

MULTI-PARAMETER ARNOLDI-TIKHONOV METHODS*

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Abstract. For the solution of linear ill-posed problems, in this paper we introduce a simple algorithm for the choice of the regularization parameters when performing multi-parameter Tikhonov regularization through an iterative scheme. More specifically, the new technique is based on the use of the Arnoldi-Tikhonov method and the discrepancy principle. Numerical experiments arising from the discretization of integral equations are presented.

Key words. multi-parameter regularization, Arnoldi-Tikhonov method, discrepancy principle

AMS subject classifications. 65F10, 65F22

1. Introduction. In the framework of Tikhonov regularization for the solution of ill-posed linear systems $Ax = b$, $A \in \mathbb{R}^{N \times N}$, the use of the multi-parameter regularization (even called multiple penalty regularization) has been introduced with the aim of acting simultaneously on different frequency bands of the solution, in the hope of reproducing all the basic features of the unknown solution with a good accuracy. Due to the wide range of applications, there is a growing interest in this kind of regularization, and many numerical schemes have been recently presented in various contexts; we cite [11] and the references therein for an overview.

In this paper we mainly focus the attention on linear discrete ill-posed problems (see [8, Chap. 1] for a background) and we assume that the available right-hand side vector b is affected by noise, caused by measurement or discretization errors. Therefore, throughout the paper we suppose that

$$b = \bar{b} + e,$$

where \bar{b} represents the unknown noise-free right-hand side, and we denote by \bar{x} the solution of the error-free system $Ax = \bar{b}$.

In the multi-parameter Tikhonov regularization setting, denoting by $\Lambda = (\lambda_1, \dots, \lambda_k)^T$ the vector of the regularization parameters ($\lambda_i \geq 0$, $i = 1, \dots, k$, $\Lambda \neq 0$)[‡] and by $\mathcal{L} = \{L_1, \dots, L_k\}$ the set of regularization matrices, a regularized solution $x_{\Lambda, \mathcal{L}}$ is defined as

$$(1.1) \quad x_{\Lambda, \mathcal{L}} = \arg \min_{x \in \mathbb{R}^N} J(x, \Lambda, \mathcal{L}), \text{ where } J(x, \Lambda, \mathcal{L}) = \|Ax - b\|^2 + \sum_{i=1}^k \lambda_i \|L_i x\|^2.$$

Here and in the sequel, the norm used is always the Euclidean norm.

While the multi-parameter regularization is theoretically superior to any single-parameter regularization which uses one of the matrices L_i in (1.1), the main problem is that in practice it may be quite difficult to work simultaneously with more than one regularization matrix and to suitably define the regularization parameters λ_i . The existing methods for the automatic choice of the parameters are essentially based on the generalized L-curve criterion (e.g., [2]) and on the generalization of the GCV criterion; see [4]. More recently an algorithm based on the knowledge of the noise structure has been introduced in [1].

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[‡]When treating multi-parameter methods, one usually requires that each component of the vector Λ is different from zero. However we prefer to present the analysis just like a generalization of the one-parameter case.

In many real applications, the noisy data b is known to satisfy

$$\|b - \bar{b}\| \leq \varepsilon,$$

so that the use of the discrepancy principle [13] may be considered even in the case of the multi-parameter regularization. Indeed, in [11] the authors introduce an algorithm for the definition of the regularization parameters based on the numerical solution with respect to Λ of the equation,

$$(1.2) \quad \|Ax_{\Lambda, \mathcal{L}} - b\| = \eta\varepsilon, \quad \eta \geq 1.$$

Up to now, to the best of our knowledge, such technique seems to be the only existing one based on the discrepancy principle in the framework of the multi-parameter regularization.

In this paper, we solve (1.1) using an iterative scheme called Arnoldi-Tikhonov (AT) method, first proposed in [5] in the case of the single-parameter regularization with $\mathcal{L} = \{I_N\}$, where I_N denotes the identity matrix of order N . This method has proved to be particularly efficient when dealing with large scale problems, as for instance the ones arising from image restoration. Indeed, it is based on the projection of the original problem (1.1) onto Krylov subspaces of smaller dimensions computed by the Arnoldi algorithm.

Using an iterative method for (1.1) we automatically introduce a new parameter to be determined, that is, the number of iterations. Let us denote by $x_{\Lambda}^{(m)}$ the m -th approximation arising from the Arnoldi-Tikhonov process (from now we omit indicating the dependency on \mathcal{L} , since this set is assumed to be fixed). The algorithm here proposed for the definition of Λ and to stop the procedure, is based on the solution of

$$\|Ax_{\Lambda}^{(m)} - b\| = \eta\varepsilon,$$

at each step, by means of a linear approximation (with respect to each parameter λ_i , $i = 1, \dots, k$) of the function,

$$\phi^{(m)}(\Lambda) = \|Ax_{\Lambda}^{(m)} - b\|.$$

This method generates a sequence of regularization vectors $\Lambda^{(m)}$, $m \geq 1$, whose components $\lambda_i^{(m)}$ are automatically defined. The idea extends the one studied in [6] for the single-parameter case, which has been shown to be competitive with existing ones for Krylov type solvers; see, e.g., [5, 10, 16].

The paper is organized as follows. In Section 2, we explain the use of the AT method for the solution of (1.1). In Section 3, we describe our scheme for the choice of the parameter vector Λ . In Section 4, we explain the algorithm associated to the new method along with a computationally cheaper variant. In Section 5, we display the main results obtained performing common test problems. Finally, in Section 6, we provide some concluding remarks. We also include an Appendix A, which reports some tables that summarize various meaningful results related to the experiments described in Section 5.

2. The Arnoldi-Tikhonov method. Let us work in the single parameter case with $\Lambda = \{\lambda\}$ and $\mathcal{L} = \{L\}$. The Arnoldi-Tikhonov (AT) method was introduced in [5] with the basic aim of reducing the problem,

$$(2.1) \quad \min_{x \in \mathbb{R}^N} \{ \|Ax - b\|^2 + \lambda \|Lx\|^2 \}, \quad \text{where } \lambda > 0 \text{ and } L = I_N,$$

to a problem of much smaller dimension. The idea is to project the matrix A onto the Krylov subspaces generated by A and the vector b , i.e., $\mathcal{K}_m(A, b) = \text{span}\{b, Ab, \dots, A^{m-1}b\}$ with

$m \ll N$. The method was also introduced to avoid the matrix-vector multiplication with A^T required by Lanczos type schemes; see, e.g., [3, 5, 9, 15]. To construct the Krylov subspaces, the AT method employs the Arnoldi algorithm (see [17, Section 6.3] for an exhaustive background), which yields the decomposition,

$$(2.2) \quad AV_m = V_{m+1}\bar{H}_m,$$

where $V_{m+1} = [v_1, \dots, v_{m+1}] \in \mathbb{R}^{N \times (m+1)}$ has orthonormal columns which span the Krylov subspace $\mathcal{K}_{m+1}(A, b)$ and v_1 is defined as $b/\|b\|$. The matrix $\bar{H}_m \in \mathbb{R}^{(m+1) \times m}$ is an upper Hessenberg matrix. Denoting by $h_{i,j}$ the entries of \bar{H}_m , in exact arithmetic the Arnoldi process terminates whenever $h_{m+1,m} = 0$, which means $\mathcal{K}_{m+1}(A, b) = \mathcal{K}_m(A, b)$.

The AT method searches for approximations of the solution of the problem (2.1) belonging to $\mathcal{K}_m(A, b)$. In this sense, substituting $x = V_m y_m$ ($y_m \in \mathbb{R}^m$) into (2.1), yields the reduced minimization problem,

$$(2.3) \quad \min_{y_m \in \mathbb{R}^m} \left\{ \|\bar{H}_m y_m - V_{m+1}^T b\|^2 + \lambda \|y_m\|^2 \right\},$$

since $V_{m+1}^T V_{m+1} = I_{m+1}$. Remembering that $v_1 = b/\|b\|$ we also have

$$V_{m+1}^T b = \|b\| e_1 \quad \text{where } e_1 = (1, 0, \dots, 0)^T \in \mathbb{R}^{m+1}.$$

Looking at (2.3), we can say that the AT method can be regarded to as a regularized version of the GMRES.

The method considered in this paper is an extension of the AT method in order to work with one or more regularization operators not necessarily equal to the identity matrix. In detail, substituting, as before, $x = V_m y_m$ ($y_m \in \mathbb{R}^m$) into (1.1) and using (2.2), we have that

$$(2.4) \quad \min_{x \in \mathcal{K}_m(A, b)} J(x, \Lambda, \mathcal{L}) = \min_{y_m \in \mathbb{R}^m} \left\{ \|\bar{H}_m y_m - \|b\| e_1\|^2 + \sum_{i=1}^k \lambda_i \|L_i V_m y_m\|^2 \right\}$$

$$(2.5) \quad = \min_{y_m \in \mathbb{R}^m} \left\| \begin{bmatrix} \bar{H}_m \\ \sqrt{\lambda_1} L_1 V_m \\ \vdots \\ \sqrt{\lambda_k} L_k V_m \end{bmatrix} y_m - \begin{bmatrix} \|b\| e_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right\|^2.$$

In the sequel we will refer to (2.5) as least squares formulation of the multi-parameter Arnoldi-Tikhonov method. We emphasize that the above strategy can be applied even when the regularization matrices are rectangular, as for instance when considering scaled finite difference approximations of the derivative operators. However, we remark that, contrary to (2.3), the original dimension of the problem is only partially reduced, since $L_i V_m \in \mathbb{R}^{(N-p_i) \times m}$ if $L_i \in \mathbb{R}^{(N-p_i) \times N}$.

Since $\bar{H}_m = V_{m+1}^T A V_m$, if $L_i \in \mathbb{R}^{N \times N}$, $i = 1, \dots, k$, one may even consider the projected operators,

$$(2.6) \quad K_i^{(m)} = V_{m+1}^T L_i V_m,$$

and hence the reduced minimization,

$$(2.7) \quad \min_{y_m \in \mathbb{R}^m} \left\{ \|\bar{H}_m y_m - \|b\| e_1\|^2 + \sum_{i=1}^m \lambda_i \|K_i^{(m)} y_m\|^2 \right\}.$$

Even if problem (2.7) is not equivalent to the original one (2.4), many numerical experiments have revealed that the use of (2.6) is worthy of further investigation. However, it is important to point out that, in fact, the computational cost associated to the solution of (2.7) is comparable with the one of (2.5), because of the operation (2.6).

Finally, we remark that if an initial approximation x_0 of the solution \bar{x} is available, then we can incorporate it into the Arnoldi-Tikhonov scheme by defining the initial residual $r_0 = b - Ax_0$ and by considering the Krylov subspaces $\mathcal{K}_m(A, r_0)$. Consequently, the approximate solution of the problem (1.1) is of the form $x_m = x_0 + V_m y_m$ and in the expressions (2.3), (2.4), (2.5), (2.7), we simply have to substitute b with r_0 ; cf. [6].

3. The parameter selection strategy. As already said in the introduction, if we assume that the quantity $\varepsilon = \|b - \bar{b}\|$ is known, it turns out that a successful strategy to define Λ , as well as a stopping criterion, is the discrepancy principle (1.2) adapted to the iterative setting of the AT method. At each iteration we can define the function $\phi^{(m)}(\Lambda) = \|b - Ax_\Lambda^{(m)}\|$, and we say that the discrepancy principle is satisfied as soon as

$$\phi^{(m)}(\Lambda) \leq \eta\varepsilon, \quad \text{where } \eta \gtrsim 1.$$

We remark that, if we rather know the noise level $\tilde{\varepsilon} = \|e\|/\|\bar{b}\|$, then the discrepancy principle reads

$$(3.1) \quad \phi^{(m)}(\Lambda) = \eta\tilde{\varepsilon}\|b\|.$$

We immediately note that, since for the AT method the approximations are of the form $x_\Lambda^{(m)} = V_m y_\Lambda^{(m)} \in \mathcal{K}_m(A, b)$, where $y_\Lambda^{(m)}$ solves (2.5), the discrepancy can be rewritten as

$$(3.2) \quad \phi^{(m)}(\Lambda) = \|b - AV_m y_\Lambda^{(m)}\| = \|c - \bar{H}_m y_\Lambda^{(m)}\|,$$

where $c = \|b\|e_1 \in \mathbb{R}^{m+1}$.

Now we briefly focus on the case $k = 1$, since the strategy derived to choose the components of the regularization vector Λ in the multi-parameter case is a generalization of the algorithm for the single-parameter case.

3.1. The one-parameter case. As in Section 2, here we denote the unique regularization parameter and operator simply by λ and L , respectively. The method that we are going to describe has been introduced in [6] and has already been used in [14]; we underline that it is able to simultaneously determine suitable values for both λ and m . Our basic hypothesis is that the discrepancy can be well approximated by

$$(3.3) \quad \phi^{(m)}(\lambda) \approx \alpha^{(m)} + \lambda\beta^{(m)},$$

i.e., by a linear function with respect to λ , in which $\alpha^{(m)}, \beta^{(m)} \in \mathbb{R}$ can be easily computed or approximated.

Since $y_\lambda^{(m)}$ solves the normal equations,

$$(\bar{H}_m^T \bar{H}_m + \lambda V_m^T L^T L V_m) y_\lambda^{(m)} = \bar{H}_m^T c,$$

associated with the least square problem (2.5) with $k = 1$, by (3.2) we obtain

$$(3.4) \quad \phi^{(m)}(\lambda) = \|\bar{H}_m (\bar{H}_m^T \bar{H}_m + \lambda V_m^T L^T L V_m)^{-1} \bar{H}_m^T c - c\|.$$

For the computation of $\alpha^{(m)}$ in (3.3), the Taylor expansion of (3.4) suggests the choice

$$\alpha^{(m)} = \phi^{(m)}(0) = \|\bar{H}_m(\bar{H}_m^T \bar{H}_m)^{-1} \bar{H}_m^T c - c\|,$$

which is just the norm of the residual of the GMRES iterate, which can be evaluated working in reduced dimension, by solving the least squares problem

$$(3.5) \quad \min_{y \in \mathbb{R}^m} \|\bar{H}_m y - c\|.$$

For the computation of $\beta^{(m)}$, suppose that, at step m , we have used the parameter $\lambda^{(m-1)}$ (obtained at the previous step or, if $m = 1$, given by the user) to compute $y_{\lambda^{(m-1)}}^{(m)}$ by solving (2.5) with $\lambda = \lambda^{(m-1)}$. The corresponding discrepancy is

$$\phi^{(m)}(\lambda^{(m-1)}) = \left\| c - \bar{H}_m y_{\lambda^{(m-1)}}^{(m)} \right\|,$$

and consequently, using the approximation (3.3), we obtain

$$(3.6) \quad \beta^{(m)} = \frac{\phi^{(m)}(\lambda^{(m-1)}) - \alpha^{(m)}}{\lambda^{(m-1)}}.$$

To select $\lambda^{(m)}$ for the next step of the Arnoldi-Tikhonov algorithm we impose

$$(3.7) \quad \phi^{(m)}(\lambda^{(m)}) = \eta \varepsilon$$

and we force the approximation

$$(3.8) \quad \phi^{(m)}(\lambda^{(m)}) = \alpha^{(m)} + \lambda^{(m)} \beta^{(m)};$$

Hence, by (3.6) and (3.7), we define

$$(3.9) \quad \lambda^{(m)} = \frac{\eta \varepsilon - \alpha^{(m)}}{\phi^{(m)}(\lambda^{(m-1)}) - \alpha^{(m)}} \lambda^{(m-1)}.$$

The method (3.9) has a simple geometrical interpretation which allows it to be seen as a zero finder. Indeed, with this choice of $\alpha^{(m)}$ and $\beta^{(m)}$, the function $\phi^{(m)}(\lambda)$ is linearly interpolated at $(0, \alpha^{(m)})$ and $(\lambda^{(m-1)}, \phi^{(m)}(\lambda^{(m-1)}))$; looking at (3.8), we understand that, at each iteration of the Arnoldi-Tikhonov method, a step of a secant-like zero-finder for the solution of (3.7) is performed; see, again, [6].

We remark that in the first iterations of (3.9) instability can occur, due to the fact that we may have $\alpha^{(m)} \gg \eta \varepsilon$. In this situation the result of (3.9) may be negative (recall that the function $\phi^{(m)}(\lambda)$ is increasing and is only defined for $\lambda > 0$); therefore, we consider

$$(3.10) \quad \lambda^{(m)} = \left| \frac{\eta \varepsilon - \alpha^{(m)}}{\phi^{(m)}(\lambda^{(m-1)}) - \alpha^{(m)}} \right| \lambda^{(m-1)}.$$

Numerically, formula (3.10) is very stable, in the sense that after the discrepancy principle is satisfied, $\lambda^{(m)} \approx \text{const}$ for growing values of m . We address the fact that this parameter choice technique can also be used together with the Range-Restricted approach [10] and even in the case of Krylov methods based on the Lanczos bidiagonalization process [5].

Finally we note that, with respect to the strategies used so far in connection with the AT method, the present one is intrinsically simpler and cheaper; indeed it essentially involves quantities that are strictly connected to the projected problem and the only additional computations are performed in reduced dimension. More specifically, the computation of the GMRES residual requires $O(m^2)$ operations (if the QR update is not employed, otherwise just $O(m)$).

3.2. The multi-parameter case. As pointed out by many works in the literature (cf., for example, [4] and [11]), the most natural way to face a multi-parameter problem is to first solve some single-parameter problems, one for each regularization matrix, and then to find a connection between all the problems. In our case, at the m -th step of the Arnoldi-Tikhonov algorithm and for a given j , $1 \leq j \leq k$, we consider the problem,

$$(3.11) \quad \min_{y_m \in \mathbb{R}^m} \left\| \begin{bmatrix} \bar{H}_m \\ \sqrt{\lambda_1^{(m)}} L_1 V_m \\ \vdots \\ \sqrt{\lambda_{j-1}^{(m)}} L_{j-1} V_m \\ \sqrt{\lambda} L_j V_m \end{bmatrix} y_m - \begin{bmatrix} \|b\| e_1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix} \right\|^2,$$

which is a j -parameter Arnoldi-Tikhonov scheme; it can also be regarded as a reduced version of the system (2.5), where the corresponding regularization vector is

$$(3.12) \quad \Lambda = \left((\Lambda_{j-1}^{(m)})^T, \lambda, 0, \dots, 0 \right)^T, \quad \text{where } \Lambda_{j-1}^{(m)} = (\lambda_1^{(m)}, \dots, \lambda_{j-1}^{(m)})^T.$$

According to the notation that we have used in the one-parameter case, this means that we have already solved, in a sequential way, $(j - 1)$ reduced problems obtained adding to the original projected problem (3.5) a new regularization term and that we have determined the suitable regularization parameters $\lambda_1^{(m)}, \dots, \lambda_{j-1}^{(m)}$, for the problems so far considered. Therefore, now the task is to determine the parameter $\lambda_j^{(m)}$. Since we only have to update one parameter, we can use the strategy employed for the single parameter AT method. We define the function

$$(3.13) \quad \phi_j^{(m)}(\lambda) = \phi^{(m)}(\Lambda) = \left\| c - \bar{H}_m y_{\Lambda, j}^{(m)} \right\|, \quad \Lambda = \left((\Lambda_{j-1}^{(m)})^T, \lambda, 0, \dots, 0 \right)^T,$$

where $y_{\Lambda, j}^{(m)}$ is the solution of (3.11). In this framework, the normal equations associated with the problem (3.11) are

$$\left(\bar{H}_m^T \bar{H}_m + \sum_{i=1}^{j-1} \lambda_i^{(m)} V_m^T L_i^T L_i V_m + \lambda V_m^T L_j^T L_j V_m \right) y_{\Lambda, j}^{(m)} = \bar{H}_m^T c.$$

As before, we are looking for a linear approximation, with respect to the parameter λ , of the discrepancy associated with the reduced multi-parameter problem so far considered, i.e.,

$$(3.14) \quad \phi_j^{(m)}(\lambda) \approx \alpha_j^{(m)} + \lambda \beta_j^{(m)}.$$

Analogously to the one-parameter case, to obtain $\alpha_j^{(m)}$ we consider $\lambda = 0$, that is,

$$\alpha_j^{(m)} = \phi_j^{(m)}(0) = \left\| \bar{H}_m \left(\bar{H}_m^T \bar{H}_m + \sum_{i=1}^{j-1} \lambda_i^{(m)} V_m^T L_i^T L_i V_m \right)^{-1} \bar{H}_m^T c - c \right\|.$$

Observing the above expression, we see that now we have to deal with the discrepancy associated to the $(j - 1)$ -parameter method with vector of the regularization parameters given by $\Lambda_{j-1}^{(m)}$. Using the definition (3.13) we also have

$$(3.15) \quad \alpha_j^{(m)} = \phi^{(m)}(\Lambda_{j-1}^{(m)}).$$

We emphasize that, to obtain the quantity $\alpha_j^{(m)}$, we have to solve again the $(j - 1)$ -parameter problem with the regularization vector given by $\Lambda_{j-1}^{(m)}$. Of course, when $j = 1$, the determination of $\lambda_1^{(m)}$ again requires the computation of the solution of the problem (3.5) as in the one-parameter case, i.e., $\alpha_1^{(m)} = \phi_1^{(m)}(0)$ is still the residual of the m -th GMRES iterate.

Regarding the quantity $\beta_j^{(m)}$, once we have solved (3.11) for $\lambda = \lambda_j^{(m-1)}$, we obtain

$$(3.16) \quad \phi_j^{(m)}(\lambda_j^{(m-1)}) = \left\| c - \bar{H}_m y_{\Lambda, j}^{(m)} \right\|, \quad \Lambda = \left((\Lambda_{j-1}^{(m)})^T, \lambda_j^{(m-1)}, 0, \dots, 0 \right)^T,$$

and consequently, using the approximation (3.14), we get

$$\beta_j^{(m)} = \frac{\phi_j^{(m)}(\lambda_j^{(m-1)}) - \alpha_j^{(m)}}{\lambda_j^{(m-1)}}.$$

Finally, imposing $\phi_j^{(m)}(\lambda_j^{(m)}) = \eta\varepsilon$ and forcing again (3.14), we compute the new j -th component of the regularization vector as

$$\lambda_j^{(m)} = \frac{\eta\varepsilon - \alpha_j^{(m)}}{\phi_j^{(m)}(\lambda_j^{(m-1)}) - \alpha_j^{(m)}} \lambda_j^{(m-1)}.$$

As in the one-parameter case, the computation of each $\lambda_j^{(m)}$, $j = 1, \dots, k$, can be meaningless for the first few iterations, since when $\eta\varepsilon$ is larger than $\alpha_j^{(m)}$, the values of $\lambda_j^{(m)}$ are negative. For this reason we consider

$$(3.17) \quad \lambda_j^{(m)} = \left| \frac{\eta\varepsilon - \alpha_j^{(m)}}{\phi_j^{(m)}(\lambda_j^{(m-1)}) - \alpha_j^{(m)}} \right| \lambda_j^{(m-1)}.$$

At this point, if $j < k$ we add a regularization term and we repeat the previous computation with $j+1$ instead of j ; otherwise, if $j = k$, the solution $y_{\Lambda, k}^{(m)}$ of (3.11) is indeed the solution of the complete multi-parameter problem (2.5). We stop the iterations as soon as $\phi^{(m)}(\Lambda) \leq \eta\varepsilon$.

3.3. Geometrical interpretation. We close this section suggesting a geometrical interpretation of the above proposed scheme. For simplicity we treat the case $k = 2$, but the exposed ideas can be generalized to an arbitrary number of regularization terms. We fix an index m and a Cartesian coordinate system $(\lambda_1, \lambda_2, z)$. Considering $z = \phi^{(m)}(\lambda_1, \lambda_2)$ we obtain a differentiable surface in \mathbb{R}^3 ; solving (1.2) means finding the intersections between the just mentioned surface and the horizontal plane $z = \eta\varepsilon$; see Figure 3.1, upper frame. The strategy described above prescribes to initially take $\lambda_2 = 0$; in this way we work on the plane (λ_1, z) and the approximate solution $\lambda_1^{(m)}$ of $\phi^{(m)}(\lambda_1, 0) = \phi_1^{(m)}(\lambda_1) = \eta\varepsilon$ is the intersection between $z = \alpha_1^{(m)} + \lambda_1 \beta_1^{(m)}$ and $z = \eta\varepsilon$ if this scalar is positive, otherwise its absolute value; see Figure 3.1, lower leftmost frame. At this point we take $\lambda_1 = \lambda_1^{(m)}$, that is, we work on the plane $(\lambda_1^{(m)}, \lambda_2, z)$; the new value $\lambda_2^{(m)}$ is the approximate solution of $\phi^{(m)}(\lambda_1^{(m)}, \lambda_2) = \phi_2^{(m)}(\lambda_2) = \eta\varepsilon$, which is the intersection between $z = \alpha_2^{(m)} + \lambda_2 \beta_2^{(m)}$ and $z = \eta\varepsilon$ if this scalar is positive, otherwise its absolute value; see Figure 3.1, lower rightmost frame; in this case we display what happens when the quantity $\alpha_2^{(m)}$ is larger than the noise level.

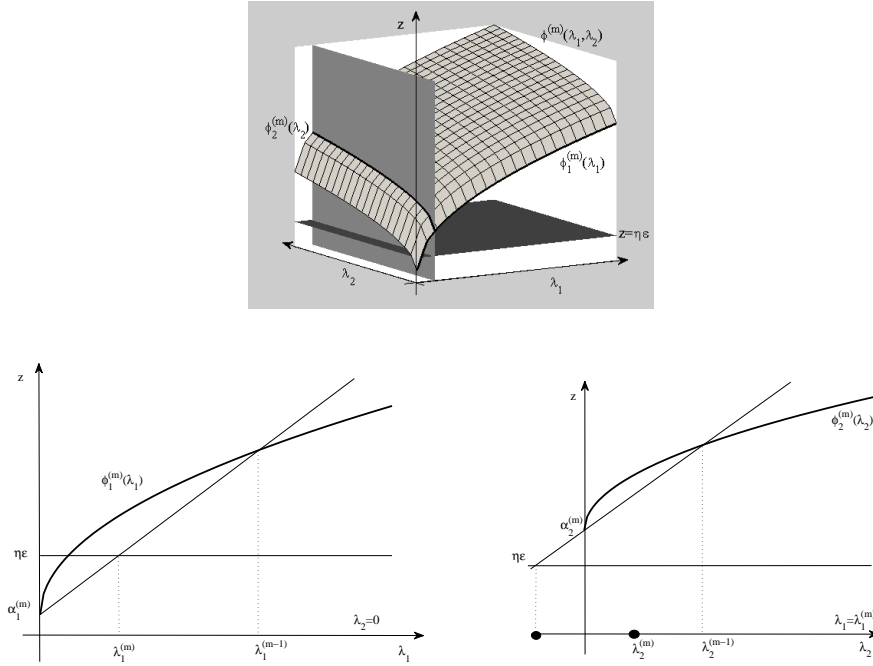


FIG. 3.1. Geometric interpretation of the strategy proposed to find the values of the regularization parameters when performing Arnoldi-Tikhonov multi-parameter method in the case $k = 2$ and for a fixed m . Upper frame: plot of the surface $z = \phi^{(m)}(\lambda_1, \lambda_2)$ along with the planes $z = \eta\varepsilon$ and $\lambda_1 = \lambda_1^{(m)}$. Lower leftmost frame: plot of the curve $\phi_1^{(m)}(\lambda_1) = \phi^{(m)}(\lambda_1, 0)$ on the plane $\lambda_2 = 0$; we also display the threshold $\eta\varepsilon$, and the considered linear approximation and the computed new value $\lambda_1^{(m)}$. Lower rightmost frame: plot of the curve $\phi_2^{(m)}(\lambda_2) = \phi^{(m)}(\lambda_1^{(m)}, \lambda_2)$ on the plane $\lambda_1 = \lambda_1^{(m)}$; we also display the threshold $\eta\varepsilon$, and the considered linear approximation and the computed new value $\lambda_2^{(m)}$ (note that, in this case, $\alpha_2^{(m)} > \eta\varepsilon$).

4. Algorithms. In this section, we summarize the method described above and we propose a computationally cheaper variant of the following algorithm.

ALGORITHM 4.1. Multi-parameter Arnoldi-Tikhonov

1. Input: $A, b, \mathcal{L} = \{L_1, \dots, L_k\}, \Lambda = (\lambda_1^{(0)}, \dots, \lambda_k^{(0)}), x_0, \varepsilon, \eta$
2. For $m = 1, 2, \dots$ until $\|c - \bar{H}_m y_\Lambda^{(m)}\| \leq \eta\varepsilon$
 - (a) Update V_m, \bar{H}_m by the Arnoldi algorithm (2.2).
 - (b) For $j = 1, \dots, k - 1$
 - i. Solve (3.11) with the parameters $((\Lambda_{j-1}^{(m)})^T, \lambda_j^{(m-1)})^T$ and evaluate $\phi_j^{(m)}(\lambda_j^{(m-1)})$ by (3.16).
 - ii. Solve (3.11) with the parameters $((\Lambda_{j-1}^{(m)})^T, 0)^T$ and evaluate $\phi_j^{(m)}(0)$ by (3.16).
 - iii. Compute the new parameter $\lambda_j^{(m)}$ by (3.17) and then $\Lambda_j^{(m)}$ (cf. (3.12)).
 - (c) Compute the vector $y_\Lambda^{(m)} := y_{\Lambda, k}^{(m)}$ by solving the complete problem (2.5), with $\Lambda = ((\Lambda_{k-1}^{(m)})^T, \lambda_k^{(m-1)})^T$.
 - (d) Compute the new parameter $\lambda_k^{(m)}$ by (3.17) and then update Λ .
3. Compute the approximate solution $x = V_m y_\Lambda^{(m)}$.

Algorithm 4.1 follows the discussion of the previous section, and hence requires the solution of each reduced system twice (for each $j = 1, \dots, k$), in order to sequentially update the values of the components of the regularization vector Λ . There is however a cheaper alternative that consists in not using the updated values of the parameter. In other words, for $j = 1, \dots, k - 1$, we do not need to replace $\lambda_j^{(m-1)}$ by $\lambda_j^{(m)}$, but we can work with the regularization vector $((\Lambda_{j-1}^{(m-1)})^T, \lambda_j^{(m-1)})^T = (\lambda_1^{(m-1)}, \dots, \lambda_{j-1}^{(m-1)}, \lambda_j^{(m-1)})^T$ at Step 2bi. The new expression of $\alpha_j^{(m)}$ is now (cf. (3.15))

$$(4.1) \quad \alpha_j^{(m)} = \phi^{(m)}(\Lambda_{j-1}^{(m-1)}).$$

This alternative approach, described by Algorithm 4.2, requires only one solution of (3.11), for $j = 1, \dots, k$, at each step.

ALGORITHM 4.2. *Multi-parameter Arnoldi-Tikhonov without intermediate update*

1. *Input:* $A, b, \mathcal{L} = (L_1, \dots, L_k), \Lambda = (\lambda_1^{(0)}, \dots, \lambda_k^{(0)}), x_0, \varepsilon, \eta$
2. *For* $m = 1, 2, \dots$ *until* $\|c - \bar{H}_m y_\Lambda^{(m)}\| \leq \eta \varepsilon$
 - (a) *Update* V_m, \bar{H}_m *by the Arnoldi algorithm (2.2).*
 - (b) *For* $j = 1, \dots, k$
 - i. *Solve (3.11) with the parameters $(\Lambda_{j-1}^{(m-1)})^T$ and evaluate $\phi_j^{(m)}(\lambda_j^{(m-1)})$ by (3.16).*
 - ii. *Take $\alpha_j^{(m)}$ as in (4.1).*
 - iii. *Compute the new parameter $\lambda_j^{(m)}$ by (3.17).*
 - (c) *Update the vector $\Lambda = (\lambda_1^{(m)}, \dots, \lambda_k^{(m)})$.*
3. *Compute the approximate solution $x = V_m y_{\Lambda^{(m-1)}}^{(m)}$.*

The numerical tests reported in Appendix A show that this strategy can compute regularized solutions whose relative error is still comparable to the one of the solutions obtained running Algorithm 4.1. However, the number of iterations required to return the solution is, on average, larger than for the former method.

REMARK 4.3. In our computations both Algorithm 4.1 and Algorithm 4.2 have been implemented with some minor changes regarding the stopping criterion. Indeed we have employed a sort of *weakened discrepancy principle*, that is, we stop the iterations as soon as

$$(4.2) \quad \phi^{(m)}(\lambda) - \eta \tilde{\varepsilon} \|b\| < 10^\theta,$$

where $\theta < 0$ is automatically determined as the sum of the order of the noise level $\tilde{\varepsilon}$ and of the order of the last significant digit of η . In this way, when applying the discrepancy principle, we neglect any quantity coming after the last significant digit of the product $\tilde{\varepsilon}\eta$. For instance, if $\tilde{\varepsilon} = 10^{-2}$ and $\eta = 1.01$ then $\theta = -4$ and we stop the iterations as soon as

$$\phi^{(m)}(\lambda)/\|b\| \leq 1.01 \cdot 10^{-2} + 9.9 \cdot 10^{-5}.$$

We remark that, if the “classical” discrepancy principle (3.1) is fulfilled, then also (4.2) is satisfied. We introduced this weakened version of the discrepancy principle because, while executing the numerical experiments, we noted that very often the discrepancy stagnates slightly above the prescribed threshold without crossing it and, when performing too many iterations, the quality of the approximate solution deteriorates. At the same time, we decide to enforce the stopping criterion in order to assure that not only the solution $y_\Lambda^{(m)}$ of the complete problem but also all the solutions of the reduced regularization problems satisfy the weakened

discrepancy principle (4.2), that is, $\phi_j^{(m)}(\lambda_j^{(m-1)}) - \eta \tilde{\varepsilon} \|b\| < 10^\theta \forall j = 1, \dots, k - 1$. This is a quite natural choice, since the solution of the multi-parameter problem is formed taking into account the k solutions of the associated one-parameter problems.

5. Numerical experiments. In this section we test the behavior of Algorithm 4.1 to solve multi-parameter problems. We believe that the best way to validate the method just described is to make suitable comparisons with what happens in the one-parameter case; in the sequel we will explain the details and the goal of each experiment. We will exclusively focus on two-parameter and three-parameter cases. All the test problems are taken from Hansen’s package *Regularization Tools* [7].

In all the examples we assume that we know the exact solution \bar{x} and that the exact right-hand side vector is either given in [7] or constructed by taking $\bar{b} = A\bar{x}$. The elements of the noise vector e are normally distributed with zero mean and the standard deviation is chosen such that $\|e\|/\|\bar{b}\|$ is equal to a prescribed level $\tilde{\varepsilon}$. Moreover, we always consider the initial guess $x_0 = 0$ and we set $\eta = 1.01$ and $\Lambda = (1, \dots, 1)^T \in \mathbb{R}^k$. Following [11], each test problem is generated 100 times to reduce the dependence of the results on the random components of the vector e . All the computations have been executed using MATLAB 7.10 with 16 significant digits on a single processor computer Intel Core i3-350M.

Before describing each test, we list the regularization matrices that we have employed:

- The identity matrix $I_N \in \mathbb{R}^{N \times N}$.
- Scaled finite difference approximations of the first and second order derivatives, i.e.,

$$(5.1) \quad D_1 := \begin{bmatrix} 1 & -1 & & \\ & \ddots & \ddots & \\ & & 1 & -1 \\ & & & \ddots & \ddots \end{bmatrix} \in \mathbb{R}^{(N-1) \times N},$$

$$(5.2) \quad D_2 := \begin{bmatrix} 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & \ddots & \ddots \end{bmatrix} \in \mathbb{R}^{(N-2) \times N},$$

whose null spaces are given by $\mathcal{N}(D_1) = \text{span}\{(1, 1, \dots, 1)^T\} \subset \mathbb{R}^N$ and $\mathcal{N}(D_2) = \text{span}\{(1, 1, \dots, 1)^T, (1, 2, \dots, N)^T\} \subset \mathbb{R}^N$.

- Square projection matrices built using the strategy suggested in [12]: given $M \in \mathbb{R}^{N \times \ell}$ we compute the “skinny” QR factorization $M = WR$ (where $W \in \mathbb{R}^{N \times \ell}$ and $R \in \mathbb{R}^{\ell \times \ell}$) and we take, as regularization matrix

$$(5.3) \quad L := I_N - WW^T \in \mathbb{R}^{N \times N}.$$

In this way the null space of L is spanned by the orthonormal columns of W . This kind of matrix is particularly useful when we want to consider a regularization operator with a given null space different from the ones of the commonly used operators (5.1) and (5.2).

5.1. Results obtained considering particular solutions. The aim of the first set of experiments is to show that, when applying the multi-parameter method to a problem whose exact solution \bar{x} lies in the null space of the regularization operator L_i , the parameter selection strategy correctly weights the i -th component of the regularization vector Λ by assigning to λ_i a value dominating the other components. Indeed, in this situation, the regularization operator L_i is the most suitable one, since the important features of the solution are not damped. Therefore, we start to consider two particular exact solutions: the constant one, $\bar{x}_c := (1, 1, \dots, 1)^T \in \mathbb{R}^N$, and the linear one, $\bar{x}_l := (1, 2, \dots, N)^T \in \mathbb{R}^N$; as recalled in the

above list, $\bar{x}_c \in \mathcal{N}(D_1) \cap \mathcal{N}(D_2)$, while $\bar{x}_l \in \mathcal{N}(D_2)$. For this reason we will employ both two- and three-parameter methods with different combinations of the regularization matrices I_N , D_1 , and D_2 .

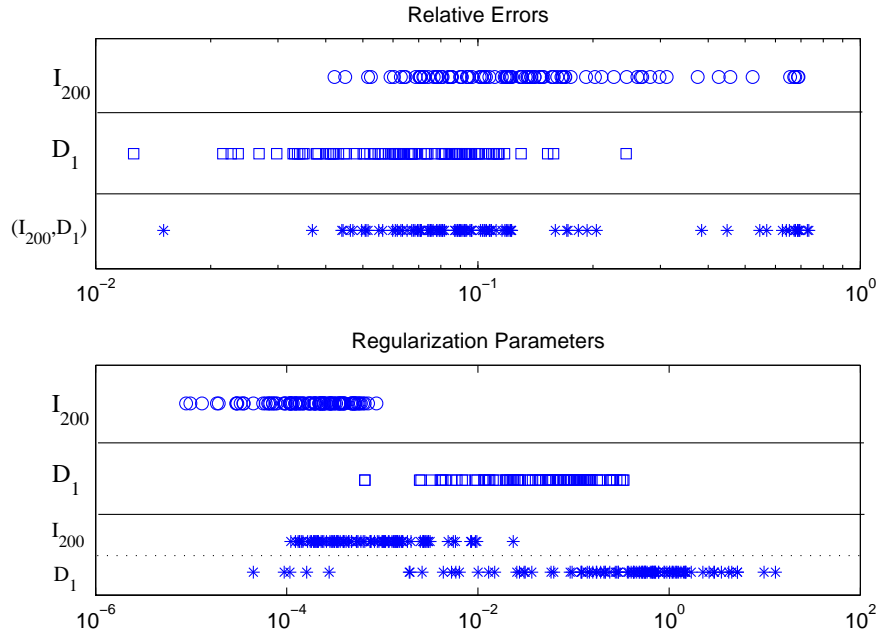


FIG. 5.1. Results obtained running 100 times the test problem `i_laplace` with the particular solution \bar{x}_c (we plot one single marker for each performed test). Upper frame: we report the values of the relative errors in logarithmic scale on the horizontal axis and, at each vertical level, we mark the values corresponding to the I_{200} one-parameter (circle), the D_1 one-parameter (square), and the (I_{200}, D_1) two-parameter (asterisk) methods. Lower frame: we report the values of the regularization parameters in logarithmic scale on the horizontal axis and, at each vertical level, we mark the values corresponding to the I_{200} one-parameter (circle), the D_1 one-parameter (square), and the (I_{200}, D_1) two-parameter (asterisk) methods; concerning the multi-parameter method, the first line (labelled by I_{200}) refers to the parameter that weights the term $\|x\|^2$, while the second line (labelled by D_1) refers to the parameter that weights the term $\|D_1 x\|^2$.

First, we take the solution \bar{x}_c and consider the matrix of size $N = 200$ associated with the problem `i_laplace`. The noise level is $\tilde{\varepsilon} = 10^{-2}$ and we determine a regularized solution by using the (I_{200}, D_1) two-parameter method. To illustrate what happens using the single-parameter Tikhonov method, for each test we also report results obtained considering exclusively $L = I_{200}$ and $L = D_1$. We display the results for 100 different noisy right-hand sides in Figure 5.1. We can clearly see that, with very few exceptions, the components of the regularization vector associated with I_{200} and D_1 replicate the behavior of the parameter of the Tikhonov method with $L = I_{200}$ and $L = D_1$, respectively. This means that, in the regularization process, the most appropriate regularization operator, in this case D_1 , gets a larger weight than the others. In almost all cases, the solutions of the I_{200} and D_1 one-parameter methods belong to Krylov subspaces of dimensions 5 and 6, respectively, while most of the solutions associated to the two-parameter method belong to Krylov subspaces of dimensions 6 or 7. In Figure 5.2 we focus on a single test and we display the course of the relative error, the regularization parameters, and the discrepancies of the examined methods at each step of the Arnoldi algorithm. Looking at both figures we can see that the quality of the solutions computed by the multi-parameter method does not improve with respect to

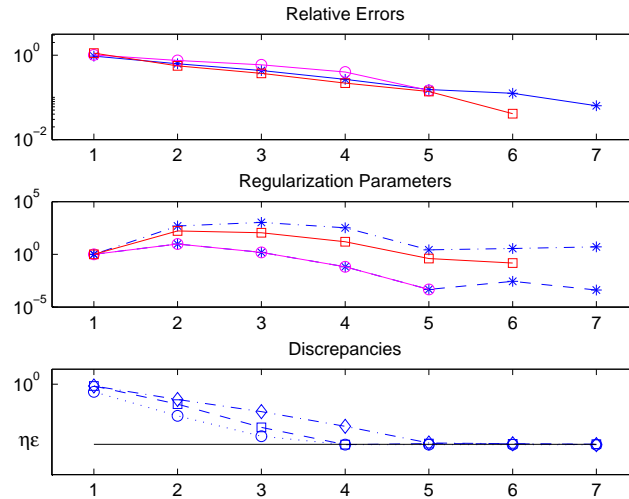


FIG. 5.2. Behavior of the relative errors, regularization parameters and discrepancies versus the number of iterations for the test problem `i_laplace` with solution \bar{x}_c . Upper box: we consider the multi-parameter method (asterisk), the I_{200} one-parameter method (circle), and the D_1 one-parameter method (square); middle box: we display the values of the parameters λ_1 associated to I_{200} (asterisk with dashed line) and λ_2 associated to D_1 (asterisk with dash-dot line) and the values of the parameters of the two one-parameter methods considered above (with the same markers as listed above); lower box: the norm of the residual of the GMRES over $\|b\|$ (circle) and the discrepancies $\phi_1^{(m)}/\|b\|$ associated to the first regularization term (square), $\phi_2^{(m)}/\|b\|$ associated to the second regularization term (diamond).

the results for the D_1 one-parameter method. However, this is quite reasonable since, as said in the introduction, the task of the multi-parameter method is to preserve many different features of the solution; when, as in this case, the solution belongs to the null space of one of the considered operators, the one-parameter method with that regularization operator is the one that works the best.

Now we consider the matrix associated to the problem `phillips` with $N = 200$ and take, as exact solution, the linear one \bar{x}_l ; the noise level is again $\tilde{\varepsilon} = 10^{-2}$. We compute the regularized solution employing the three-parameter method with regularization matrices $L_1 = I_{200}$, $L_2 = D_1$, and $L_3 = D_2$. We display the results in Figure 5.3 together with our results for the same problem with the I_{200} , D_1 , D_2 one-parameter methods. Even in this case the parameter selection strategy assigns the largest parameter value to the matrix whose null space contains the exact solution (in this case, D_2). Regarding the number of iterations required to satisfy the weakened discrepancy principle, the three-parameter method needs in most of the cases 8, 11, or 13 iterations, the I_{200} one-parameter method requires 7 or 8 iterations, while both the D_1 and D_2 one-parameter methods demand 8 or 9 iterations. In Figure 5.4 we show the relative errors of the regularization parameters and of the discrepancies versus the number of iterations for the problem `shaw` of size 200. We take again the linear vector \bar{x}_l as exact solution.

The method has been applied to the most popular test problems of [7], all of dimension $N = 200$, using the two particular solutions \bar{x}_c and \bar{x}_l . We also consider two different noise levels ($\tilde{\varepsilon} = 10^{-2}$ and $\tilde{\varepsilon} = 5 \cdot 10^{-2}$) and several combinations of regularization operators. We summarize the obtained results in Tables A.1, A.2, A.3, and A.4 reported in Appendix A.

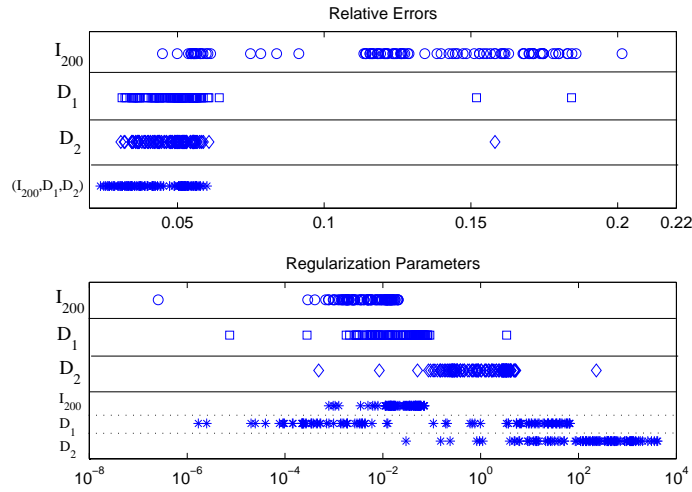


FIG. 5.3. Results obtained running 100 times the test problem `phillips` with the particular solution \bar{x}_1 (we plot one single marker for each performed test). Upper frame: we report the values of the relative errors on the horizontal axis and, at each vertical level, we mark the values corresponding to the I_{200} one-parameter (circle), the D_1 one-parameter (square), the D_2 one-parameter (diamond), and the (I_{200}, D_1, D_2) three-parameter (asterisk) methods. Lower frame: we report the values of the regularization parameters in logarithmic scale on the horizontal axis and, at each vertical level, we mark the values corresponding to the I_{200} one-parameter (circle), the D_1 one-parameter (square), the D_2 one-parameter (diamond), and the (I_{200}, D_1, D_2) three-parameter (asterisk) methods; concerning the multi-parameter method, the first line (labelled by I_{200}) refers to the parameter that weights the term $\|x\|^2$, the second line (labelled by D_1) refers to the parameter that weights the term $\|D_1 x\|^2$, and the third line (labelled by D_2) refers to the parameter that weights the term $\|D_2 x\|^2$.

Finally, we consider experiments with the artificial solutions

$$(5.4) \quad \bar{x}_{\sin} = x^{(a)} + x^{(b)} := 10 \sin\left(\frac{x}{2}\right) + x \in \mathbb{R}^N,$$

$$(5.5) \quad \bar{x}_{\tan} = x^{(a)} + x^{(b)} := \frac{1}{10} \tan\left(\frac{x}{N+1} \frac{\pi}{2}\right) + x \in \mathbb{R}^N.$$

Here \bar{x}_{\sin} is oscillating while \bar{x}_{\tan} is quickly increasing. These experiments are motivated by the fact that the pair of matrices (5.1) and (5.2) considered so far represents a particular situation, since $\mathcal{N}(D_1) \subset \mathcal{N}(D_2)$. Taking instead the solution (5.4) or (5.5), by (5.3) we can build two particular regularization matrices $L^{(a)}$ and $L^{(b)}$ such that $x^{(a)} \in \mathcal{N}(L^{(a)})$, $x^{(b)} \in \mathcal{N}(L^{(b)})$ and $\mathcal{N}(L^{(a)}) \cap \mathcal{N}(L^{(b)}) = \{0\}$. Consequently, neither \bar{x}_{\sin} nor \bar{x}_{\tan} belong to the null space of the matrices $L^{(a)}$ or $L^{(b)}$. In this way we can really appreciate that the essence of the multi-parameter methods is, as said in the introduction, to preserve many different features of the solution of the original problem that may be distorted imposing only one regularization operator. For both solutions we consider the matrix $A \in \mathbb{R}^{200 \times 200}$ associated to the test problem `foxgood`, a noise level $\tilde{\varepsilon} = 10^{-2}$, and the regularization matrices $L_1 = L^{(a)}$, $L_2 = L^{(b)}$. We display the results for (5.4) and (5.5) in Figure 5.5.

5.2. Results for more general solutions. In the second set of computed experiments we simply consider the most common test problems in [7] with their appropriate solution. We are just going to display some graphs that compare the performances of the new multi-parameter method and the usual Arnoldi-Tikhonov method. We consider the regularization matrices I_N , D_1 , and D_2 .

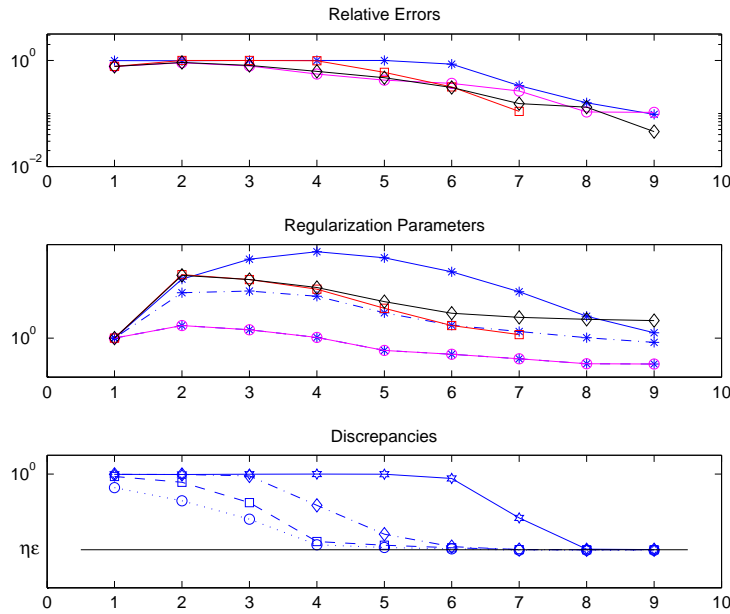


FIG. 5.4. Behavior of the relative errors, regularization parameters and discrepancies versus the number of iterations for the test problem `shaw` with solution \bar{x}_1 . The displayed quantities are the same as in Figure 5.2 and are denoted by the same markers. In addition: in the upper box we visualize the D_2 one-parameter method (diamond); in the middle box we visualize the parameter λ_3 (asterisk with solid line) that weights the term $\|D_2x\|^2$ of the multi-parameter method along with the regularization parameter associated to the D_2 one-parameter method (diamond); in the lower box we visualize the discrepancy $\phi_3^{(m)}/\|b\|$ (hexagram) associated to the third regularization term.

Figure 5.6 displays the behavior of the relative errors and the values of the regularization parameters obtained when solving the test problem `i_laplace` of dimension $N = 200$ with noise of level $\tilde{\varepsilon} = 10^{-2}$ in the right-hand-side vector. We consider the I_{200} and D_1 one-parameter methods and the (D_1, I_{200}) two-parameter method. We remark that, when performing the multi-parameter method, the results can be affected by the order in which the regularization matrices appear. Indeed, looking at the parameters selection strategy described in subsection 3.2, we can understand that the first regularization matrix (in this case, L_1) is weighted similarly to the one-parameter case, while the following ones work as corrections. This is a consequence of the fact that many reduced problems are solved sequentially and each one is based on the solutions and on the parameters associated to the previous ones; in this sense the first regularization operator is somehow advantaged with respect to the others. Therefore, if one has some intuition about the regularity of the solution, we suggest to put in the first place the most suitable regularization matrix. Tables A.5 and A.6 reported in Appendix A collect results obtained by considering one-, two-, and three-parameter methods with various combinations of the usual regularization matrices and two different noise levels.

5.3. Further considerations. In this subsection we highlight a couple of important features of the new method that we noted while carrying out the numerical experiments just described.

The first property is that the AT multi-parameter method is very robust with respect to the initial choice of the regularization vector Λ , that is, considering different values of the components of Λ , the accuracy of the results and the number of iterations are basically stable. In Figure 5.7 we display the values of the regularization parameters obtained by solving the

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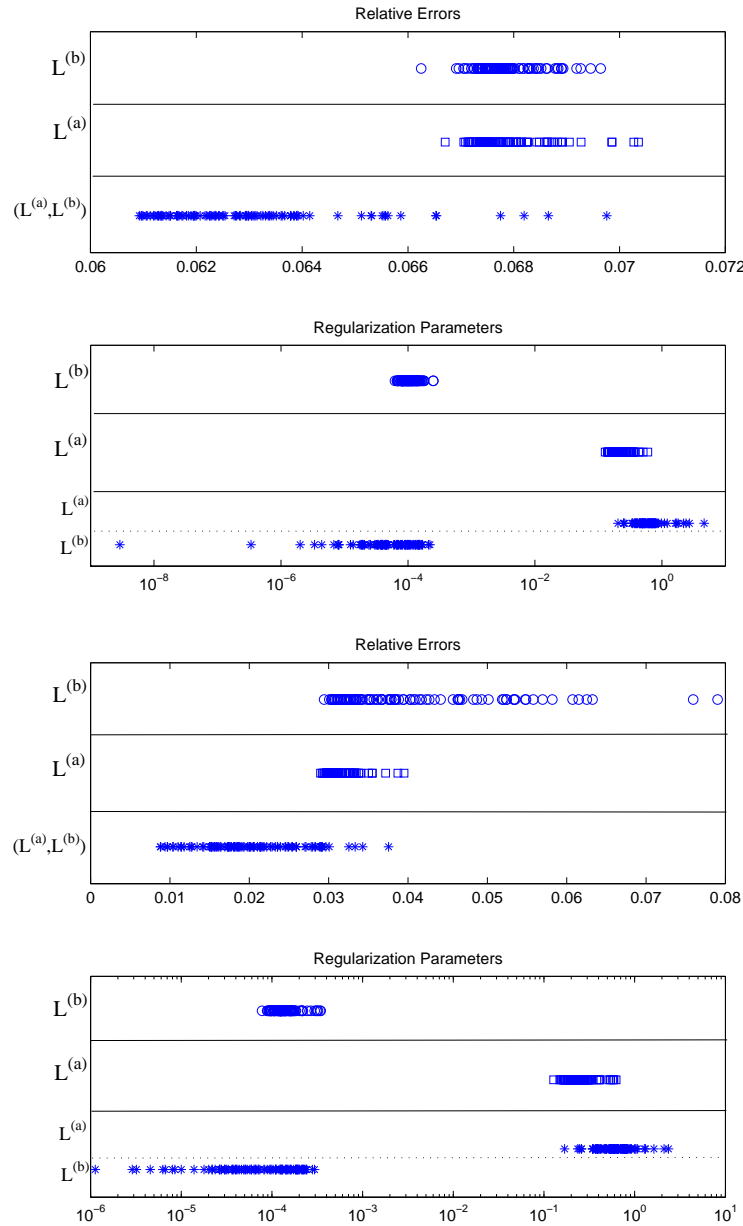


FIG. 5.5. Results obtained running 100 times the test problem foxgood with the particular solutions \bar{x}_{\sin} (first and second frames) and \bar{x}_{\tan} (third and fourth frames); as before, we plot one single marker for each performed test. The regularization operators $L^{(a)}$ and $L^{(b)}$ are projection operators of the form (5.3). First and third frames: we report the values of the relative errors on the horizontal axis and, at each vertical level, we mark the values corresponding to the $L^{(b)}$ one-parameter (circle), the $L^{(a)}$ one-parameter (square), and the $(L^{(a)}, L^{(b)})$ two-parameter (asterisk) methods. Second and fourth frames: we report the values of the regularization parameters in logarithmic scale on the horizontal axis and, at each vertical level, we mark the values corresponding to the $L^{(b)}$ one-parameter (circle), the $L^{(a)}$ one-parameter (square), and the $(L^{(a)}, L^{(b)})$ two-parameter (asterisk) methods; concerning the multi-parameter method, the first line (labelled by $L^{(a)}$) refers to the parameter that weights the first regularization term (i.e., the one that acts on the $x^{(a)}$ component of the solutions (5.4) and (5.5)), and the second line (labelled by $L^{(b)}$) refers to the parameter that weights the second regularization term (i.e., the one that acts on the $x^{(b)}$ component of the solutions (5.4) and (5.5)).

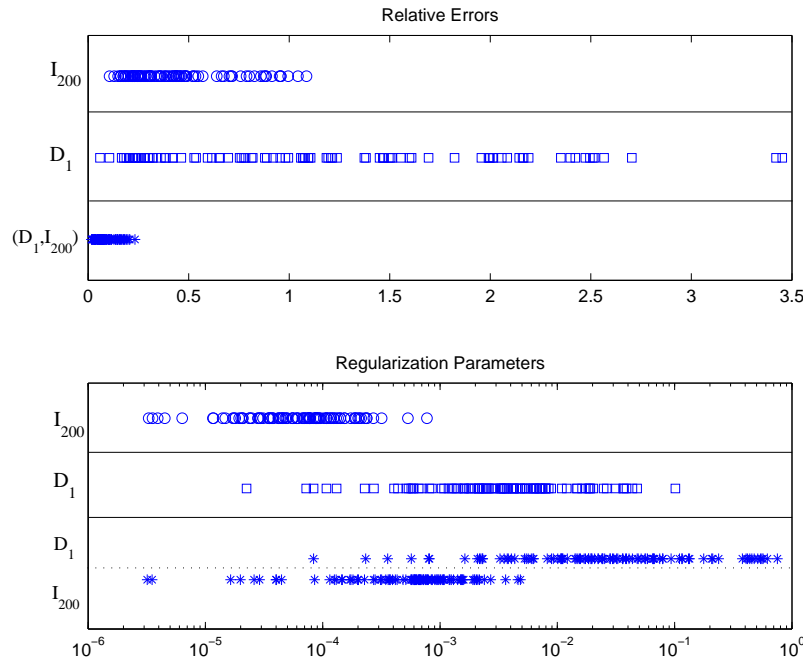


FIG. 5.6. Results obtained running 100 times the test problem `i_laplace` (we plot one single marker for each performed test). Upper frame: we report the values of the relative errors on the horizontal axis and, at each vertical level, we mark the values corresponding to the I_{200} one-parameter (circle), the D_1 one-parameter (square), and the (D_1, I_{200}) two-parameter (asterisk) methods. Lower frame: we report the values of the regularization parameters in logarithmic scale on the horizontal axis and, at each vertical level, we mark the values corresponding to the I_{200} one-parameter (circle), the D_1 one-parameter (square), and the (D_1, I_{200}) two-parameter (asterisk) methods; concerning the multi-parameter method, the first line (labelled by D_1) refers to the parameter that weights the term $\|D_1 x\|^2$, while the second line (labelled by I_{200}) refers to the parameter that weights the term $\|x\|^2$.

test problem `shaw` of dimension $N = 200$ and taking as exact solution the one given in [7]; the noise level is $\tilde{\varepsilon} = 10^{-2}$. We have employed the (I_{200}, D_1, D_2) three-parameter method and carried out four tests with initial vector Λ whose three entries are all equal to 0.5, 1, 10, or 100. We can see that, except in the very first iterations, the behavior of each λ_i , $i = 1, 2, 3$, is very similar independently of the initial value $\lambda_i^{(0)}$. We have also considered different components of the initial vector Λ and the results, even if not shown, are identical to the ones just described.

The second property is about the performance of the method when many extra iterations are executed after the stopping criterion is fulfilled. Despite that we had to review the stopping criterion introducing the weakened discrepancy principle (cf. Section 4), we can appreciate that in many cases the behavior of the method is very stable even when we decide to go on with an arbitrary number of iterations. For instance, in Figure 5.8 we display what happens when solving the problem `shaw` by the three-parameter method and letting, as above, $N = 200$, $\tilde{\varepsilon} = 10^{-2}$, $L_1 = I_{200}$, $L_2 = D_1$, and $L_3 = D_2$. Similar results have been obtained for `phillips` and `foxgood`.

6. Conclusion. We have described a new strategy to work with multi-parameter Tikhonov methods when an iterative scheme based on the Arnoldi algorithm is applied. The parameter selection method is based on the discrepancy principle and the algorithm to determine suitable regularization parameters at each step of the Arnoldi algorithm is computationally very

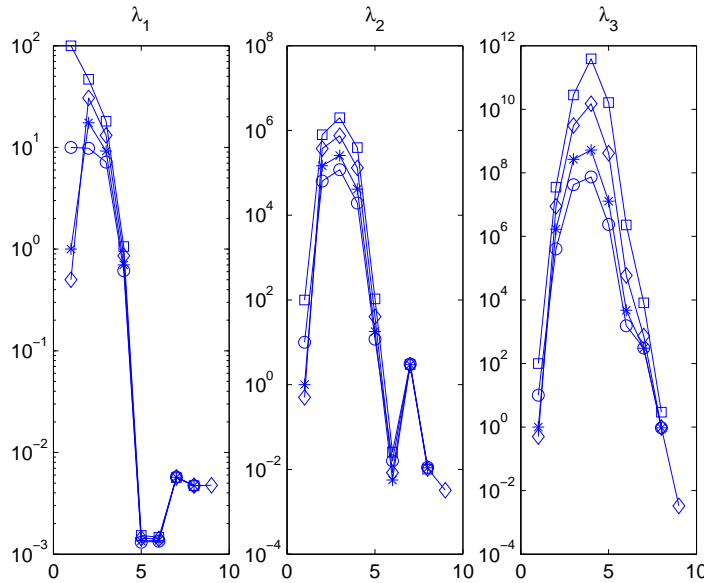


FIG. 5.7. Values of the components of the regularization vector Λ versus the number of iterations (each frame corresponds to a different component). The test problem is `shaw` and we consider the (I_{200}, D_1, D_2) multi-parameter AT method. The initial values for the regularization vector are $\Lambda = (0.5, 0.5, 0.5)^T$ (diamond), $\Lambda = (1, 1, 1)^T$ (asterisk), $\Lambda = (10, 10, 10)^T$ (circle), $\Lambda = (100, 100, 100)^T$ (square).

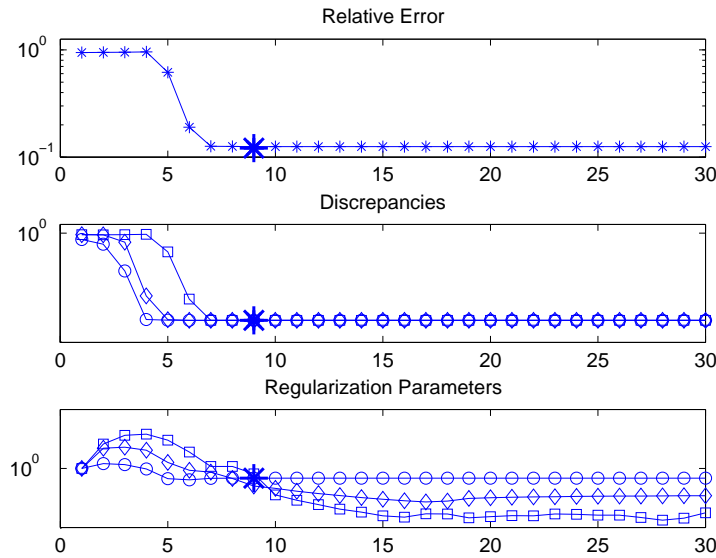


FIG. 5.8. Values of the relative error, of the discrepancies and of the regularization parameters versus the number of iterations for the test problem `shaw` solved by the (I_{200}, D_1, D_2) multi-parameter method. In the second and third boxes, the circle denotes the quantities associated to the first regularization matrix (I_{200}), the diamond denotes the quantities associated to the second regularization matrix (D_1), and the square denotes the quantities associated to the third regularization matrix (D_2). This method would stop at the 9th iteration (denoted by the large asterisk), but we decide to run it until the 30th iteration.

cheap, since it exclusively involves computations in reduced dimension. We have verified that the new method is able to automatically weight different regularization terms, assigning larger values of the regularization parameters to the most suitable regularization matrices. The numerical experiments performed also show that, in many cases, the new method is able to improve the solution computed by means of the one-parameter Arnoldi-Tikhonov method.

Appendix. A.

We report some tables for the experiments described in Section 5. The results are obtained performing, for each problem, 100 tests and taking the average of the relative errors, the average of each regularization parameter that appears in the method, and the average of the number of iterations. The parameters λ_1 , λ_2 , and λ_3 are always associated with the regularization matrices I_N , D_1 , and D_2 , respectively. When the multi-parameter method is used, we report the results obtained applying both Algorithm 4.1 and Algorithm 4.2 (we mark the latter with the abbreviation WU within brackets next to the test name). The dimension of the problem is always $N = 200$. Tables A.1, A.2, A.3, and A.4 show tests for particular solutions (constant and linear), while Tables A.5 and A.6 use solutions given by the routines of [7]. We consider different noise levels and we highlight the most interesting results with boldface.

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TABLE A.1
 Constant solution \bar{x}_c with noise level $\tilde{\varepsilon} = 10^{-2}$.

	Relative Errors	λ_1	λ_2	λ_3	Iterations
baart	1.0378e-001	6.7818e-004	-	-	3.00
baart	3.1941e-002	-	2.9526e+002	-	3.36
baart	4.6184e-002	-	-	1.5322e+003	3.08
baart	3.3079e-002	4.1362e-003	2.3190e+003	-	3.40
baart (WU)	3.8475e-002	2.3079e-003	1.0314e+003	-	4.31
baart	3.5972e-002	5.8633e-003	-	8.8528e+004	3.34
baart (WU)	4.6334e-002	6.8556e-004	-	1.5115e+004	3.01
baart	5.4689e-003	-	3.9761e+002	1.5605e+005	4.01
baart (WU)	6.3468e-003	-	3.3345e+002	6.4547e+005	4.00
baart	3.2744e-002	3.9987e-003	2.7437e+003	8.9722e+007	3.48
baart (WU)	2.5777e-003	3.7114e-003	8.3275e+003	2.0124e+009	5.30
gravity	7.6927e-002	2.7235e-002	-	-	4.05
gravity	3.5608e-002	-	1.2120e+002	-	4.89
gravity	3.7409e-002	-	-	7.5008e+003	5.01
gravity	3.6233e-002	4.3953e-002	5.0042e+001	-	5.06
gravity (WU)	3.6591e-002	3.5814e-002	9.1060e+001	-	4.82
gravity	3.7397e-002	4.6282e-002	-	1.8640e+002	4.94
gravity (WU)	3.7525e-002	3.7270e-002	-	2.6912e+003	4.92
gravity	3.0131e-002	-	2.9360e+002	1.8309e+004	6.08
gravity (WU)	2.7768e-002	-	3.8358e+002	2.3200e+004	7.08
gravity	3.1157e-002	5.7598e-002	4.7711e+001	3.1995e+003	6.50
gravity (WU)	2.6016e-002	6.3788e-002	2.6957e+002	7.3402e+003	8.02
shaw	1.9111e-001	8.2282e-004	-	-	11.96
shaw	1.0719e-001	-	9.6939e-001	-	6.82
shaw	1.4307e-001	-	-	1.7511e+002	7.12
shaw	1.2701e-001	1.1500e-003	6.5296e+000	-	6.91
shaw (WU)	9.5561e-002	8.9523e-004	1.2847e1	-	7.65
shaw	1.1748e-001	9.5530e+000	-	1.3175e+003	7.44
shaw (WU)	1.2813e-001	6.1538e+000	-	2.2507e+003	7.82
shaw	1.1748e-001	-	9.5530e+000	1.3175e+003	7.44
shaw (WU)	1.2813e-001	-	6.1538e+000	2.2507e+003	7.82
shaw	1.7063e-001	1.0023e-003	3.0629e+000	1.2808e+003	7.65
shaw (WU)	1.0891e-001	9.5358e-004	7.0005e+000	1.5660e+003	8.38

TABLE A.2
 Constant solution \bar{x}_c with noise level $\tilde{\varepsilon} = 5 \cdot 10^{-2}$.

	Relative Errors	λ_1	λ_2	λ_3	Iterations
baart	4.7271e-002	1.8289e-002	-	-	3.03
baart	4.6467e-002	-	2.6946e+002	-	3.00
baart	4.8727e-002	-	-	3.1295e+001	3.00
baart	2.8299e-002	3.5002e-002	2.8047e+003	-	3.81
baart (WU)	4.5396e-002	1.8319e-002	3.1644e+002	-	3.01
baart	5.6287e-002	3.5177e-002	-	6.1848e+004	3.81
baart (WU)	4.5595e-002	1.8319e-002	-	2.0673e+004	3.01
baart	4.1186e-002	-	2.6891e+003	3.5107e+006	3.12
baart (WU)	4.2843e-002	-	1.2127e+003	4.1811e+006	3.09
baart	2.9684e-002	3.4540e-002	2.8129e+003	7.0676e+006	3.95
baart (WU)	4.5433e-002	1.8319e-002	3.1644e+002	1.4420e+005	3.01
gravity	1.4412e-001	6.2068e-002	-	-	3.00
gravity	7.3863e-002	-	1.0178e+003	-	3.38
gravity	7.6596e-002	-	-	5.8340e+002	3.30
gravity	7.5657e-002	8.9338e-002	2.6968e+001	-	3.52
gravity (WU)	5.9147e-002	1.7299e-001	1.4920e+003	-	4.61
gravity	7.6178e-002	9.4794e-002	-	7.9399e+002	3.41
gravity (WU)	7.7175e-002	6.9617e-002	-	1.6570e+003	3.23
gravity	5.6443e-002	-	3.4291e+003	1.0032e+005	5.13
gravity (WU)	5.7096e-002	-	2.1291e+003	1.7057e+005	5.14
gravity	7.5426e-002	1.1257e-001	3.4710e+001	1.6360e+004	3.90
gravity (WU)	5.5631e-002	3.2129e-001	7.2494e+002	5.6887e+004	10.39
shaw	3.8658e-001	1.1241e-002	-	-	4.73
shaw	3.7087e-001	-	1.0679e+001	-	4.30
shaw	3.7499e-001	-	-	1.1396e+002	4.08
shaw	3.4765e-001	4.0968e-002	6.2112e+000	-	5.77
shaw (WU)	3.2295e-001	2.8325e-002	8.9987e+000	-	6.71
shaw	3.6824e-001	9.7160e-002	-	5.0404e+002	4.85
shaw (WU)	3.5303e-001	1.8491e-002	-	1.3922e+003	5.06
shaw	2.2610e-001	-	8.0840e+001	1.0614e+003	6.59
shaw (WU)	2.8593e-001	-	2.4070e+001	2.7850e+003	6.02
shaw	3.4812e-001	3.0250e-002	6.1392e+000	5.6965e+002	7.06
shaw (WU)	3.2119e-001	3.3386e-002	3.6780e+000	1.0717e+003	9.23

TABLE A.3
 Linear solution \bar{x}_1 with noise level $\tilde{\varepsilon} = 10^{-2}$.

	Relative Errors	λ_1	λ_2	λ_3	Iterations
gravity	9.1882e-002	9.9070e-003	-	-	5.88
gravity	4.3925e-002	-	6.2429e+000	-	6.60
gravity	4.4210e-002	-	-	8.3509e+002	6.60
gravity	4.8555e-002	3.0927e-002	-	1.5557e+001	6.32
gravity (WU)	4.5759e-002	2.1120e-002	-	2.0771e+003	6.85
gravity	4.0287e-002	-	3.9018e+001	7.2829e+003	7.96
gravity (WU)	3.5810e-002	-	6.9289e+001	7.7211e+003	9.39
gravity	4.0742e-002	3.3236e-002	5.2950e+000	1.8860e+003	8.15
gravity (WU)	3.6273e-002	4.3565e-002	6.7350e+000	2.0170e+003	12.37
phillips	8.3395e-002	7.5351e-004	-	-	3.88
phillips	5.1312e-002	-	6.0850e+000	-	4.79
phillips	2.5810e-002	-	-	1.0223e+004	3.70
phillips	4.9806e-002	1.1568e-003	-	1.5404e+002	3.76
phillips (WU)	2.9860e-002	7.8084e-004	-	1.1637e+005	3.73
phillips	2.0121e-002	-	1.3793e+001	3.0215e+005	5.34
phillips (WU)	7.3637e-003	-	1.0211e+001	7.1454e+007	5.82
phillips	2.1245e-002	1.1547e-003	5.1765e+000	7.0991e+005	4.03
phillips (WU)	4.9555e-003	1.0063e-003	2.6263e+000	1.3782e+009	6.12
shaw	1.6558e-001	5.6169e-004	-	-	8.04
shaw	9.8639e-002	-	2.0738e+000	-	7.05
shaw	1.1969e-001	-	-	2.8091e+002	7.90
shaw	1.6111e-001	9.4367e-004	-	2.4475e+002	7.60
shaw (WU)	1.4970e-001	6.4663e-004	-	3.0588e+002	8.65
shaw	1.8624e-001	-	1.4567e+003	7.5914e+003	10.66
shaw (WU)	1.8275e-001	-	1.6192e+003	6.4621e+004	12.87
shaw	1.5545e-001	7.2387e-004	1.1118e+000	3.0236e+002	8.34
shaw (WU)	8.5492e-002	6.8840e-004	2.3488e-001	9.2377e+002	10.08

TABLE A.4
 Linear solution \bar{x}_1 with noise level $\tilde{\epsilon} = 5 \cdot 10^{-2}$.

	Relative Errors	λ_1	λ_2	λ_3	Iterations
gravity	2.8768e-001	5.5438e-002	-	-	4.05
gravity	7.9760e-002	-	8.3692e+001	-	4.99
gravity	9.9241e-001	-	-	2.0821e+003	6.47
gravity	9.9263e-001	3.0098e-002	-	3.0273e+002	8.08
gravity (WU)	9.9256e-001	3.0199e-002	-	3.9649e+002	9.23
gravity	7.0756e-002	-	5.1613e+002	5.8957e+004	6.88
gravity (WU)	6.9625e-002	-	5.1480e+002	8.2787e+004	7.32
gravity	7.1772e-002	2.7579e-001	3.3161e+001	3.5037e+003	8.09
gravity (WU)	6.9084e-002	2.8820e-001	1.6383e+001	2.2734e+003	15.31
phillips	1.3393e-001	6.9273e-003	-	-	4.98
phillips	4.6177e-002	-	1.9380e+001	-	4.00
phillips	6.2626e-002	-	-	1.5541e+002	3.00
phillips	5.9475e-002	1.2138e-002	-	3.8318e+003	3.04
phillips (WU)	4.4428e-002	7.1280e-003	-	7.3170e+005	3.96
phillips	4.4724e-002	-	8.0428e+001	2.8338e+006	5.74
phillips (WU)	3.0147e-002	-	4.9414e+001	9.6469e+006	5.51
phillips	5.9309e-002	1.1927e-002	1.9741e+001	2.6932e+004	3.15
phillips (WU)	5.1288e-002	8.9332e-003	5.1621e+000	2.0490e+007	6.68
shaw	4.2575e-001	5.0157e-003	-	-	5.40
shaw	3.3582e-001	-	9.5404e+000	-	5.81
shaw	3.8572e-001	-	-	1.2562e+003	5.41
shaw	3.7063e-001	1.6175e-002	-	5.2509e+002	6.60
shaw (WU)	3.3534e-001	1.8732e-002	-	1.0808e+003	8.03
shaw	1.9170e-001	-	3.4898e+001	1.0244e+003	7.64
shaw (WU)	1.5476e-001	-	3.7043e+001	3.9485e+003	8.22
shaw	3.3859e-001	1.8235e-002	5.7642e+000	5.6926e+002	7.68
shaw (WU)	3.1797e-001	2.1206e-002	3.7208e+000	2.1282e+003	12.32

TABLE A.5
 Given solution with noise level $\tilde{\varepsilon} = 10^{-2}$.

	Relative Errors	λ_1	λ_2	λ_3	Iterations
baart	5.0485e-002	5.9453e-004	-	-	4.00
baart	9.6425e-002	-	4.2167e-001	-	6.00
baart	6.2569e-002	-	-	1.0876e+003	5.01
baart	1.5099e-001	1.0683e-003	6.3735e-002	-	5.50
baart (WU)	1.5135e-001	1.0854e-003	1.0809e-001	-	6.10
baart	8.8097e-002	8.3136e-004	-	1.3274e+002	4.38
baart (WU)	1.2243e-001	1.0936e-003	-	2.3528e+002	5.67
baart	1.2223e-001	-	8.5082e-001	1.6022e+002	7.57
baart (WU)	1.2907e-001	-	8.9299e-001	1.1968e+002	8.93
baart	1.4903e-001	1.1395e-003	1.5122e-002	9.7826e+001	6.63
baart (WU)	2.0029e-001	1.2088e-003	2.5714e-003	3.3557e+001	15.88
gravity	1.2013e-001	9.7765e-003	-	-	5.27
gravity	4.0751e-002	-	3.4584e+000	-	6.24
gravity	4.0657e-002	-	-	5.4844e+002	6.19
gravity	4.3901e-002	3.3339e-002	7.3607e-001	-	6.15
gravity (WU)	4.2829e-002	2.7101e-002	3.6701e+000	-	6.50
gravity	4.2992e-002	4.1944e-002	-	9.7444e+001	6.04
gravity (WU)	4.1431e-002	2.8425e-002	-	2.3548e+003	6.60
gravity	4.5887e-002	-	1.1104e+001	2.0749e+003	7.92
gravity (WU)	4.6282e-002	-	1.2389e+001	2.5341e+003	8.83
gravity	3.7745e-002	4.0109e-002	8.4321e-001	4.1857e+002	7.80
gravity (WU)	3.5941e-002	5.1580e-002	6.8753e-001	8.0771e+002	13.03
phillips	2.8920e-002	1.8711e-002	-	-	5.00
phillips	2.5621e-002	-	5.2041e+000	-	5.05
phillips	2.5663e-002	-	-	5.5949e+002	5.00
phillips	2.5654e-002	5.5102e-002	2.2946e+000	-	7.52
phillips (WU)	2.5428e-002	4.2635e-002	2.2588e+000	-	8.06
phillips	2.6108e-002	5.0990e-002	-	2.7694e+002	7.48
phillips (WU)	2.6021e-002	4.1527e-002	-	3.0252e+002	8.05
phillips	2.7134e-002	-	1.0548e+001	1.4744e+002	7.54
phillips (WU)	2.7043e-002	-	9.1030e+000	1.3533e+002	8.43
phillips	2.5571e-002	4.6571e-002	9.4471e-001	4.5558e+001	9.71
phillips (WU)	2.5307e-002	5.1642e-002	3.8008e-001	5.2265e+001	12.56
shaw	1.3445e-001	7.5858e-004	-	-	5.85
shaw	1.2074e-001	-	5.4351e-001	-	6.29
shaw	1.2074e-001	-	-	1.2207e+002	6.01
shaw	1.3477e-001	1.8739e-003	2.5149e-001	-	6.73
shaw (WU)	1.4452e-001	3.1749e-003	2.6832e-001	-	8.02
shaw	1.3466e-001	2.0832e-003	-	5.8343e+001	6.71
shaw (WU)	1.4767e-001	3.6720e-003	-	5.1928e+001	8.18
shaw	2.0162e-001	-	1.8871e-001	2.9227e+000	9.59
shaw (WU)	2.0445e-001	-	1.8076e-001	4.0254e+000	10.85
shaw	1.3631e-001	3.1890e-003	2.6252e-001	1.7495e+001	7.71
shaw (WU)	1.3297e-001	3.6163e-003	2.2794e-002	9.6222e+000	15.36

TABLE A.6
 Given solution with noise level $\tilde{\epsilon} = 5 \cdot 10^{-2}$.

	Relative Errors	λ_1	λ_2	λ_3	Iterations
baart	2.5915e-001	5.5184e-003	-	-	3.88
baart	3.5281e-001	-	4.1254e+001	-	22.62
baart	1.4907e-001	-	-	7.8514e+001	3.90
baart	3.1181e-001	1.0697e-002	1.6995e+000	-	5.41
baart (WU)	3.1079e-001	1.0679e-002	1.8720e+001	-	6.17
baart	2.5738e-001	7.0589e-003	-	1.4668e+003	4.04
baart (WU)	2.4875e-001	6.3857e-003	-	1.8854e+003	4.16
baart	3.6233e-001	-	4.2956e+001	6.7892e+005	11.53
baart (WU)	3.6189e-001	-	4.2750e+001	9.5807e+005	12.31
baart	3.0971e-001	1.2027e-002	9.7625e-001	8.6695e+002	6.34
baart (WU)	3.0669e-001	1.4359e-002	5.6894e+000	2.7463e+006	22.44
gravity	2.0667e-001	7.6931e-002	-	-	4.20
gravity	7.1581e-002	-	6.4767e+001	-	5.00
gravity	6.5899e-002	-	-	1.0511e+002	4.96
gravity	7.0950e-002	1.5823e-001	2.6622e+000	-	5.89
gravity (WU)	6.9396e-002	9.8279e-002	2.2876e+001	-	5.08
gravity	6.7248e-002	1.4980e-001	-	1.3094e+003	5.15
gravity (WU)	6.5526e-002	9.7083e-002	-	2.3641e+003	5.03
gravity	8.9110e-002	-	1.5691e+002	7.3888e+003	7.24
gravity (WU)	9.2507e-002	-	1.5515e+002	9.6310e+003	8.28
gravity	6.7490e-002	3.0044e-001	7.9010e+000	4.7311e+002	8.24
gravity (WU)	6.6388e-002	3.1555e-001	7.0614e-001	1.0583e+003	16.10
phillips	1.7706e-001	5.4795e-002	-	-	4.00
phillips	5.2064e-002	-	2.7421e+001	-	4.86
phillips	4.9188e-002	-	-	1.2585e+002	4.79
phillips	5.1560e-002	2.2233e-001	3.0768e+000	-	8.89
phillips (WU)	4.5868e-002	9.5929e-002	1.1118e+001	-	5.33
phillips	5.0609e-002	2.1969e-001	-	3.3818e+002	7.30
phillips (WU)	5.3031e-002	8.1022e-002	-	3.5514e+003	5.04
phillips	6.2712e-002	-	6.8085e+001	3.2822e+002	7.74
phillips (WU)	6.2458e-002	-	6.7112e+001	3.4593e+002	8.65
phillips	4.9898e-002	2.5948e-001	1.8172e+000	5.1243e+001	10.62
phillips (WU)	4.9975e-002	2.6521e-001	2.4459e-001	9.0852e+001	16.69
shaw	1.8119e-001	7.5811e-003	-	-	5.00
shaw	2.0664e-001	-	1.2412e+001	-	6.91
shaw	2.0299e-001	-	-	1.9892e+003	6.81
shaw	1.8248e-001	2.9196e-002	1.1667e+000	-	9.45
shaw (WU)	1.7661e-001	2.9472e-002	1.3307e+000	-	8.14
shaw	1.7095e-001	3.2668e-002	-	3.7580e+002	8.77
shaw (WU)	1.7345e-001	3.0384e-002	-	2.4513e+002	9.91
shaw	3.6022e-001	-	1.9433e+001	2.1029e+002	8.31
shaw (WU)	4.1838e-001	-	1.6601e+001	6.2015e+002	9.97
shaw	1.6869e-001	2.7108e-002	1.3957e+000	6.2512e+001	8.53
shaw (WU)	1.7007e-001	2.9894e-002	1.6217e-001	6.3068e+001	15.61