A framework for studying the regularizing properties of Krylov subspace methods

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IIT TR-14/2004

Technical report

Dicembre 2004
A framework for studying the regularizing properties of Krylov subspace methods

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Abstract

Krylov subspace iterative methods have recently received considerable attention as regularizing techniques for solving linear systems with a coefficient matrix of ill-determined rank and a right-hand side vector perturbed by noise. For many of them little is known from this point of view. In this paper the regularizing properties of some methods of Krylov type (CGLS, GMRES, QMR, CGS, BiCG, Bi-CGSTAB) are examined in comparison with other regularization methods (truncated SVD, Tikhonov method, Landweber iteration) for which a complete theoretical analysis is available. Tools for measuring the regularization efficiency are introduced. An extensive experimentation validates the proposed measures on the studied methods. The problem of the choice of the regularization parameter is also addressed by examining the consistency with the discrepancy principle.

1 Introduction

Let

\[ Ax = b, \]  

be an \( n \times n \) linear system with a nonsymmetric coefficient matrix \( A \) and a right-hand side (r.h.s.) vector \( b \) belonging to the range of \( A \). We assume that \( A \) is a large matrix of ill-determined rank, i.e. \( A \) has singular values gradually decaying to zero, so that it is difficult to determine the numerical rank of \( A \). Let \( x^* = A^\dagger b \) be the minimal norm solution of (1). In many applications \( b \) is not exactly known, a perturbed vector \( b_\eta \) being available instead. For this kind of problems, known in the literature as discrete ill-posed problems \cite{6}, the solution \( A^\dagger b_\eta \) is often a poor approximation of \( x^\dagger \). In this case special techniques, called regularization methods, are used.

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Besides classical regularization techniques such as truncated SVD, Tikhonov method and Landweber iteration, iterative methods of Krylov type are presently receiving considerable attention (see for example [3, 4, 5, 6]).

The regularizing properties of conjugate gradient are well known, but little is known for other Krylov subspace methods, from this point of view. Recently the regularizing properties of GMRES method have been analyzed in [5] from a theoretical point of view. The regularizing properties of BiCG and QMR methods have been tested in [3] on an experimental basis. A theoretical analysis of some biconjugate methods would be interesting, but this task seems to be present difficult, taking into account that even convergence proofs are lacking. This paper aims to give a contribution to this discussion from an experimental point of view. The regularizing properties of different iterative methods of Krylov type are examined in comparison with the three classical methods: truncated SVD, Tikhonov method and Landweber iteration, by introducing tools for measuring the regularization efficiency.

For these three classical methods the filters are explicitly known and do not depend on the perturbed right-hand side. This fact allows us to give in a probabilistic setting an expression for the mean error of the solution of the perturbed problem, varying the noise, with respect to $x^*$. The definition of a measure of the regularizing efficiency based on the mean error provides the ground for validating the use of an analogous measure in a statistical setting, where it can be applied to the Krylov subspace methods, for which no explicit expression of the filters is available.

In Section 2 the general definitions and properties of the regularization methods are given. In Section 3 the error behaviour and the consistency with the discrepancy principle for the three classical methods are analyzed in the probabilistic setting. The statistical approach is introduced in Section 4 and the experimentation is described in Section 5, together with the conclusions.

## 2 Regularization methods

We consider the problem

$$Ax = b + \eta, \quad \text{(2)}$$

where $A$ is a rank-deficient or an ill-conditioned matrix and $\eta = \eta d$ is an unknown noise vector with $||d|| = 1$ and $\eta \leq 1$. Classical examples of ill-conditioned problems (2) arise from the discretization of Fredholm integral equations of the first kind (see [6], which is one of the starting points of the present paper).

Due to the presence of the noise, the vector $x^{(n)} = A^t(b + \eta)$ may differ much from $x^*$ and a regularized solution of (2) should be sought instead. In order to define what we mean by regularized solution and regularization method, we follow [2] and consider a family $\{A^{(n)}\}$ of linear operators, depending on the noise and on a regularization parameter $\omega \geq 0$. Each operator $A^{(n)}$ has a
bounded inverse $R^{(n)}_\omega$, approximating $A^\dagger$ in the sense that for any $\eta$

$$\lim_{\omega \to \infty} R^{(n)}_\omega b = A^\dagger b.$$  

(3)

Hence when the operators $R^{(n)}_\omega$ are applied to the r.h.s. of system (1), they produce better and better reconstructions of the exact solution $x^*$ for increasing values of $\omega$. When they are applied to the noisy r.h.s. vector, a different convergence behaviour occurs. In fact, let us consider the two systems

$$A^{(n)}_\omega x = b, \quad (4)$$
$$A^{(n)}_\omega x = b + \eta. \quad (5)$$

Let $y^*_\omega$ and $y^{(n)}_\omega$ be the solutions of (4) and (5) respectively. The error of $y^{(n)}_\omega$ with respect to $x^*$ is

$$e^{(n)}_\omega = ||x^* - y^{(n)}_\omega|| \leq ||x^* - y^*_\omega|| + ||y^*_\omega - y^{(n)}_\omega||.$$ 

Then $e^{(n)}_\omega$ is bounded from above by the sum of

1. an approximation error $\gamma^{(n)}_\omega = ||x^* - y^*_\omega|| = ||A^\dagger b - R^{(n)}_\omega b||$, due to the approximation of $A^\dagger$ by $R^{(n)}_\omega$,
2. a noise-propagation error $\delta^{(n)}_\omega = ||y^*_\omega - y^{(n)}_\omega|| = ||R^{(n)}_\omega \eta||$, due to the presence of the noise in the r.h.s. vector.

The two errors have an opposite behaviour as functions of $\omega$: typically, when $\omega \to \infty$ by (3) $\gamma^{(n)}_\omega$ has a behaviour decreasing, on the average, to 0, while $\delta^{(n)}_\omega$ has an increasing behaviour and, since $R^{(n)}_\omega$ approximates $A^\dagger$ and $A$ is ill-conditioned, $\delta^{(n)}_\omega$ assumes, on the average, large values for large $\omega$. Hence an optimal value $\omega_0$ exists such that $e^{(n)}_\omega$ has a minimum value.

To ensure that this error behaviour can be exploited in practice, for any $\eta$ the operators $A^{(n)}_\omega$ should enjoy the semiconvergence property. According to this property, a value $\omega_0$ exists such that, when $\omega \geq \omega_0$ exists until $\omega_0$, the computed solutions $y^{(n)}_\omega$ approach, on the average, the exact solution $x^*$, then go away. Then we say that a family $\{A^{(n)}_\omega\}$ represents a regularization method if it satisfies (3) and enjoys the semiconvergence property. The solution $y^{(n)}_\omega$, corresponding to the optimal choice of $\omega$, is called the regularized solution.

For a practical implementation of a regularization method the semiconvergence property is not enough: a technique which allows a sufficiently good approximation of $\omega_0$ is also required. Since our interest lies mainly in iterative methods, among the many available techniques for estimate $\omega_0$ the discrepancy principle will be here addressed. Let

$$res^{(n)}_\omega = ||b + \eta - Ay^{(n)}_\omega|| \equiv ||b + \eta d - Ay^{(n)}_\omega||$$  

(6)
be the residual norm of $y_\omega^{(n)}$. According to the discrepancy principle the optimal value $\omega_\eta$ should be chosen in such a way that the corresponding residual norm is approximately equal to $\eta$, i.e.

$$\text{res}_\omega^{(n)} \sim \alpha \eta,$$

for $\alpha > 0$ independent from $\eta$. For an effective use of this principle, the residual norm should have, on the average, a decreasing behaviour with respect to $\omega$. In this case we will say that the method is consistent with the discrepancy principle if it satisfies (7).

In [5] the regularization property is characterized through the consistency with the discrepancy principle. More precisely, a method is defined a regularization method if an $\alpha$ exists such that:

$$\lim_{\eta \to 0} \sup_d \epsilon_\omega^{(n)} = 0,$$

where $\omega$ is the lowest value for which $\|\text{res}_\omega^{(n)}\| \leq \alpha \eta$.

A simple classification of the operators $A_\omega^{(n)}$ can be made.

1. The operator $A_\omega^{(n)}$ is independent from the r.h.s. vector of (2), hence it does not depend directly on $\eta$, but only indirectly through the choice of $\omega$ which is usually related to $\eta$. These methods are extensively analyzed in the literature (see for example [6] and its large bibliography). Among them we focus our attention on three classical methods which represent different regularization strategies. In the following they will be collectively referred to as methods of Class I and for the corresponding operator we will drop the $\eta$ superscript. They share the property that the explicit expression of their filter factors is known.

(a) Truncated SVD technique. For this method $A_\omega$ is the matrix reconstructed from the SVD of $A$ by taking the $k$ largest singular values, where $k = \omega$. Hence $\omega \leq r$, where $r$ is the rank of $A$. In order to give a meaning to the limit in (3) also in this case, we should let $\omega$ vary on the natural numbers and set $k = \min \{r, \omega\}$. We set also $y_0^{(n)} = 0$ as the solution corresponding to the null operator.

(b) Tikhonov method. For this method $R_\omega = (A^TA + \lambda I)^{-1}A^T$, where $\lambda = 1/\omega$. It is reasonable to assume $y_0^{(n)} = 0$, since $R_0(b + \eta) = \lim_{\lambda \to \infty} R_{1/\lambda}(b + \eta) = 0$.

(c) Landweber iteration, as an example of a stationary iterative regularization method. In this case $\omega$ is the number $m$ of performed iterations. Then $y_{\omega}^{(1)}$ is the $m$th iteration vector and $y_{\omega}^{(n)} = R_\omega(b + \eta)$, where $R_\omega = (I - (I - \tau A^TA)^m A^T$. We assume that $y_0^{(n)}$ is the null vector.
2. The operator $A_\omega^{(1)}$ depends on the r.h.s. vector of (4), hence on $\eta$. Non stationary iterative regularization methods belong to this class. Also in this case $\omega$ is the number $m$ of performed iterations and $y_\omega^{(m)} = 0$. Among Krylov subspace methods for nonsymmetric problems, only CGLS and GMRES [5] have been shown to enjoy regularizing properties. Other Krylov subspace methods experimentally show a regularization behaviour, even if a theoretical analysis is lacking. Actually, we are particularly interested in studying these methods which, together with CGLS and GMRES, in the following are collectively referred to as methods of Class 2.

Throughout the paper the Euclidean norm for vectors and the Frobenius norm for matrices will be used.

3 Analysis of the methods of Class 1.
From the point of view of the regularization, the behaviour of the methods of Class 1 is well-known. The analysis of the regularizing properties makes extensive use of the filter factors, which can be explicitly expressed. Hence we start by considering these methods, in order to find a simple framework, suitable to be used also for the more complex methods of Class 2. In this way a comparative evaluation of the methods of the two classes can be made.

The behaviour of the error $e_\omega^{(1)}$ is generally analyzed for a given $\eta$, letting $\omega$ vary, as outlined in the previous section. Instead, we are interested in studying the behaviour of $e_\omega^{(1)}$ as function of $\eta$ for a given $\omega$ and a given direction $d$ of the noise.

3.1 The error behaviour.
The graph of $e_\omega^{(1)}$ versus $\eta$ roughly consists of two parts:

1. for $\eta$ sufficiently small, when the approximation error $\gamma_\omega^{(1)}$ dominates, the graph appears to be a horizontal line, since for the methods of Class 1 $\gamma_\omega^{(1)}$ does not depend on $\eta$.

2. for larger values of $\eta$, when the noise-propagation error $\delta_\omega^{(1)} = \eta \| R_\omega d \|$ dominates, the graph appears to be an oblique straight line.

When $\omega$ increases, the horizontal part lowers and the oblique part rises. For large values of $\omega$, for example when Tikhonov method is applied with values of $\lambda$ approximately zero or an iterative method is carried out for a very large number of iterations, the approximation error is negligible and

$$e_\omega^{(1)} \sim \eta \| A^t d \|.$$ 

Hence for large values of $\omega$, in the graph of $e_\omega^{(1)}$ the horizontal part nearly disappears.
An example of the behaviour just described is shown in Figure 1 for a synthetic problem. A matrix $A$ with condition number $10^5$, a solution $x^*$ and a r.h.s. vector $b$ have been constructed as explained in Section 5.1. Moreover a white Gaussian noise unitary vector $d$ has been generated and vectors $\eta = \eta d$ have been considered for $\eta = 10^t$, $t = -7, \ldots, -1$. The corresponding problems (2) have been solved by Tikhonov method with increasing values of the parameter $\omega$ ($\omega = 1/\lambda = 10^i$, $i = 5, 7, 9, 11$). The figure shows the (log, log) plots of $\epsilon_{\omega}^{(\eta)}$ versus $\eta$.

![Figure 1: Graphs of the errors produced by Tikhonov method.](image)

The log scale transforms the oblique straight lines into straight lines with angular coefficient 1 shifted by $-\log ||R_{\omega}d||$. The solid line corresponds to the graph of $\eta \|A_{\omega}d\|$. Let $\epsilon_{\omega_{\text{opt}}}^{(\eta)} = \epsilon_{\omega_{\text{opt}}} = \min_{\omega} \epsilon_{\omega}^{(\eta)}$ be the error corresponding to the optimal value $\omega_{\text{opt}}$ of $\omega$. The graph of $\epsilon_{\omega_{\text{opt}}}^{(\eta)}$ versus $\eta$ is the lower envelope of the error graphs varying $\omega$. Figure 2 shows $\epsilon_{\omega_{\text{opt}}}^{(\eta)}$ (dotted line) for the error graphs of Figure 1. The dotted line then sketches the errors produced by $A_{\omega_{\text{opt}}}$. For comparison the solid line, still corresponding to the graph of $\eta \|A_{\omega}d\|$, sketches the errors which would result if problem (2) was solved without regularization.

![Figure 2: Lower envelope of the error graphs of Fig. 1.](image)

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3.2 Mean errors for random noise vectors

From (1) and (5) we get
\[ e_\omega^0 = \| B_1 x^* - \eta B_2 d \|, \quad \text{where} \quad B_1 = I - R_\omega A, \quad B_2 = R_\omega, \]
and
\[ e_\omega^0 = \| B_1 x^* \|^2 + \eta^2 \| B_2 d \| - 2 \eta x^* B_1^T B_2 d. \]  
(9)

Let \( A = U \Sigma V^T \), where \( \Sigma = \text{diag}[\sigma_1, \ldots, \sigma_n] \), be the SVD of \( A \), with \( \sigma_i = 0 \) for \( i > r \). Following [6], we write
\[ R_\omega = V \Sigma_\omega U^T, \quad \Sigma_\omega = F \Sigma^T, \]
where \( F \) is a diagonal matrix whose principal elements \( f_i, \ i = 1, \ldots, n \), are called the filter factors of the regularization method. Then
\[ B_1 = V (I - \Sigma_\omega \Sigma) V^T, \quad B_2 = V \Sigma_\omega U^T. \]

In order to give a measure of the regularization efficiency of a method of Class I, we analyze the error behaviour in a probabilistic setting. The probabilistic tool is present in the literature concerning regularization, see for example [8].

Let \( E(e_\omega^0) \) be the expected value of \( e_\omega^0 \). We call mean error \( E_\omega^0 \) the square root of this expected value.

We assume hence that in problem (2) the components of \( d \) are independent stochastic variables, normally distributed with mean zero. Then the expected value of the last term of (9) is zero and
\[ (E_\omega^0)^2 = E(e_\omega^0) = \beta_1(\omega) + \eta^2 \beta_2(\omega), \quad \text{where} \quad \left\{ \begin{array}{l} \beta_1(\omega) = E(\| B_1 x^* \|), \\ \beta_2(\omega) = E(\| B_2 d \|). \end{array} \right. \]
(10)

Hence \( \beta_1(\omega) \) corresponds to the square of the approximation error and \( \eta^2 \beta_2(\omega) \) corresponds to the square of the noise-propagation error.

Being \( \| d \| = 1 \), the components \( d_i \) of \( d \) have variance \( 1/n \) and \( E(d_i^2) = 1/n \). Let \( c = U^T d \). Since the multiplication by an orthogonal matrix represents a rotation in \( \mathbb{R}^n \), the components of \( c \) and of \( d \) have the same distribution. Then also \( E(c_i^2) = 1/n \) and
\[ \beta_2(\omega) = E(\| F \Sigma^T e \|)^2 = E \left( \sum_{i=1}^r \frac{f_i^2}{\sigma_i^2} e_i^2 \right) = \sum_{i=1}^r \frac{f_i^2}{\sigma_i^2}. \]
(11)

\( \beta_1(\omega) \) depends, in addition to the filter factors, on the Fourier coefficients of \( b \) with respect to the columns \( u_i \) of \( U \). In fact, by denoting \( z = V^T x^* \), we have \( z_i = 0 \) for \( i = r + 1, \ldots, n \) and
\[ \beta_1(\omega) = \| B_1 x^* \|^2 = \sum_{i=1}^r (1 - f_i)^2 z_i^2. \]
(12)
Since $z = \sum_{i} u_i^T b$, then $|z_i| = |u_i^T b / \sigma_i|$ for $i = 1, \ldots, r$, i.e. the components of $z$ are the ratios of the Fourier coefficients of $b$ to the singular values of $A$. The components of $z$ play an important role in the regularization, because if the coefficients $|u_i^T b|$ decay to zero slower than the corresponding $\sigma_i$, then we cannot expect to compute an acceptable regularized solution. In fact, a *discrete Picard condition* [6] is generally assumed when the problem is obtained by discretizing a Fredholm integral equation. It reflects the Picard condition, which should be satisfied by the right-hand side of the continuous problem in order to assure the existence of a square integrable solution. According to the discrete Picard condition, the coefficients $|u_i^T b|$ should, on the average, decay to zero faster than the corresponding $\sigma_i$.

We consider two different cases.

1. In the *partially stochastic* case the solution $\mathbf{x}^*$ is fixed and only the components of $\mathbf{d}$ vary stochastically.

2. In the *completely stochastic* case also the components of $z$ are independent stochastic variables, normally distributed with mean zero and variance $\zeta_i^2$, where $\zeta_i$ is decreasing with $i$. In this way the expected values of $|z_i|$ decrease to zero and the discrete Picard condition holds. The solution $\mathbf{x}^* = Vz$ is then computed. Since $E(z_i^2) = \zeta_i^2$, equation (12) holds also in this case provided that $z_i$ is replaced by $\zeta_i$.

Function (10) can be explicitly expressed for the methods of Class 1.

- For truncated SVD (*tsvd*) the filter factors are $f_i = 1$ for $i \leq k$ and $f_i = 0$ for $i > k$, where $k$ is the number of singular values taken.

- For Tikhonov method (*tikh*) the filter factors are $f_i = \sigma_i^2 / (\sigma_i^2 + \lambda)$, $i = 1, \ldots, n$.

- For Landweber iteration (*land*) the filter factors are $f_i = 1 - (1 - \tau \sigma_i^2)^m$, $i = 1, \ldots, n$, where $m$ is the number of performed iterations and $0 < \tau < 2 / \sigma_1$ for convergence.

Substituting the filter factors into (10), (11) and (12), in the partially stochastic case we have

$$
E_{\text{tsvd}}^2 = \sum_{i=k+1}^{r} z_i^2 + \frac{\eta^2}{n} \sum_{i=1}^{k} \frac{1}{\sigma_i^2}
$$

$$
E_{\text{tikh}}^2 = \sum_{i=1}^{r} \frac{\lambda^2 z_i^2}{(\sigma_i^2 + \lambda)^2} + \frac{\eta^2}{n} \sum_{i=1}^{r} \frac{\sigma_i^2}{(\sigma_i^2 + \lambda)^2}
$$

$$
E_{\text{land}}^2 = \sum_{i=1}^{r} (1 - \tau \sigma_i^2)^{2m} z_i^2 + \frac{\eta^2}{n} \sum_{i=1}^{r} \frac{(1 - (1 - \tau \sigma_i^2)^m)^2}{\sigma_i^2}
$$

In the completely stochastic case $z_i$ is replaced by $\zeta_i$. 

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3.3 Optimal mean error

The following properties hold:

- \( \lim_{\omega \to \infty} A_\omega = A \) (in the case of truncated SVD the limit is for \( \omega \to n \)),
- \( \beta_1(\omega) \) is a decreasing function of \( \omega \) with \( \lim_{\omega \to \infty} \beta_1(\omega) = 0 \),
- \( \beta_2(\omega) \) is an increasing function of \( \omega \) with \( \lim_{\omega \to \infty} \beta_2(\omega) = \beta_\infty = \|A^\dagger\|^2 \).

Hence for any \( \eta \) the squared mean error \( \beta_1(\omega) + \eta^2 \beta_2(\omega) \) has a unique minimum point \( \omega_{opt} \), which is the optimal value of the parameter.

For any \( \eta \) we define

1. the optimal mean error

\[
E^{(\eta)}_{opt} = \min_{\omega \in \mathcal{R}} E^{(\eta)}_\omega,
\]

where \( \mathcal{R} \) is the variability range of \( \omega \). The optimal mean error describes the error behaviour of the method when the parameter \( \omega \) is given the optimal value \( \omega_{opt} \) for the mean case.

2. the limiting mean error

\[
E^{(\eta)}_\infty = \lim_{\omega \to \infty} E^{(\eta)}_\omega = \eta \sqrt{\frac{\beta_\infty}{n}} = \eta \frac{\|A^\dagger\|}{\sqrt{n}},
\]

which would affect the unregularized solution \( x^{(\eta)} \) of (2). In the log scale the graph of the limiting mean error appears as an oblique line shifted by \( -\log_{10}(\|A^\dagger\|/\sqrt{n}) \).

3. the zero solution mean error \( E_0 \) such that

\[
E_0^2 = E^{(\eta)}_0 = \mathcal{E}(\|x^*\|^2),
\]

which is the mean error one would obtain if the zero vector was taken as the regularized solution. Any solution affected by an error greater than \( E_0 \) can not be considered as an acceptable regularized solution. In the partially stochastic case \( E_0 = \|A^\dagger\| \) and in the completely stochastic case \( E_0 = \|\zeta\| \), where \( \zeta \) is the vector whose components are the standard deviations \( \zeta_i \).

The graph of \( E^{(\eta)}_{opt} \) corresponds to the lower envelope of the graphs of \( E^{(\eta)}_\omega \) versus \( \eta \). In Figure 3 the graph of \( E^{(\eta)}_{opt} \) (dotted line) of Tikhonov method applied to problem shaw [7] (see Section 5.1), the graph of \( E^{(\eta)}_\infty \) (solid line) and the graph of \( E_0 \) (dashed line) are given.

Problem shaw belongs to the set of problems dealt with in the experimentation of Section 5 with size \( n = 32 \). Figure 3 refers to a size \( n = 10 \) problem, because with a greater size the limiting mean error and the optimal mean error
would not be visible in the same graph for values of $\eta$ in the usual variability range of the noise. In fact, due to the large ill-conditioning of the matrix $\mathbf{A}$, the limiting mean error would be shifted too much toward the left.

Under suitable hypotheses an estimate of the optimal value $\omega_{opt}$ can be found for the methods of Class 1.

**Truncated SVD.** In the partially stochastic case the squared optimal mean error is

\[
(E^{(\eta)}_{opt})^2 = \min_{k \in \mathbb{R}} (E^{(\eta)}_k)^2 = \min_{1 \leq k \leq r} \left( \sum_{i=k+1}^{r} \frac{\sigma_i^2}{\sigma_i^2 + \frac{n}{\eta} \sum_{i=1}^{k} \frac{1}{\sigma_i^2}} \right).
\]

It is easy to see that

\[
(E^{(\eta)}_k)^2 \leq \min \left\{ (E^{(\eta)}_{k-1})^2, (E^{(\eta)}_{k+1})^2 \right\} \quad \text{if} \quad \frac{\sigma_k^2}{\sigma_{k+1}^2} < \frac{n}{\eta} \leq \frac{\sigma_{k+1}^2}{\sigma_k^2}. \tag{13}
\]

By the discrete Picard condition the sequence $\sigma_k^2 / \sigma_{k+1}^2 = \|u_k^T b\|^2$ on the average decays to zero faster than the sequence $\sigma_k^2$. We assume that only an index $k$ exists satisfying (13) (i.e., we assume a monotonical decay of $\|u_k^T b\|$ for values close to $\eta^2/n$). In this case the optimal value $\omega_{opt}$ coincides with the index $k$ verifying (13).

**Tikhonov method.** The squared optimal mean error is

\[
(E^{(\eta)}_{opt})^2 = \min_{\omega \in \mathbb{R}} (E^{(\eta)}_\omega)^2 = \min_{\lambda \in [0,1]} \sum_{i=1}^{r} \frac{1}{\sigma_i^2 + \lambda \sigma_i^2} \left( \lambda^2 \frac{\sigma_i^2}{\sigma_i^2} + \frac{n}{\eta} \sigma_i^2 \right).
\]

The minimum is attained for $\lambda$ satisfying

\[
\sum_{i=1}^{r} \frac{\lambda \sigma_i^2}{(\sigma_i^2 + \lambda \sigma_i^2)^3} = \frac{n}{\eta} \sum_{i=1}^{r} \frac{\sigma_i^2}{(\sigma_i^2 + \lambda \sigma_i^2)^3}.
\]
The optimal value \( \lambda \) verifies \( \sum_{i=1}^{r} \alpha_i z_i^2 / \sum_{i=1}^{r} \alpha_i = \frac{\eta^2}{n \lambda} \), where \( \alpha_i = \frac{\sigma_i^2}{\sigma_i^2 + \lambda} \). Then \( \frac{\eta^2}{n \lambda} \) is equal to a weighted mean and an index \( j \) exists for which \( z_j^2 \sim \frac{\eta^2}{n \lambda} \). For this index \( j \) we have
\[
\sum_{i=1}^{r} \frac{\sigma_i^2 z_i^2}{(\sigma_i^2 + \lambda)^3} \sim \sum_{i=1}^{r} \frac{\sigma_i^2 z_j^2}{(\sigma_i^2 + \lambda)^3}.
\] (14)

If the two sums are equally well approximated by their dominant term and the corresponding indices coincide with \( i \) such that \( \sigma_i^2 \sim \lambda \) (this usually happens when the singular values decay exponentially), and we replace the sums in (14) by the single \( i \)th terms, we see that \( i = j \) and \( \eta^2 / n \sim \sigma_j^2 z_j^2 \). By comparison with (13) it follows that \( j \sim k \), i.e. the optimal value of \( \lambda \) is close to \( \sigma_k^2 \). The corresponding filter factors \( f_i \) are close to 1 for \( i \leq k \), and close to 0 for \( i > k \).

Hence the optimal Tikhonov filter factors approximate the optimal TSVD filter factors.

**Landweber iteration** The \( i \)th filter factor is \( f_i = 1 - (1 - \tau \sigma_i^2)^m \). We assume here that \( \tau \sigma_i^2 < 1 \) for \( i = 1, \ldots, n \). This assumption guarantees both the method converges and all the filters are less than 1. We have
\[
\frac{1}{1 - f_i} = \frac{1}{(1 - \tau \sigma_i^2)^m} = 1 + m \tau \sigma_i^2 + O(\tau^2 \sigma_i^4), \quad \text{where} \quad O(\tau^2 \sigma_i^4) > 0,
\]
then
\[
f_i = \frac{m \tau \sigma_i^2}{1 + m \tau \sigma_i^2}.
\]
Writing \( m \tau = 1 / \lambda \), we see that the Landweber filters are close to the Tikhonov filters, the approximation being better for larger indices \( i \). Then we expect that the minimum of the mean error of Landweber iteration is attained for an optimal value \( \omega_{opt} \) close to \( 1 / (\tau \sigma_k^2) \). This explains why, when \( \eta \) is small, such a large number of iterations are required by the Landweber method to obtain an error of the same order than the error obtained by Tikhonov method with optimal \( \lambda \). In [2] this result is obtained by working in the frequency domain.

To illustrate the filters behaviour, a completely stochastic problem has been generated with size \( n = 100 \) and a noise magnitude \( \eta = 10^{-1} \). The index for which condition (13) holds is \( k = 37 \). Figure 4 shows the optimal filter factors with indices \( i \) in the range [20, 50] for the methods of Class I (triangles for TSVD, gray squares for Tikhonov method, stars for Landweber iteration)

### 3.4 Regularizing efficiency

The optimal mean error \( E_{opt}^{(n)} \) can be used to measure the regularizing efficiency of a method applied to a problem of form (2).

First of all we note that if in the log scale the graph of \( E_{opt}^{(n)} \) lies above the line of the zero solution error \( E_0 \) for a value of \( \eta \), the regularizing efficiency of
the method for that value of $\eta$ can be considered null, since taking the zero solution as the regularized solution would give a lower error. Hence to measure the regularizing efficiency of a method we consider the area of the region lying over the graph of $E_{\text{opt}}^{(\eta)}$ and under the graph of $E_0$ (see Figure 3). The greatest the area, the more regularizing the method.

More exactly, for a given problem we define regularizing efficiency of a method on a given interval $[10^{t_1}, 10^{t_2}]$ the integral mean

$$\rho = \log_{10} E_0 - \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} \log_{10} E_{\text{opt}}^{(\eta)} \, dt,$$

where $t = \log_{10} \eta$. (15)

For a practical use of this measure, $\eta$ should vary in intervals which encompass the usual variability range of the noise. In the experiments we choose noises ranging from $10^{-2}\|b\|$ to $10^{-1}\|b\|$ (high-level noise) and from $10^{-4}\|b\|$ to $10^{-2}\|b\|$ (low-level noise). The corresponding regularizing efficiencies are denoted by $\rho_h$ and $\rho_l$ respectively. For example, for the problem 

\[\text{shaw},\] whose graphs are given in Figure 3, the regularizing efficiencies of truncated SVD, Tikhonov method and Landweber iteration with high-level noise are

$$\rho_h^{\text{trsvd}} = 0.75, \quad \rho_h^{\text{tikh}} = 0.77, \quad \rho_h^{\text{land}} = 0.78.$$

Actually, the experiments performed in Section 5 on a collection of classical problems [7] and on a collection of randomly generated problems, show a substantial equivalence of the three methods of Class 1 for what concerns the regularizing efficiency with high-level noise. Of course the computational costs of finding the optimal value for $\omega$ and of implementing the method are not taken into consideration in this context.

3.5 Discrepancy principle

The error analysis performed in the previous section assumes the knowledge of the optimal value $\omega_\eta$ of the parameter $\omega$. However, in practice, this optimal
value is not known and we can only achieve the regularization induced by the chosen value of \( \omega \). When an estimate of the norm of the noise is available, the discrepancy principle is suggested (see [2]) for the choice of a suitable \( \omega \). For Tikhonov method the suggestion is based on the property that the solution obtained with a value \( \tilde{\omega} \) such that

\[
\text{res}_{\tilde{\omega}} = \| \eta - \hat{y}_{\omega} \| = \eta
\]

coincides with the solution of the constrained problem

\[
\text{minimize } \| x \| \\
\text{subject to } \| b + \eta - A \tilde{x} \| = \eta.
\]

The solution of this problem, having minimal norm, appears to be sufficiently close to the required optimal solution \( \hat{y}_{\omega} \) and, consequently, \( \tilde{\omega} \) appears to be a good approximation of \( \omega \).

We examine now in the probabilistic setting the effectiveness of the discrepancy principle in the choice of the optimal parameter for the methods of Class I by studying the behaviour of the mean residual norm, i.e. the square root of the expected value of \( \text{res}_{\omega} \). We have

\[
\text{res}_{\omega} = \| AB_1 \tilde{x} + \eta (I - AB_2) d \|^2,
\]

and

\[
\mathcal{E}(\text{res}_{\omega}) = \mathcal{E}(\| \Sigma (I - F) z \|^2) + \frac{\eta^2}{\mathcal{E}(\| I - \Sigma \Sigma \|^2)}.
\]

In the partially stochastic case we have

\[
\mathcal{E}(\text{res}_{\omega}) = \frac{\eta^2}{n} (n - r) + \sum_{i=1}^{r} (1 - f_i)^2 (\sigma_i^2 x_i^2 + \frac{\eta^2}{n}).
\]

In the completely stochastic case \( z_i \) is replaced by \( \zeta_i \).

For \( \omega \) sufficiently close to \( \omega_{\text{opt}} \) we may assume that the filter factors \( f_i \) with \( i \leq k \), where \( k \) satisfies (13), are close to 1, then

\[
q_{\omega} = \sum_{i=1}^{r} (1 - f_i)^2 \sigma_i^2 x_i^2 - \sum_{i=k+1}^{r} (1 - f_i)^2 \sigma_i^2 x_i^2.
\]

Since on the average \( \sigma_i^2 x_i^2 \leq \sigma_k^2 x_k^2 \sim \eta^2 / n \), for \( i > k \), it follows that \( q_{\omega} \leq c \eta^2 \), for a constant \( c \), independent from \( \eta \). By comparing (16) with (7) we see that the discrepancy principle can be effectively applied with

\[
\alpha^2 \sim c + \frac{1}{n} \left[ n - r + \sum_{i=1}^{r} (1 - f_i)^2 \right].
\]

This confirms the well known result of effectiveness of the discrepancy principle for the methods of Class I.
4 Error behaviour of the methods of Class 2.

Conjugate gradient (CG) method applied to the normal equations $A^TAx = A^T(b + \eta d)$ is a classical Krylov subspace method for finding a regularized solution of system (1) when $A$ is not symmetric. Its regularizing effect is due to the fact that CG reconstructs first the components of the solution in the direction of the singular vectors corresponding to the largest singular values of $A$. We refer here to the CGLS implementation, which avoids the explicit construction of the matrix $A^TA$. The filter factors of this method are well-known, but they depend on the r.h.s. of the system. The dependence of the filter factors on $\eta$ does not allow us to get a simple expression for the mean error like (10).

Quoting from [1] “many iterative methods have been developed and it is impossible to cover them all”. This is true also if we restrict ourselves to Krylov subspace methods, with their many variants. Hence we decided to select only the Krylov subspace methods covered in [1], i.e. GMRES and the biconjugate methods QMR, CGS, BiCG and Bi-CGSTAB, and to implement them according to the pseudocodes listed there. For simplicity sake, in the tables the names of the methods of Class 2 will be denoted by a low-case abbreviation as follows: cgls, gmres, qmr, cgs, bcg, sta.

4.1 Statistical approach

For the methods of Class 2 the probabilistic approach followed in Section 3 can not be adopted, due to the lack of explicit expressions for the filter factors. Hence we have to resort to statistics to analyze the consistency of a method with the discrepancy principle and to evaluate its regularizing efficiency, by applying it to a sample of test problems. The two approaches differ on an important detail:

- in the probabilistic approach the computation of the mean error $E_p^{(\eta)}(\omega)$ is performed before the computation of the optimal value $\omega_{opt}$ of the corresponding optimal error $E_{opt}^{(\eta)}$ and of the mean residual norm for $\omega = \omega_{opt}$.

- in the statistical approach one deals with a problem of the sample at the time and computes for it the optimal value $\omega_{opt}$, the corresponding optimal error $E_{opt}^{(\eta)}$ and the residual norm $re_{\omega_{opt}}^{(\eta)}$. When all the sample problems have been processed, the average $E_{av}^{(\eta)}$ of all the computed $E_{opt}^{(\eta)}$ and the average $re_{av}^{(\eta)}$ of all the computed $re_{\omega_{opt}}^{(\eta)}$ are found.

Hence, in addition to the probabilistic regularizing efficiency $\rho$ defined in the previous section, we can consider an analogous statistical measure $\mu$ taken on the graph of $E_{av}^{(\eta)}$. The quantity $E_0$ of (15) is replaced by the average of $||x^*||$ for all the problems of the sample. We expect in general $E_{av}^{(\eta)}$ to be close to $E_{opt}^{(\eta)}$. Figure 5 shows the results obtained by applying Tikhonov method to problem shaw. The shaded area contains the graph of the optimal error $E_{opt}^{(\eta)}$ of all the
generated sample problems varying \( \mathbf{d} \). The dashed line corresponds to the graph of \( \epsilon_{av}(\eta) \). The solid line corresponds to the graph of \( E_{opt}(\eta) \).

![Graph of the \( \epsilon_{opt}(\eta) \) (shaded area), of \( \epsilon_{av}(\eta) \) (dashed line) and of \( E_{opt}(\eta) \) (solid line).](image)

The figure suggests that the graphs of \( E_{opt}(\eta) \) and \( \epsilon_{av}(\eta) \) have the same behaviour. The experiments of Section 5 confirm that this behaviour is shared by the truncated SVD and Landweber iteration. In Section 5.2 the probabilistic and statistical measures \( \mu \) and \( \rho \) are compared for the methods of Class 1 and for all the test problems.

In order to compare the performances of the methods of Class 2 with those of the methods of Class 1 on a fair basis, the statistical measures will be used for both classes.

## 5 Numerical experiments

The experiments aim to compare the methods with respect to the regularizing efficiency and the consistency with the discrepancy principle.

### 5.1 Test problems

The problems used for the experiments belong to two different sets, which correspond to the two cases examined in subsection 3.2.

1. The first set, which corresponds to the partially stochastic case, contains five test problems of size \( n = 32 \) taken from REGULARIZATION TOOLS [7], namely baart, foxgood, ilaplace, phillips, shaw. The matrix \( \mathbf{A} \) and the solution \( \mathbf{x}^* \) are given. Then the exact r.h.s. vector \( \mathbf{b} = \mathbf{A}\mathbf{x}^* \) is computed and a perturbation \( \eta = \eta \mathbf{d} \) is added, \( \mathbf{d} \) being a white Gaussian noise unitary vector and \( \eta = 10^{-t}\|\mathbf{b}\| \), with \( 1 \leq t \leq 4 \). For problem ilaplace all the solutions listed in [7] have been considered, because they exhibit different smoothness degree. In the tables the results of this problem are shown under the names ilaplace1, ..., ilaplace4.
A great part of the problems of this set have singular values decaying exponentially. For example, the singular values of problem $A$ with $n = 32$ are approximately equal to $\sigma_i = 3.5 \kappa \left( \frac{\kappa}{n-1} \right)^{1.6}$, with $k = 10^{32}$. Problem phillips does not verify the discrete Picard condition: the ratios of the Fourier coefficients and the singular values oscillate and an average decay to zero does not appear.

2. The second set corresponds to the completely stochastic case. Each problem depends on three parameters: $\kappa$ controls the conditioning, $\nu$ controls the decay speed of the singular values and $\theta$ controls the convergence rate to zero of the quantities involved into the discrete Picard condition. First the random matrix $A$ of size $n = 100$ is generated, with the singular values $\sigma_i$, $i = 1, \ldots, n$:

$$\sigma_i = \frac{\varphi_i}{s}, \quad \text{where} \quad \varphi_i = \kappa \left( \frac{\kappa}{n-1} \right)^{\nu} \quad s = \left( \sum_{i=1}^{n} \varphi_i^{2(\theta+1)} \right)^{1/2}.$$ 

To preserve the sign changes behaviour of the singular vectors characteristic of the discretized ill-posed problems, we follow the suggestions given in [6]. A bidiagonal matrix $B$ with nonzero elements normally distributed with unit variance and mean 3a is generated. Unitary matrices $U$ and $V$ are obtained by computing the SVD decomposition of $B$. The matrix $A$ is computed as $A = U \Sigma V^T$, where $\Sigma = \text{diag}(\sigma_i)$.

Then a vector $z$ is generated whose $i$th component is a stochastic variable normally distributed with mean zero and variance

$$\zeta^2_i = \varphi_i^{2\theta}.$$ 

Finally the solution $x^* = Vz$ and the r.h.s $b = Ax^*$ are computed. Since $||b|| = ||\Sigma z||$, then

$$\mathcal{E}(||b||^2) = \sum_{i=1}^{n} \sigma_i^2 \mathcal{E}(\zeta_i^2) = \sum_{i=1}^{n} \sigma_i^2 \varphi_i^{2\theta} = 1.$$ 

The relation among the Fourier coefficients of $b$ and the singular values of $A$ for these problems has been suggested by the model problem (4.30) of [6].

The values of the parameters considered in the experiments are $\kappa = 10^{20}$, $\nu = \{1, 1.5\}$ and $\theta = \{0.8, 1, 1.2\}$. The perturbation $\eta = \eta d$ is added to $b$, with $d$ varying as for the first set of problems and $\eta = 10^{-t}$, $1 \leq t \leq 4$. In the tables the results for these problems are shown under the names $\sigma - \nu - \theta$.

5.2 Testing the regularizing efficiency

First we compare the regularizing efficiencies of the methods of Class 1, in order to confirm the substantial equivalence between the probabilistic and the statistical measures and among the different methods. In Table 1, which refers to high-level noise, the values of $\rho_h$ and $\mu_h$ are shown for each test problem and each method of Class 1. The quantities $\rho_h$ and $\mu_h$ are identified by a superscript
denoting the method used. Table 2 shows the analogous quantities $\mu$ for low-level noise. In this table the statistical data of Landweber iteration are missing because the method is too slow and requires too many iterations to reach the optimal error with this level of noise. A good agreement between the probabilistic and experimental measures is evident for all the problems. Moreover the three methods of Class 1 seem to be substantially equivalent from the point of view of the regularizing efficiency.

<table>
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<th>$\rho_{twd}$</th>
<th>$\rho_{tsvd}$</th>
<th>$\rho_{tikh}$</th>
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<td>1.18</td>
<td>1.27</td>
<td>1.31</td>
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</tbody>
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Table 1: Probabilistic and statistical regularizing efficiencies at high-level noise of the methods of Class 1.

Next we compare the statistical regularizing efficiency $\mu_{h}$ and $\mu$ of the methods of Class 2 with the corresponding measure of Tikhonov method, taken as reference. In Table 3, which refers to high-level noise, the first column displays the values $\rho_{tikh}$, the other columns display the values $\mu_{meth}$ for method $meth$ in Class 2. Table 4 shows the analogous quantities for low-level noise. CGLS shows a behaviour comparable with that of Tikhonov method. GMRES and QMR show a worse behaviour, but sometimes acceptable. The other three methods perform slightly worse.

Another group of experiments has been performed to study on a statistical base if there are relevant differences in the behaviour of the methods when the noise has a Poissonian distribution, instead of a Gaussian one, as frequently happens in the practical cases. The detailed results are not reported here for the sake of brevity, but they point out that the distribution of the noise is not
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<th>$l_{adv}^{*}$</th>
<th>$l_{thh}$</th>
<th>$l_{thh}^{*}$</th>
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Table 2: Probabilistic and statistical regularizing efficiencies at low-level noise of the methods of Class 1.

influential on the error behaviour and on the reconstruction efficiency for all the problems and all the methods.

5.3 Testing the discrepancy principle

Now we analyze a statistical base the consistency with the discrepancy principle (which for the methods of Class 1 has been studied in the probabilistic setting in Section 3.5). For each problem and each method the averages $q(\eta) = \text{res}^{(\eta)}$ of the residual norms in the optimal values of the parameter are computed for a discrete set $\eta = 10^{-t_i}\|b\|$ with $t_i$ equispaced in the interval $[1, 4]$ (except for the Landweber method where the interval is $[1, 3]$). The hypothesis to be statistically tested is that $q(\eta)$ results to be well approximated by a linear function, according to (7). As customary, the linearity of the function is tested in the $(\log, \log)$ scale, in order to get equispaced abscissas. The standard deviation $sd$ of the vector $\log_{10} q(\eta_k) - t_i$ is taken as a measure of dispersion. The results are shown in Table 5. As expected, the methods of Class 1 result to be consistent. Also CGLS and GMRES show a good consistency behaviour. The other methods show a lower degree of consistency with the discrepancy principle. In particular, QMR performs worse on the problems of the second set, CGS and Bi-CGSTAB perform worse on the problems of the first set, while BiCG behaves
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Table 3: Statistical regularizing efficiencies at high-level noise of the methods of Class 2 compared with Tikhonov method (first column).

poorly on both sets.

The worst performances (corresponding to \( sd > 0.2 \)) of the last three methods can be attributed both to the behaviour of the residual norm, whose monotonic decrease is not guaranteed, and to the large convergence speed, which does not allow enough iterations before the noise contaminates the computed solution. If the use of the discrepancy principle implies an overestimation on the number of iterations to be performed, too many iterations would completely alter the result.

Conclusions
In summary, we think that the last three methods (CGS, BiCG and Bi-CGSTAB) are not consistent regularizing methods according to the definition given in Section 2. The large sensitivity, which does not affect slower iterative methods, suggests special care in their use. CGLS method shows the same good behaviour of the methods of Class 1 from the point of view of both efficiency and consistency. The other two Krylov methods (GMRES and QMR) show intermediate features, but anyway they should be taken into consideration on account of their low computational cost.

Of course the choice among the methods can not be based only on the above considerations. Other features should be considered: Truncated SVD is not suitable for problems of large size, Tikhonov method requires an extra
computation effort for a good determination of the regularization parameter. Landweber method may require too many iterations when the noise is low. CGLS, GMRES and QMR methods do not suffer from these drawbacks and, seen the results of our analysis, can be suggested in practice, taking into account that the greater consistency and efficiency of CGLS are paid by a greater number of iterations.

On the other hand, Krylov methods may have breakdowns, due to the fact that the generated Krylov subspace cannot be expanded furthermore. Moreover, a possible drawback of GMRES is the large storage requirement, when too many iterations are performed. However, these difficulties in general do not arise in the first iterations and are not so serious in our context where few iterations are often sufficient to get the regularized solution.

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Table 5: Measure of dispersion for the consistency of the methods.


