means of the following update formula:

\[ \lambda_{k+1} = \lambda_k + \text{sign}(\hat{\gamma} - \gamma_k)\mu, \quad \mu > 0 \]  

The first strategy to obtain the value of \( \mu \) is derived by the variational form (5). Let \( z^{(m)} \) be the \( m \)-th iterate of the CG method applied to the normal equations (4) started with \( z^{(0)} = x_{k-1} \) and \( \lambda = \lambda_k \), then:

\[ (H^*H + \lambda_k L^*L)z^{(m)} = H^*y^\delta - r^{(m)} \]  \hspace{1cm} (14)

which is equivalent to the variational formulation:

\[ (Hz^{(m)}, Hv) + \lambda_k (Lz^{(m)}, Lv) = (y^\delta, Hv) \quad \forall v \in X. \]  \hspace{1cm} (15)

We define \( \lambda_{k+1} \) such that:

\[ (r^{(m)}, v) = 0 \quad \forall v \in X. \]

i.e.

\[ (Hz^{(m)}, Hv) + \lambda_{k+1} (Lz^{(m)}, Lv) = (y^\delta, Hv) \quad \forall v \in X. \]  \hspace{1cm} (16)

Subtracting (15) from (16) we have that:

\[ (\lambda_{k+1} - \lambda_k) (Lz^{(m)}, Lv) = (r^{(m)}, v) \quad \forall v \in X. \]

We define a suitable value for the parameter \( \mu \) by computing \( |\lambda_{k+1} - \lambda_k| \) and choosing \( v = z^{(m)} \):

**Rule 1.** \[ \mu = \frac{|(r^{(m)}, z^{(m)})|}{\|Lz^{(m)}\|^2}. \]  \hspace{1cm} (17)

An alternative rule to compute \( \mu \) is obtained by imposing that \( \lambda_{k+1} \) and \( z^{(m)} \) satisfy the normal equations system:

\[ (H^*H + \lambda_{k+1} L^*L)z^{(m)} = H^*y^\delta. \]  \hspace{1cm} (18)

Subtracting (14) from (18), we have:

\[ (\lambda_{k+1} - \lambda_k) L^*Lz^{(m)} = r^{(m)}. \]

We solve the least squares problem

\[ \min_{\sigma} \|\sigma L^*Lz^{(m)} - r^{(m)}\|^2 \]

and set \( \mu = |\sigma| \):

**Rule 2.** \[ \mu = \frac{|(Lz^{(m)})^*Lr^{(m)}|}{\|L^*Lz^{(m)}\|^2}. \]  \hspace{1cm} (19)

In several applications, when the Rule 1 produces small values of \( \mu \), we propose an alternative update formula:

**Rule 3.** \[ \mu = \lambda_k |(r^{(m)}, z^{(m)})|/\|r^{(m)}\|^2. \]  \hspace{1cm} (20)
The index $m$ where the CG iterations are stopped is such that $\mu < \lambda_k$ in order to satisfy the proposition 1.

In the case of Rule 1 and Rule 2 we observe that $r(m)$ is the residual vector of the normal equations system (18) where the matrix is symmetric positive definite, then $\|r(m)\| \to 0$ when $m \to \infty$ and it is possible to find an index $m$ such that $(r(m), z(m))$ or $(Lz(m), Lr(m))$ is sufficiently small. In the case of Rule 3, the condition $\lambda_k+1 > 0$ is equivalent to the condition:

$$\|(r(m), z(m))\|/\|r(m)\|^2 < 1.$$  

This condition is likely to be satisfied only in the first few CG iterations, where the residual norm is still large and the solution norm is small. Since it may not be verified for large values of $m$, in the algorithm implementation, we stop the CG iterations at the first index $m$ that satisfies Rule 1 or Rule 3.

**Definition 4.** We define the steps of the inexact Tikhonov CG Algorithm (TKTRCG) as follows:

**Algorithm 2 (TKTRCG Algorithm).**

Choose $\gamma > 0$, $z(0) = 0$ and $\lambda_0 > 0$.

for $k = 0, 1, 2, \ldots$

1. **Computation of the approximate solution** $x_k$
   
   Perform CG iterations in (14) until:
   
   $\mu < \lambda_k$ (17) or (19) or (20).
   
   Let $m$ be number of performed iterations and
   
   $z(m)$ the computed solution;
   
   Set $x_k = z(m)$.

2. **Computation of the weight factor** $\gamma_k$
   
   $\gamma_k = \|Lx_k\|^2/\Theta(x_k, \lambda_k)$;

3. **Update the regularization parameter by** (13)

4. Set $k = k + 1;

end

The starting value of $\lambda_0$ has usually been set equal to 1. In the case the algorithm requires too many external iterations, the value $\lambda_0$ may be changed to a more suitable value. Good heuristic initial estimates have been computed by performing one CG iteration and computing $\lambda_0 = \|(r(1), z(1))\|$ where $r(1) = H^*y^\delta - H^*Hz(1)$.

The TKTRCG algorithm relies on matrix vector products only and has fixed storage requirements features that make it suitable for large scale computations. All the values required by the update formulas of the regularization parameter are computed in the inner CG iterations. The outer iterations can be terminated using criteria based on the value of $\mu$ as well as $\Theta(x_k, \lambda_k)$ as presented in [9];

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1. $|\lambda_{k+1} - \lambda_k| < \tau_\lambda$ with $\tau_\lambda \simeq 10^{-6}$;
2. $|\Theta(x_k, \lambda_k) - \Theta(x_{k+1}, \lambda_{k+1})| < \tau_\Theta \Theta(x_k, \lambda_k)$ with $\tau_\Theta \simeq 10^{-3}$.

4 Numerical results

In this section we report some numerical results showing the behavior of the algorithms 1 and 2 presented in the previous sections.

The first test problem is the blur test problem from the Regularization Tool [4]. It arises from the discretization of a first kind Fredholm integral equation on 100 points. White noise of levels $10^{-4}$ and $10^{-3}$ have been added in order to simulate noisy data. It has been solved both with the TKCG and the TKTRCG methods, by using the proposed criteria 17 (TKTRCG(1)) and 19(TKTRCG(2)). The algorithms has been stopped after a fixed number of external iterations and the best results in terms of relative error $E_{\text{rel}}$:

$$E_{\text{rel}} = \frac{\|x - \tilde{x}\|_2}{\|x\|_2}$$

between the exact and the computed solutions ($x$ and $\tilde{x}$, respectively) has been considered. The value of the parameter $\tilde{\gamma}$ used in this test problem is $\tilde{\gamma} = 10^{-6}$. Figure 1 shows the exact (continuous line) and reconstructed signal with TKTRCG (dotted line) in the case of $L = I$ and noise of level $1.e^{-3}$. Table 1 reports all the results obtained on this test problem. The second column indicates the order $d$ of the differential operator used as regularization matrix: $d = 0$ is used to indicate the identity operator $L = I$, $d = 1$ is a first order differential operator $L = \nabla$ and $d = 2$ indicates the second order Laplace operator $L = \nabla^2$. The third column is the level of white noise introduced, the fourth column reports the number of performed iterations (external between parentheses), and $\lambda$ is the value of the regularization parameter obtained by the method and used in the computation of the solution. When $d = 0$ ($L = I$) the two criteria are the same and only one of the two results is reported. From the table, we can conclude that the TKCG method converge towards a good regularized solution. Moreover, when the TKTRCG algorithm is used the number of iterations (and the computational time) dramatically decreases without affecting the accuracy of the solution, for at least one of the two stopping criteria. Usually the rule 1 (17) works better.

In table 2 we report the results obtained on the same test problem by computing the regularization parameter with the Lcurve [5] and the Generalized Cross Validation (GCV) [2] methods. We used the functions implemented in the Regularization Toolbox. The $E_{\text{relLc}}$ and $E_{\text{relGCV}}$ values are the relative errors between the exact solution and the solutions obtained with the regularization parameter computed by the Lcurve ($\lambda_{\text{Lc}}$) and GCV ($\lambda_{\text{GCV}}$) methods, respectively. From the table it is evident that the GCV method gives better results than L-curve in this test problem and the L-curve fails in some cases (see, for example, the case $d = 2$ with noise $10^{-3}$). The GCV results are similar.
to those of the TKTRCG method, but the computational time required by the GCV method is extremely high, especially when the problem size increases.

The last test problem is an image restoration problem. The discrete model, deriving from the discretization of a Fredholm integral equation of the first kind, is given by:

\[ Hf = g \]

where \( H \) represents the Point Spread Function (PSF), \( f \) is the object, i.e. the exact image, and \( g \) is the blurred and noisy image. We considered two different objects \( f \): a 256 \( \times \) 256 pixels photographic image (the peppers image, figure 2) and a 128 \( \times \) 128 pixels Magnetic Resonance image (the mri image, figure 3). The blurred image \( g \) was obtained by convolving \( f \) with a gaussian PSF implemented in the blur function of the Regularization Tool [4] and by adding gaussian white noise.

In this case we used only the identity operator (\( L = I \)) and the rule (20) for the regularization parameter update. The images have been restored by using both the TKCG and the TKTRCG methods. In these test problems we used the value: \( \hat{\gamma} = 10^{-5} \). The Tikhonov method has also been applied with a suitable heuristic choice of the regularization parameter, in order to compare the results obtained (the L-curve and GCV method have prohibitive costs in the case of images). The errors have been measured through the relative error \( E_{rel} \) between the exact and reconstructed images. The results are presented in table 3. The table shows that the errors obtained with the TKTRCG method are lower than the best result with the Tikhonov method. The computed values of the regularization parameter are very similar to the best heuristic value for the peppers image, while they differ in the case of the mri image.

We can finally observe that in the numerical experiments considered the TKTRCG method usually gives better results with a lower computational cost. The value of the regularization parameter \( \lambda \) obtained with the two proposed method, TKCG and TKTRCG, is different. The value of \( \lambda \) obtained with the TKTRCG method is smaller, because the truncated algorithm acts itself as regularization. In order to recover a more accurate approximation of the regularization parameter some heuristic a posteriori techniques need to be applied.

5 Conclusions

In this paper we presented a new method for the solution of an ill conditioned problem with the Tikhonov regularization method. The proposed TKCG method is an iterative method that estimates a suitable value for the regularization parameter in the absence of information on the noise and computes the solution of the Tikhonov functional. An inexact version, the TKTRCG method, has also been proposed. The method is efficient especially for large size problems, because of its low computational cost when compared with some methods known in literature, such as the L-curve or the GCV methods.

The methods have been tested on simulated problems represented by signal and image reconstructions. The numerical experiments showed the efficiency of
the methods in terms of both precision and computational time required.

References


Figure 1: Shaw test problem.

Figure 2: peppers test problem.
Figure 3: MRI test problem.

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Table 1: Numerical results for the Shaw test problem with the proposed TKCG and TKTRCG methods.
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<td>1.66e-1</td>
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<td>9.91e-2</td>
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<td>1.0e-4</td>
<td>1.167e-1</td>
<td>3.46e-1</td>
<td>9.683e-2</td>
<td>6.17e-2</td>
</tr>
<tr>
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<td>1.0e-3</td>
<td>6.548e-1</td>
<td>5.06e+1</td>
<td>1.688e1</td>
<td>9.18e-1</td>
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</tbody>
</table>

Table 2: Numerical results for the Shaw test problem when the regularization parameter is chosen by the Lcurve and GCV methods.

<table>
<thead>
<tr>
<th>test problem</th>
<th>method</th>
<th>noiselev</th>
<th>it (it.est)</th>
<th>$\text{erel}$</th>
<th>$\lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td>peppers</td>
<td>TKCG</td>
<td>3.e-2</td>
<td>197 (10)</td>
<td>7.6e-2</td>
<td>3.43e-2</td>
</tr>
<tr>
<td>peppers</td>
<td>TKTRCG</td>
<td>3.e-2</td>
<td>78(11)</td>
<td>6.28e-2</td>
<td>2.61e-2</td>
</tr>
<tr>
<td>peppers</td>
<td>Tikh</td>
<td>3.e-2</td>
<td>89</td>
<td>7.64e-2</td>
<td>3.2e-2</td>
</tr>
<tr>
<td>mri</td>
<td>TKCG</td>
<td>5.e-2</td>
<td>230 (6)</td>
<td>1.33 e-1</td>
<td>2.05e-2</td>
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<tr>
<td>mri</td>
<td>TKTRCG</td>
<td>5.e-2</td>
<td>13 (6)</td>
<td>1.29 e-1</td>
<td>4.44e-3</td>
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<tr>
<td>mri</td>
<td>Tikh</td>
<td>5.e-2</td>
<td>137</td>
<td>1.47e-2</td>
<td>2.e-2</td>
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</tbody>
</table>

Table 3: Numerical results for the image restoration problems.