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RESIDUAL NORM BEHAVIOR FOR HYBRID LSQR REGULARIZATION

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Abstract: Hybrid LSQR represents a powerful method for regularization of large-scale discrete inverse problems, where ill-conditioning of the model matrix and ill-posedness of the problem make the solutions seriously sensitive to the unknown noise in the data. Hybrid LSQR combines the iterative Golub-Kahan bidiagonalization with the Tikhonov regularization of the projected problem. While the behavior of the residual norm for the pure LSQR is well understood and can be used to construct a stopping criterion, this is not the case for the hybrid method. Here we analyze the behavior of norms of approximate solutions and the corresponding residuals in Hybrid LSQR with respect to the Tikhonov regularization parameter. This helps to understand convergence properties of the hybrid approach. Numerical experiments demonstrate the results in finite precision arithmetic.

Keywords: inverse problem, noise, Hybrid LSQR, Tikhonov regularization

MSC: 15A29, 65F22, 65F50

1. Introduction

We are concerned with an ill-posed inverse linear approximation problem

$$Ax \approx b, \quad A \in \mathbb{R}^{m\times n},\ b \in \mathbb{R}^{m}, \tag{1}$$

where $m \geq n$, $m, n \in \mathbb{N}$. The matrix A represents a (possibly large-scale) discretized smoothing operator, b stands for the data typically polluted by unknown additive noise e. Formally,

$$b = b^{\text{exact}} + e,$$

where b^{exact} denotes noise-free data. Further, denote $\eta = \|e\|/\|b\|$ the noise level, with $\|.\|$ being the standard Euclidean norm. Problems of the form (1) arise in many applications such as medical imaging or gravity surveying, see for example [4, 6]. Since the approximate solution is here seriously sensitive to the noise in b, regularization needs to be applied in order to obtain a meaningful solution. A wide variety

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of regularization techniques have been developed, where for large-scale problems, iterative schemas are often the methods of choice. Here regularization is achieved by early termination of the process. Determining a reliable stopping criteria is crucial, because iterative methods applied on (1) typically exhibit semiconvergence. Alternatively, iterations can be further combined with direct regularization yielding the so-called hybrid methods such as Hybrid LSQR or Hybrid GMRES, see [1] for an overview. Hybrid methods are known for their ability to stabilize the computation and making it less sensitive to stopping criteria. Analysis of the properties of hybrid methods is, however, significantly more complicated.

In this paper we focus on Hybrid LSQR combining iterative projection on a Krylov subspace with the Tikhonov regularization of the projected small problem. We analyze residual norm behavior, since its stagnation indicates stabilization of the method and is thus used in stopping criteria when solving ill-posed problems. While properties of the residuals for standard LSQR regularization have already been analyzed (see, e.g, [2, 8]), this is not the case for Hybrid LSQR, where the behavior is highly dependent on the inner Tikhonov regularization parameter λ_k that changes in each outer iterative step k. Note that some analysis of LSQR combined with Tikhonov regularization for constant λ_k was provided already in [10]. A variety of parameter-choice methods have been introduced for selecting λ_k, e.g., the Discrepancy principle, L-curve or Generalized Cross Validation, see [4, 9, 12]. Their suitability for hybrid framework was studied in [3]. Here we, however, do not restrict ourselves to a particular parameter-choice strategy. We provide conditions on parameters λ_k to guarantee a decrease of the residual norm in hybrid LSQR and discuss its meaning in regularization process. Throughout the paper we assume exact arithmetic. Numerical experiments then demonstrate the presented properties in finite precision arithmetic.

2. Krylov projection and Tikhonov regularization

Hybrid LSQR represents a combination of the well known Golub-Kahan iterative bidiagonalization [10, 11] with the Tikhonov regularization. The Golub-Kahan bidiagonalization starting with $s_1 = b/\|b\|$ produces after k iterations the matrices W_k and S_{k+1}, having orthogonal basis of $\mathcal{K}_k(A^TA, A^Tb)$ and $\mathcal{K}_k(AA^T, b)$ in their columns, respectively. Assuming that the algorithm does not stop early, bidiagonalization coefficients $\alpha_i > 0,\ \beta_i >$ are stored in a lower bidiagonal matrix L_k,

$$L_k = \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_k & \alpha_k \end{bmatrix} \in \mathbb{R}^{k\times k}, \quad \text{and we denote} \quad L_{k+} = \begin{bmatrix} L_k \\ e_k^T\beta_{k+1} \end{bmatrix} \in \mathbb{R}^{(k+1)\times k},$$

where e_k is the k-th Euclidean vector of an appropriate size. Then it holds that

$$AW_k = S_{k+1}L_{k+}, \qquad A^TS_k = W_kL_k^T. \tag{2}$$

In the standard LSQR, the original problem (1) is replaced by the problem

$$\min_{y \in \mathbb{R}_k} \{\|AW_k y - b\|\}. \tag{3}$$

Using relations (2) and the orthogonality of S_k, we have

$$\|AW_k y - b\| = \|S_{k+1} L_{k+} y - b\| = \left\|S_{k+1}^T S_{k+1} L_{k+} y - S_{k+1}^T b\right\| = \|L_{k+} y - \beta_1 e_1\| \tag{4}$$

for any $y \in \mathbb{R}^k$. The projected problem (3) thus translates to

$$\min_{y \in \mathbb{R}_k} \{\|L_{k+} y - \beta_1 e_1\|\}, \quad \text{where} \quad \beta_1 = \|b\|,$$

having a unique solution y_k.

For inverse problems, however, the projected problem subsequently inherits their ill-posedness and noise gradually propagates to the projections, see [7]. Thus, Hybrid LSQR further applies Tikhonov regularization on the projected problem and solves

$$\min_{y \in \mathbb{R}^k} \{\|L_{k+} y - \beta_1 e_1\|^2 + \lambda_k^2 \|y\|^2\}, \tag{5}$$

for some regularization parameter $\lambda_k > 0$, $\lambda_k \in \mathbb{R}$. The obtained minimization problem has also a unique solution, further denoted $\overline{y}_k$. Putting the initial approximation $x_0 = 0$, the approximate solution to the original problem (1) is then obtained by

$$x_k = W_k y_k \quad \text{and} \quad \overline{x}_k = W_k \overline{y}_k \tag{6}$$

for LSQR and Hybrid LSQR, respectively.

Let us further clarify some notation. Denote the residuals corresponding to LSQR and Hybrid LSQR in the iteration k as follows

$$\begin{aligned} r_k(x) &= b - Ax, & p_k(y) &= \beta_1 e_1 - L_{k+} y, \\ \bar{r}_k(x) &= \begin{pmatrix} b \\ 0 \end{pmatrix} - \begin{pmatrix} A \\ \lambda_k I \end{pmatrix} x, & \bar{p}_k(y) &= \begin{pmatrix} \beta_1 e_1 \\ 0 \end{pmatrix} - \begin{pmatrix} L_{k+} \\ \lambda_k I \end{pmatrix} y, \end{aligned}$$

where for each k we have $x = W_k y,\ y \in \mathbb{R}^k$. We deliberately include the index k in the notation of the residuals for clarity when discussing their properties throughout iterations. Using (4), we get

$$\|r_k(x)\| = \|p_k(y)\|, \quad \|\overline{r}_k(x)\| = \|\overline{p}_k(y)\| \tag{7}$$

for any $x = W_k y,\ y \in \mathbb{R}^k$. Moreover, clearly it holds

$$\begin{aligned} \|\overline{r}_k(x)\|^2 &= \|r_k(x)\|^2 + \lambda_k^2 \|x\|^2, \\ \|\overline{p}_k(y)\|^2 &= \|p_k(y)\|^2 + \lambda_k^2 \|y\|^2. \end{aligned} \tag{8}$$

2.1. Interchangeability of projection and regularization

The above presented Hybrid LSQR applies the so called first project then regularize approach. It is well known that for selected hybrid methods this is equivalent to the first regularize then project approach, see [4, Chap. 6], even though the meaning of the equivalency is for various methods slightly different. Here, we briefly explain why for Hybrid LSQR the two approaches are fully interchangeable. The important consequence of this relationship is that many properties of LSQR hold also for Hybrid LSQR with a constant λ_k.

The first regularize then project approach starts with an application of the Tikhonov regularization to the original problem, schematically

$$\min_x\{\|Ax-b\|\} \to \min_x \left\{ \left\| \begin{pmatrix} b \\ 0 \end{pmatrix} - \begin{pmatrix} A \\ \lambda I \end{pmatrix} x \right\| \right\}.$$

Subsequently, k iterations of the Golub-Kahan bidiagonalization are computed for the extented problem above yielding the projected problem

$$\min_{y\in\mathbb{R}^k} \left\{ \left\| \begin{pmatrix} b \\ 0 \end{pmatrix} - \begin{pmatrix} A \\ \lambda I \end{pmatrix} \overline{W}_k y \right\| \right\}, \tag{9}$$

where $\overline{W}_k$ is an orthogonal basis of $\mathcal{K}_k \left(\begin{pmatrix} A \\ \lambda I \end{pmatrix}^T \begin{pmatrix} A \\ \lambda I \end{pmatrix}, \begin{pmatrix} A \\ \lambda I \end{pmatrix}^T \begin{pmatrix} b \\ 0 \end{pmatrix} \right)$. This shows the main disadvantage of the first regularize strategy - the parameter λ must be selected apriori based on the large problem (1). However, the obtained minimization (9) is clearly equivalent to

$$\min_{y\in\mathbb{R}_k}\{\left\|A\overline{W}_k y - b\right\|^2 + \lambda^2\left\|y\right\|^2\}, \tag{10}$$

thanks to the orthogonality of $\overline{W}_k$. It remains to show that $\overline{W}_k = W_k$. From a simple multiplication and application of shift invariance of Krylov subspaces it follows that

$$\mathcal{K}_k \left(\begin{pmatrix} A \\ \lambda I \end{pmatrix}^T \begin{pmatrix} A \\ \lambda I \end{pmatrix}, \begin{pmatrix} A \\ \lambda I \end{pmatrix}^T \begin{pmatrix} b \\ 0 \end{pmatrix} \right) = \mathcal{K}_k(A^TA, A^Tb).$$

Thus, the first column of orthogonal matrices W_k and $\overline{W}_k$ is the same and their first i columns span the same subspace for any admissible i. It follows from the sequential form of the bidiagonalization process that in such a case $W_k = \overline{W}_k$. Using (4), the minimization problem (10) (first regularize then project approach) is equivalent to

$$\min_{y\in\mathbb{R}^k}\{\|L_{k+}y - \beta_1 e_1\|^2 + \lambda^2\left\|y\right\|^2\}.$$

Consequently, provided λ is the same, the minimization problem is identical to the one in Hybrid LSQR (5) (first project then regularize approach).

Some further relations can be derived. Similarly to (2) we have

$$\begin{pmatrix} A \\ \lambda I \end{pmatrix} W_k = \overline{S}_{k+1}\overline{L}_{k+}, \quad \begin{pmatrix} A \\ \lambda I \end{pmatrix}^T \overline{S}_k = W_k \overline{L}_k^T,$$

and therefore similarly to (4) we obtain

$$\left\| \begin{pmatrix} A \\ \lambda I \end{pmatrix} - \begin{pmatrix} b \\ 0 \end{pmatrix} W_k y \right\| = \left\| \overline{S}_{k+1} \overline{L}_{k+} y - b \right\| = \left\| \overline{L}_{k+} y - \beta_1 e_1 \right\| .$$

The Hybrid LSQR minimization (5) can be thus equivalently written as

$$\min_{y \in \mathbb{R}_k} \{ \left\| \overline{L}_{k+} y - \beta_1 e_1 \right\| \}, \tag{11}$$

where $\overline{L}_{k+}$ has the same properties as L_{k+}, but its entries depend on λ (unlike for L_{k+}). Clearly, for $\lambda = 0$ it holds that $L_{k+} = \overline{L}_{k+}$.

3. Behavior of residual and solution norms

Recall that we assume $x_0 = 0$. It is well known [11] that then for LSQR the norm of the solution is strictly increasing,

$$\|x_{k+1}\| > \|x_k\| ,$$

and the corresponding residual norm is strictly decreasing,

$$\|r_{k+1}(x_{k+1})\| < \|r_k(x_k)\| .$$

In combination with (6), (7) and the orthogonality of W_k the same holds for the projected problem, i.e.,

$$\|y_{k+1}\| > \|y_k\| ,$$
$$\|p_{k+1}(y_{k+1})\| < \|p_k(y_k)\| .$$

Assume for a moment a constant regularization parameter, i.e., $\lambda_k = \lambda$ for all iterations k. It follows from the equivalency between project then regularize and regularize then project strategy (see Section 2), that the above described properties of LSQR hold also for Hybrid LSQR. Specifically,

$$\|\overline{x}_{k+1}\| > \|\overline{x}_k\| , \tag{12}$$
$$\|\overline{r}_{k+1}(\overline{x}_{k+1})\| < \|\overline{r}_k(\overline{x}_k)\| , \tag{13}$$

and similarly for the residual and solution of the projected problem

$$\left\|\overline{y}_{k+1}\right\| > \|\overline{y}_k\| , \tag{14}$$
$$\left\|\overline{p}_{k+1}(\overline{y}_{k+1})\right\| < \|\overline{p}_k(\overline{y}_k)\| . \tag{15}$$

It is useful to recall some properties of the Tikhonov regularization. Consider the minimization problem (5) for some fixed k. The corresponding solution can be expressed as a function of the regularization parameter λ_k as $\overline{y}_k(\lambda_k)$. Then

$$\|\overline{y}_k(\lambda_k)\| \text{ is decreasing with increasing } \lambda_k, \tag{16}$$
$$\|\overline{p}_k(\overline{y}_k(\lambda_k))\| \text{ is increasing with increasing } \lambda_k. \tag{17}$$

For the proof using the SVD decomposition see, e.g., [4].

3.1. Hybrid LSQR residual monotonicity

Hybrid LSQR minimizes the residual norm (8) which consists of two terms, the solution norm and the data fidelity term $p_k(\overline{y}_k)$. Thus (unlike LSQR) Hybrid LSQR does not minimize the residual corresponding to the original problem (1). Furthermore, the residual norm can generally oscillate and then it is hard to design a reliable stopping criterion for the iterations. For large-scale problems direct computation of $\|r_k(\overline{x}_k)\|$ may be infeasible. Thus we study the projected residual norm $\|p_k(\overline{y}_k)\|$ and then take advantage of (7). Stabilization of the inner residual norm can be used as a marker of stabilization of the method and for setting appropriate stopping criteria. The behavior of $\|p_k(\overline{y}_k)\|$ for Hybrid LSQR is highly dependent on the choice of the regularization parameter λ_k which is often chosen heuristically. We now investigate the behavior of $\|p_k(\overline{y}_k)\|$ with respect to the choice of λ_k.

Let us start with the case of constant regularization parameter, i.e., $\lambda_k = \lambda$.

Lemma 1. *Let $\overline{y}_k$ be the solution of (5) with $\lambda_k = \lambda,\ k = 1, 2, \ldots$. Then it holds*

$$\left\|p_{k+1}(\overline{y}_{k+1})\right\| < \|p_k(\overline{y}_k)\| .$$

Proof. Combining together (15) and (8) yields

$$\left\|p_{k+1}(\overline{y}_{k+1})\right\|^2 + \lambda^2 \left\|\overline{y}_{k+1}\right\|^2 < \|p_k(\overline{y}_k)\|^2 + \lambda^2 \|\overline{y}_k\|^2 ,$$

Using (14) then gives the result. □

A straightforward corollary of Lemma 1 and the property of Tikhonov regularization (17) is that

$$\lambda_{k+1} \leq \lambda_k \quad \Rightarrow \quad \left\|p_{k+1}(\overline{y}_{k+1})\right\| < \|p_k(\overline{y}_k)\| .$$

In other words, if the value of λ_k is non-increasing, for Hybrid LSQR both $\|\overline{p}_k(\overline{y}_k)\|$ and $\|p_k(\overline{y}_k)\|$ are strictly decreasing (and thus also $\|\overline{r}_k(\overline{x}_k)\|$ and $\|r_k(\overline{x}_k)\|$). Moreover, it follows from (14) and (16) that

$$\lambda_{k+1} \leq \lambda_k \quad \Rightarrow \quad \left\|\overline{y}_{k+1}\right\| > \|\overline{y}_k\| . \tag{18}$$

In practice, however, the regularization parameter λ_k is typically increasing rather then decreasing, because stronger regularization is needed with increasing k as noise subsequently propagates to the projected problem. In the paper [6], we have shown that

$$\left\|\overline{y}_{k+1}\right\| = \|\overline{y}_k\| \quad \Rightarrow \quad \left\|p_{k+1}(\overline{y}_{k+1})\right\| \leq \|p_k(\overline{y}_k)\| .$$

Thus, also $\|r_{k+1}(\overline{x}_{k+1})\| \leq \|r_k(\overline{x}_k)\|$. In words, stabilization of the inner solution norm is a sufficient condition for the residual norm to be nonincreasing. Theorem 2 generalizes this and states our main result.

Theorem 2. *Let λ_k, λ_{k+1} be such that the solutions $\overline{y}_k$, $\overline{y}_{k+1}$ of (5) satisfy $\|\overline{y}_k\| \leq \|\overline{y}_{k+1}\|$. Then*

$$\|p_{k+1}(\overline{y}_{k+1})\| \leq \|p_k(\overline{y}_k)\|, \quad k = 1,\, 2,\, 3,\, \ldots.$$

Given $\overline{x}_k = W_k\overline{y}_k$, it also holds that

$$\|r_{k+1}(\overline{x}_{k+1})\| \leq \|r_k(\overline{x}_k)\| \quad k = 1,\, 2,\, 3,\, \ldots.$$

Proof. Denote $y^*_{k+1} = [\overline{y}_k^T, 0]^T$. Then directly $\|y^*_{k+1}\| = \|\overline{y}_k\|$ and

$$\|p_{k+1}(y^*_{k+1})\| = \|L_{(k+1)+}y^*_{k+1} - \beta_1 e_1\| = \|L_{(k)+}\overline{y}_k - \beta_1 e_1\| = \|p_k(\overline{y}_k)\|.$$

Since $\overline{y}_{k+1}$ is a minimizer of (5), we obtain

$$\|p_{k+1}(\overline{y}_{k+1})\|^2 + \lambda_{k+1}^2 \|\overline{y}_{k+1}\|^2 \leq \\ \|p_{k+1}(y^*_{k+1})\|^2 + \lambda_{k+1}^2 \|y^*_{k+1}\|^2 = \|p_k(\overline{y}_k)\| + \lambda_{k+1}^2 \|\overline{y}_k\|^2.$$

Because $\|\overline{y}_{k+1}\|^2 \geq \|\overline{y}_k\|^2$, we get

$$\|p_{k+1}(y_{k+1})\|^2 \leq \|p_k(y_k)\|^2$$

and thus also $\|r_{k+1}(x_{k+1})\|^2 \leq \|r_k(x_k)\|^2$, see (7). □

Let us discuss how to satisfy the condition in Theorem 2. Clearly, by setting $\lambda_{k+1} = \lambda_k = 0$ we obtain standard LSQR for which the solution norm is increasing. Generally, it is possible to select the regularization parameter λ_{k+1} such that $\|\overline{y}_k\| = \|\overline{y}_{k+1}\|$, which also satisfies the condition. In such a case, the value of λ_k must be increasing. This holds because if λ_k was non-increasing, $\|\overline{y}_k\|$ would be increasing, see (18). In summary, Theorem 2 states that in order to maintain the residual norm $\|r_k(\overline{x}_k)\|$ decreasing, λ_k can be increasing but not too much. Provided monotonicity of the residual norm can then simplify the detection of stabilization of the regularization process. It is also important to note that the assumption in Theorem 2 is sufficient but not necessary.

4. Numerical experiments

Now we illustrate the above presented behavior in finite precision arithmetic. We consider two standard benchmark discrete ill-posed problems from the Regularization toolbox in MATLAB. For simplicity, a fixed number of iterations k is computed. The 1D problem *gravity* with $A \in \mathbb{R}^{50\times 50}$ and the noise level $\eta = 10^{-3}$ is solved in 30 iterations. For the 2D problem *blur* with $A \in \mathbb{R}^{2500\times 2500}$, $\eta = 10^{-1}$ and the Gaussian blur parameter $\sigma = 1$, we compute 50 iterations. The parameter λ_k for the Tikhonov regularization is chosen from 1000 samples logarithmically distributed in the interval $(0.0001, 10)$. We use the L-curve criterion [4, Chap. 5] for the *gravity* problem and the prescribed norm criterion [6] for the *blur* problem.

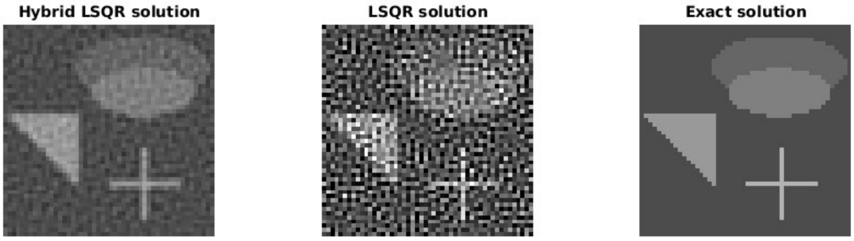

Figure 1: Comparison of approximate solutions of *blur* computed by Hybrid (left) and pure (middle) LSQR in 50 iterations. Hybrid method clearly provides a better reconstruction of the exact solution (right).

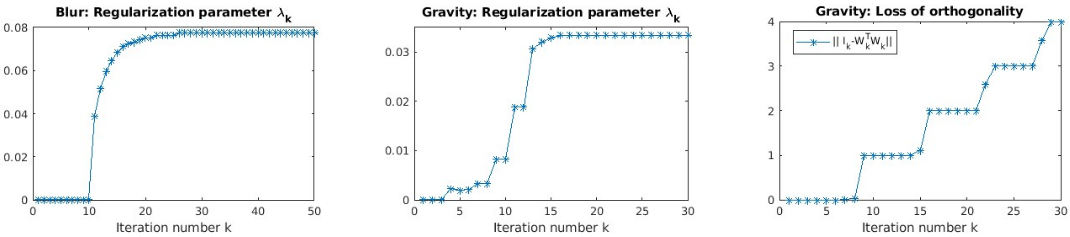

Figure 2: Regularization parameters λ_k computed for the two studied problems (left and middle). As expected, λ_k is mostly increasing. The right image illustrates significant loss of orthogonality among the columns of W_k for the *gravity* problem.

The effect of the inner regularization on improvement of the approximation is illustrated in Figure 1 comparing Hybrid LSQR and LSQR approximations for the problem *blur*. Figure 2 (left) then shows the corresponding regularization parameters λ_k determined during Hybrid LSQR. As expected, λ_k is non-decreasing and in latter iterations it stabilizes. The middle figure shows analogous behavior for the *gravity* problem. The effect is present despite the serious loos of orthogonality between the constructed bidiagonalization vectors, see the figure on the right. Figure 3 provides norms of the computed approximate solutions and the corresponding residuals for both testing problems. Their behavior corresponds nicely to the presented theory. If the solution norm increases, the residual norm is decreasing. A detailed view given in figures on the right for *gravity* shows, that from iterations 12 to 13 and 14 to 15 the solution norm decreases. Even though the assumption of Theorem 2 does not hold here, the corresponding residual norm still decreases from iteration 12 to 13 (but increases from iteration 14 to 15). This illustrates that the assumption is sufficient but not necessary. Note also how small the discrepancy is between the inner and outer residual and solution norms in finite precision, despite the severe loss of orthogonality. This property of Hybrid methods is explained in details in [5, Chap. 5] and [6]. If necessary, several re-orthogonalization strategies can be applied to improve orthogonality of the computed bidiagonalization vectors. For comparison, we illustrate the behavior when full re-orthogonalization (against all previous vectors)

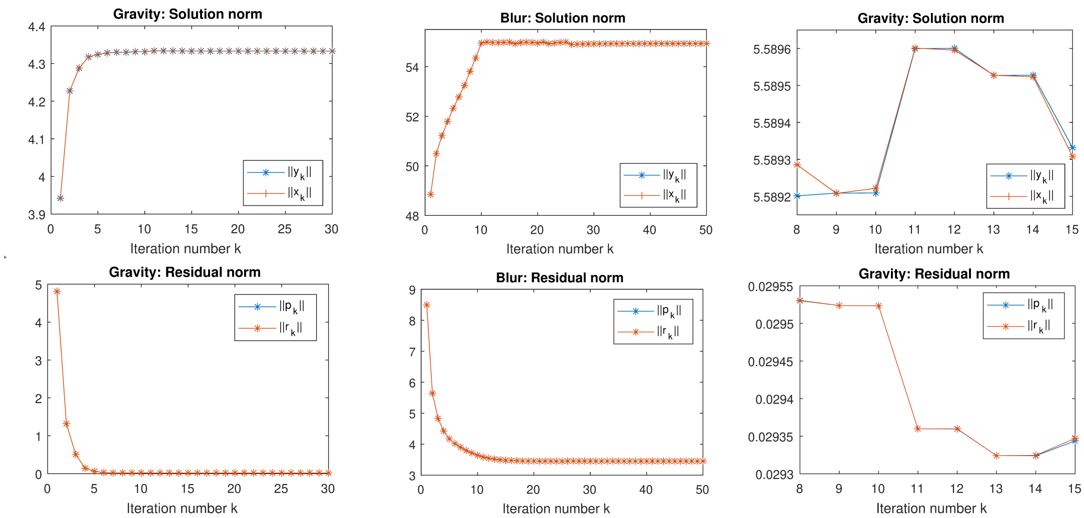

Figure 3: Behavior of the norm of the computed solutions and the corresponding residuals for the two studied problems. The right images show in detail several iterations for the *gravity* problem.

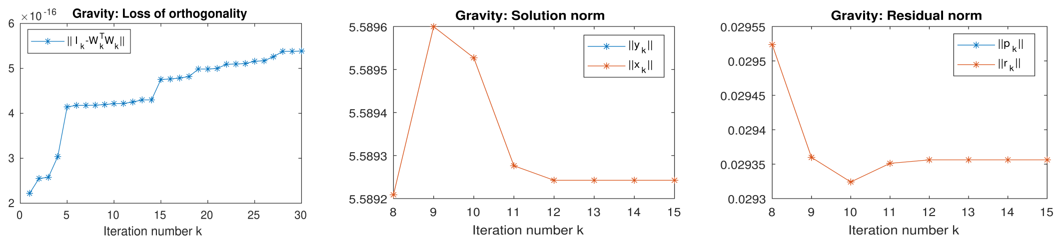

Figure 4: Illustration of the effect of re-orthogonalization. Orthogonality among the columns of W_k is at the machine precision (left). The discrepancy between the inner and outer norms is negligible (middle and right). Compare to Figure 3.

is applied on both sets W_k and S_k, see Figure 4. The orthogonality between the columns of W_k is at the machine precision (left figure). Consequently, the inner and outer solution norms match and the residual norms behave similarly as we observed in computations without re-orthogonalization.

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