

Approximating Splitting Pseudo-iterations

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Abstract

In this paper, a direct method for approximating linear least squares solutions is derived and formulated as a regularizing non-iterated variant of the Approximating Splitting Iteration method with a certain previously chosen number of iterates. Furthermore, a heuristic formula is developed for the a priori numerical estimation of the number of an iterate, at which Approximating Splitting Iteration sequences would reach a good trade-off between numerical accuracy and stability. This formula is discussed as an a priori parameter estimator of the number of iterates for the new method. By previously choosing the number of iterates through such an a priori estimation, the general formula of a conditionedness-free regularizing method is derived from the general Approximating Splitting Iteration formula.

Keywords: Linear least squares, Conditionedness, Approximating Splitting Iterations, Regression, Approximation, Regularization.

1 Introduction

It is a well-known fact that the solution of many contemporary optimization, regression, approximation and inverse problems leads to large-scale unstructured linear least squares problems [2, 4, 7, 8, 12]. The strategy for solving such kind of problems cannot be based on the previous identification of the conditionedness of the problem matrix, because the compact cluster of small singular values of the problem matrices causes the conditionedness to be ill-determined. So, exact solutions obviously cannot be expected [2, 4, 8, 9] and the choice among known methods becomes unreliable.

If the problem were in fact ill-conditioned, "orthodox" methods from Linear Algebra (for instance, Pseudo-Inverse type and Truncated Singular Value Decomposition-wise methods) might give numerically unstable approximate solutions. On the other hand, if the problem were in fact well-conditioned, classical

regularization methods might provide numerically inaccurate approximates [2, 4, 5, 8]. So, obviously, effective methods for approximating solutions of both well- and ill-conditioned linear least squares problems are needed. The point is that those methods have to be as free as possible from conditionedness and noise in order to ensure both the numerical accuracy and stability of approximates.

The idea of such conditionedness-free algorithms has been latent in most of the voluminous linear least squares and algebraic regularization literature since long (the reader is invited to a useful review of [1], [11] and the works cited therein). Only recently however, it has become more explicit in a few papers, such as [3, 5, 6, 9] and particularly [11], which provided important results concerning iterative regularization methods with improved accuracy for well-conditioned linear least squares problems. Nevertheless, the purpose of ensuring both the numerical accuracy and stability of linear least squares approximates has not been reached yet.

In this paper, a direct method for approximating linear least squares solutions is derived and formulated as a conditionedness-free regularizing non-iterated variant of the Approximating Splitting Iteration method [10] with a certain previously chosen number of iterates.

2 Improvement of the numerical robustness of Approximating Splitting Iterations. Approximating Splitting Pseudo-Iterations

In [10], it was proved that for every positive definite matrix $V \in \mathbb{R}^{n \times n}$, the splitting linear stationary iteration formula [2, 5, 12]

$$x^{[k+1]} = (V + A'A)^{-1} (V - A'A) x^{[k]} + 2(V + A'A)^{-1} A'b, \quad (1)$$

$$k = 0, 1, 2, \dots$$

produces globally convergent sequences of monotonically improved approximates of solutions of linear least squares problems

$$\min_{x \in \mathbb{R}^n} f(x) = \|Ax - b\|_2^2 \quad (2)$$

where $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$, $m, n \in \mathbb{N}$.

Indeed, it was proved there that, for $k = 0, 1, 2, \dots$ and from any initial guess $x^{[0]}$,

$$f(x^{[k+1]}) < f(x^{[k]}) \quad (3)$$

at any $x^{[k+1]} \neq x^{[k]}$,

$$\lim_{k \rightarrow +\infty} x^{[k]} = \arg \min_{x \in \text{Argmin}_{x \in \mathbb{R}^n} \|Ax - b\|_2^2} (x - x^{[0]})' V (x - x^{[0]}) = x^* \in \mathbb{R}^n \quad (4)$$

and, given a certain non-singular matrix P , $P \in \mathbb{R}^{n \times n}$, such that $V = P'P$,

$$\|R^{-1} (x^{[k+1]} - x^*)\|_2 < \|R^{-1} (x^{[k]} - x^*)\|_2 \tag{5}$$

at any $x^{[k]} \neq x^*$ and

$$\begin{aligned} x^{[k+1]} = & R \left(\begin{array}{cc} [I - 2S'_{A+} S_{A+}]^{k+1} & 0 \\ 0 & I \end{array} \right) R^{-1} x^{[0]} + \\ & + R \left(\begin{array}{cc} \left\{ I - [I - 2S'_{A+} S_{A+}]^{k+1} \right\} S_{A+}^{-1} & 0 \\ 0 & I \end{array} \right) L'_A b \end{aligned} \tag{6}$$

where I is the identity matrix and L_A , S_A and R are certain real matrices which follow from the Generalized Singular Value Decomposition (GSVD) [4, 6, 7] of the matrices A and P .

The formula (6) is the formula of the Approximating Splitting Iteration method [10].

Once the GSVD of the matrices A and P has been performed, the computation of approximate solutions with the formula (6) requires neither the solution of a system of equations nor some matrix inversion (and not even iterations in the usual way) [10]. This makes formula (6) numerically quite robust, because it essentially avoids the error propagation [10], inherent to most iteration methods (including the so-called iterated Tikhonov's regularization and Landweber's iteration-wise methods) [7, 8, 11].

Furthermore, for a previously given k , the formula (6) already could be assumed to be the general formula of a certain class of special direct (non-iterated) methods for approximating solutions of (2) for any matrix A , any vector b and any preliminary approximate $x^{[0]}$.

At this point, one should notice two important facts:

–The numerical robustness of the results would be further improved if V were chosen well-conditioned enough and formula (6) had been derived from the Singular Value Decomposition (SVD) [4, 6, 7] of the matrix AP^{-1} instead of the GSVD of the matrices A and P . That way, even for regularization purposes, the problem conditionedness could be handled through the conditionedness of the only matrix AP^{-1} [3, 7, 8, 11].

–It would be appropriate to have some formula for the a priori numerical estimation of the number of some iterate at which Approximating Splitting Iteration sequences reached a good trade-off between numerical accuracy and stability.

Obviously, whereas P is a certain non-singular matrix, $P \in \mathbb{R}^{n \times n}$, such that $V = P'P$, the iteration formula (1) can be rewritten in the following way

$$x^{[k+1]} = \left(I + (AP^{-1})' (AP^{-1}) \right)^{-1} \left(I - (AP^{-1})' (AP^{-1}) \right) Px^{[k]} + \\ + 2P^{-1} \left(I + (AP^{-1})' (AP^{-1}) \right)^{-1} (AP^{-1})' b$$

Notice that, after performing the SVD of AP^{-1} , one has

$$AP^{-1} = L \begin{pmatrix} S_h & 0 & 0 & 0 \\ 0 & I_{q_1 \times q_1} & 0 & 0 \\ 0 & 0 & S_l & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_{m \times n} R'$$

where S_h , I and S_l are those non-overlapping diagonally consecutive square submatrices of the central SVD matrix-factor of AP^{-1} , whose entries are all strictly positive and respectively greater than 1, equal to 1 (the identity matrix) and less than 1; L and R are respectively the left and right SVD real orthogonal matrices; and q_h , q_l , q_1 , $q_0 \in \mathbb{N}$ are the orders respectively of S_h , I , S_l and of the zero matrix on the right-bottom corner. Of course,

$$q_h + q_1 + q_l = \text{rank}(A)$$

and

$$q_0 = \min(m, n) - \text{rank}(A)$$

So, the iteration formula (1) can then be finally written as follows

$$x^{[k+1]} = P^{-1} R \begin{pmatrix} I - 2(I + S'_h S_h)^{-1} S'_h S_h & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & I - 2(I + S'_l S_l)^{-1} S'_l S_l & 0 \\ 0 & 0 & 0 & I \end{pmatrix} R' P x^{[k]} + \\ + P^{-1} R \begin{pmatrix} 2(I + S'_h S_h)^{-1} S'_h & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 2(I + S'_l S_l)^{-1} S'_l & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} L' b \quad (7)$$

Let us denote

$$D_h = I - 2(I + S'_h S_h)^{-1} S'_h S_h$$

and

$$D_l = I - 2(I + S'_l S_l)^{-1} S'_l S_l$$

Obviously,

$$-1 < D_h < 0 \tag{8}$$

and

$$0 < D_l < 1 \tag{9}$$

the latter inequalities meaning that each diagonal entry of matrices D_h and D_l strictly lies respectively between -1 and 0 and 0 and 1 .

Notice that the formula (7) is the formula of the $(k + 1)$ -st term of a certain globally convergent generalized geometric progression for any matrix A .

Indeed, one has by induction,

$$\begin{aligned}
 x^{[k+1]} = P^{-1}R & \begin{pmatrix} D_h^{k+1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & D_l^{k+1} & 0 \\ 0 & 0 & 0 & I \end{pmatrix} R'Px^{[0]} + \\
 + P^{-1}R & \begin{pmatrix} [I - D_h^{k+1}]S_h^{-1} & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & [I - D_l^{k+1}]S_l^{-1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} L'b \tag{10}
 \end{aligned}$$

Moreover, since x^* is the limit of the sequence $\{x^{[k]}\}_{k=0,1,2,\dots} \subset \mathbb{R}^n$, x^* is a fixed point of the map (1). From this and the equality (7) it follows that

$$x^{[k+1]} - x^* = P^{-1}R \begin{pmatrix} D_h & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & D_l & 0 \\ 0 & 0 & 0 & I \end{pmatrix} R'P(x^{[k]} - x^*) \tag{11}$$

at any $x^{[k]} \neq x^*$; for $k = 0, 1, 2, \dots$; and from any initial guess x^* .

So, according to (8)-(9), whereas V is a real positive definite matrix, such that $V = P'P$, the iteration formula (10) satisfies (3)-(4). Only condition (5) appears slightly modified according to (11) as follows

$$\left\| P(x^{[k+1]} - x^*) \right\|_2 < \left\| P(x^{[k]} - x^*) \right\|_2 \tag{12}$$

at any $x^{[k]} \neq x^*$; for $k = 0, 1, 2, \dots$; and from any initial guess x^* . Therefore, by simple induction,

$$f(x^{[k+1]}) < f(x^{[k]}) \tag{13}$$

and

$$\|P(x^{[k+1]} - x^*)\|_2 < \|P(x^{[0]} - x^*)\|_2 \quad (14)$$

at any $x^{[0]} \neq x^*$ and for $k = 0, 1, 2, \dots$.

Once the GSVD-based formula (6) has been reformulated into the equivalent SVD-based formula (10), one can naturally define Approximating Splitting Pseudo-Iterations as a direct method for approximating solutions of (2), whose formula is (10) with a certain previously chosen number of iterates τ , that is,

$$\begin{aligned} \widehat{x^*} = & P^{-1}R \begin{pmatrix} D_h^\tau & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & D_l^\tau & 0 \\ 0 & 0 & 0 & I \end{pmatrix} R'Px^{[0]} + \\ & + P^{-1}R \begin{pmatrix} [I - D_h^\tau]S_h^{-1} & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & [I - D_l^\tau]S_l^{-1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} L'b \end{aligned} \quad (15)$$

The number of iterates τ which becomes a parameter of the Approximating Splitting Pseudo-Iteration method and which has to be previously specified is hence named Number of Pseudo-Iterates.

So, the Approximating Splitting Pseudo-Iteration method (15) with a given Number of Pseudo-Iterates is a non-iterated variant of the Approximating Splitting Iteration method (10) with a certain previously chosen number of iterates.

Notice that the Approximating Splitting Pseudo-Iteration method (15) improves any preliminary numerical approximate solution of (2). In other words, for any given A , b and $x^{[0]} \neq x^*$; and any given non-singular P , $\widehat{x^*}$ approximates x^* better than $x^{[0]}$ does.

In effect, by setting $k = \tau - 1$ respectively in (13) and (14),

$$\|A\widehat{x^*} - b\|_2^2 < \|Ax^{[0]} - b\|_2^2$$

and

$$\|P(\widehat{x^*} - x^*)\|_2 < \|P(x^{[0]} - x^*)\|_2$$

for any given A , $x^{[0]} \neq x^*$ and any non-singular P .

3 Regularizing properties of the Approximating Splitting Pseudo-Iterations

In every real-world least squares problem (2), the data vector is always contaminated by various types of unknown errors, commonly called perturbations, such as measurement

and approximation errors or, even, rounding-off errors propagated along some previous computations. Hence, while solving (2), one is finding in fact an approximate solution of a certain other problem instead namely

$$\widetilde{x}^* = \arg \min_{x \in \mathbb{R}^n} \widetilde{f}(x) = \|Ax - \widetilde{b}\|_2^2 \tag{16}$$

$$\widetilde{b} = b + \Delta b \tag{17}$$

where $\Delta b \in \mathbb{R}^m$ is the vector of unknown perturbations [7, 8, 11].

The major difficulty with severely ill-conditioned linear least squares problems is, on the one hand, that they are essentially ill-determined because of the cluster of small singular values of the matrix and, on the other hand, that perturbations have components, as a rule, along all the left singular vectors of A [8].

Let us formally rewrite (15) for approximating the solution of the perturbed problem (16)-(17)

$$\begin{aligned} \widetilde{x}^* &= P^{-1}R \begin{pmatrix} D_h^\tau & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & D_l^\tau & 0 \\ 0 & 0 & 0 & I \end{pmatrix} R'Px^{[0]} + \\ &+ P^{-1}R \begin{pmatrix} [I - D_h^\tau]S_h^{-1} & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & [I - D_l^\tau]S_l^{-1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} L'\widetilde{b} \end{aligned} \tag{18}$$

The Approximating Splitting Pseudo-Iteration method has the following properties which make it suitable for regularization purposes [7, 8, 11].

\widehat{x}^* continuously depends on data. Indeed, according to (15) and (18),

$$\widehat{x}^* - \widetilde{x}^* = P^{-1}R \begin{pmatrix} [I - D_h^\tau]S_h^{-1} & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & [I - D_l^\tau]S_l^{-1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} L'(b - \widetilde{b})$$

Therefore, whereas

$$\left\| P^{-1}R \begin{pmatrix} [I - D_h^\tau]S_h^{-1} & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & [I - D_l^\tau]S_l^{-1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} L' \right\| < \infty$$

at any given τ , one has that

$$\forall \widehat{x}^*, \widetilde{x}^* \in \mathbb{R}^n, b = \widetilde{b} \Rightarrow \widehat{x}^* = \widetilde{x}^*$$

and

$$\lim_{\|\Delta b\| \rightarrow 0} \left\| \widehat{x^*} - \widetilde{x^*} \right\| = 0$$

at any given τ and for any given A , $x^{[0]}$ and any positive definite V , where $\|\dots\|$ denotes any prefixed norm.

Filter factors. It is not hard to realize that the matrix

$$\Phi[\tau, S] = \begin{pmatrix} I - \left(I - 2(I + S'_h S_h)^{-1} S'_h S_h \right)^\tau & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I - \left(I - 2(I + S'_i S_i)^{-1} S'_i S_i \right)^\tau & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

is the matrix of the so-called filter factors which play a central role in regularization theory [7, 8, 11], characterizing, in each specific case, any Approximating Splitting Pseudo-Iteration formula as the formula of a particular regularization method.

In effect, for a given $\tau > 0$, each diagonal entry of the matrix $\Phi[\tau, S]$ can be viewed as a discrete value of a continuous parametric filter function $\phi_\tau : \mathbb{R}^+ \rightarrow [0, 2) \subset \mathbb{R}^+$,

$$\phi_\tau[s] = 1 - \left(1 - 2 \frac{s^2}{1 + s^2} \right)^\tau$$

which has the following filtering properties:

$$\lim_{s \rightarrow +0} \phi_\tau[s] = 0$$

$$\lim_{s \rightarrow 1} \phi_\tau[s] = 1$$

and

$$\lim_{s \rightarrow +\infty} \phi_\tau[s] = 0$$

Finally, notice that

$$x^{[k]} - x^{[0]} = P^{-1} R \Phi[\tau, S] R' P (x^* - x^{[0]})$$

4 Previously choosing the number of iterates

Most iterative methods have an a posteriori stopping rule [4, 12]. As a logic consequence, when the iteration is stopped, propagated errors have fatally contaminated the results of all the performed computations. This happens even in the case of regularization-wise methods with a stopping rule based on the number of iterates

[7, 8, 11].

Fortunately, in the case of both the Approximating Splitting Iteration formulas (6) and (10), the error propagation is essentially avoided, because iterations are not required (at least not in the usual way) while computing each approximate solution of (2) and they both should have an a priori stopping rule.

Of course, in the latter case, the overall number of useful iterates could be chosen in several distinct ways, according to various criteria for diverse purposes.

Below, a heuristic formula is developed for the a priori numerical estimation of the number of an iterate, at which Approximating Splitting Iteration sequences would reach a good trade-off between numerical accuracy and stability.

Let us denote

$$y = R'Px = \begin{pmatrix} y_h \\ y_1 \\ y_l \\ y_0 \end{pmatrix}$$

Thus, according to (11),

$$\begin{pmatrix} y_h^{[k]} - y_h^* \\ 0 \\ y_l^{[k]} - y_l^* \\ y_0^{[0]} - y_0^* \end{pmatrix} = \begin{pmatrix} D_h^k & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & D_l^k & 0 \\ 0 & 0 & 0 & I \end{pmatrix} \begin{pmatrix} y_h^{[0]} - y_h^* \\ y_1^{[0]} - y_1^* \\ y_l^{[0]} - y_l^* \\ y_0^{[0]} - y_0^* \end{pmatrix}$$

Whereas $y_1^{[k]}$ and $y_0^{[0]}$ do not vary with k , one can directly state

$$y_1^* = [L'b]_1$$

and

$$y_0^* = y_0^{[0]}$$

where $[L'b]_1$ denotes that sub-vector of the vector $L'b$, whose components correspond to those of y_1 .

So, the attention can then be focused on the remaining components of y , that is, just on those which do vary with k , namely:

$$\begin{pmatrix} y_h^{[k]} - y_h^* \\ y_l^{[k]} - y_l^* \end{pmatrix} = \begin{pmatrix} D_h^k & 0 \\ 0 & D_l^k \end{pmatrix} \begin{pmatrix} y_h^{[0]} - y_h^* \\ y_l^{[0]} - y_l^* \end{pmatrix}$$

Let us additionally denote

$$y_{hl} = \begin{pmatrix} y_h \\ y_l \end{pmatrix}$$

$$D_{hl} = \begin{pmatrix} D_h^k & 0 \\ 0 & D_l^k \end{pmatrix} = \begin{pmatrix} \delta_1 & 0 & \dots & 0 \\ 0 & \delta_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \delta_q \end{pmatrix}$$

where $q = q_h + q_l$.

Notice that, according to (4) and (12), a sequential monotonic improvement of accuracy of approximates must be expected.

However, in spite of the mathematical simplicity of (10), an undesirable distortion of the plot of the iterative approximates may appear at late iterates (not far from x^*) as an instability symptom.

So, on the one hand, too early iterates may provide stable but inaccurate approximates, while, on the other hand, too late iterates may provide accurate but unstable approximates.

In order to more deeply investigate the aforementioned distortion, many numerical simulation experiments were performed with the Approximating Splitting Iteration formula (10) and the same well-conditioned matrix P (for instance, matrices P from factorization of $V = 2\lambda I + A'A$ and $V = \lambda I$, $\lambda \in \mathbb{R}$, $\lambda > 0$ etc.) on diverse well- and ill-conditioned linear least squares problems with and without noise. The results of those experiments revealed a clear link between the distortion and the unreliable floating point computation of powers of the diagonal entries of the approximating splitting iteration matrix

$$\begin{pmatrix} D_h & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & D_l & 0 \\ 0 & 0 & 0 & I \end{pmatrix}$$

in (10) at large values of k , that is, while computing late approximates x^* (near x^*) by means of any of formulas (6) or (10).

Even more so, the results of the performed experiments specifically with the formula (10) showed that the distortion arises at about a certain iterate τ^* , which satisfies either

$$\text{cond}(D_{hl})^{-\tau^*} \approx \varepsilon$$

if $\text{cond}(D_{hl}) \neq 1$ or

$$|\delta|^{\tau^*} \approx \varepsilon, \delta = \delta_i < 1, i = 1, 2, \dots, q$$

if $\text{cond}(D_{hl}) = 1$; where ε is the computer floating point relative accuracy (the distance from 1.0 to the next largest floating-point number) [4, 12].

So, the experimental facts described above suggest that the iterative improvement of accuracy of approximates should be kept only until $k = \tau^*$, when the conditionedness of the sub-matrix D_{hl} reach a top value about ε^{-1} , in order to prevent the plot distortion. That way, the formula

$$\tau^* = \begin{cases} \lceil \text{integer} \left(\frac{-\log(\varepsilon)}{\log(\text{cond}(D_{hl}))} \right) \rceil, & \text{cond}(D_{hl}) \neq 1 \\ \lceil \text{integer} \left(\frac{\log(\varepsilon)}{\log(|\delta|)} \right) \rceil, & \text{cond}(D_{hl}) = 1 \end{cases} \quad (19)$$

results the heuristic formula of a good a priori numerical estimator of the number of the iterate about which the plot distortion might originate with the Approximating Splitting Iteration method.

Thus, τ^* can be assumed as an appropriate a priori numerical estimator of the number of that iterate, at which each sequence (10) would reach a good trade-off between numerical accuracy and stability with the Approximating Splitting Iteration method.

Therefore, the general Approximating Splitting Pseudo-Iteration formula (15) with τ^* as the Number of Pseudo-Iterates becomes the general formula of a certain conditionedness-free method for approximating solutions of (2).

Indeed, notice that, choosing V well-conditioned enough, according to (19), well-conditioned problems must yield large numbers of iterates while ill-conditioned problems must yield small ones. So, conditionedness-free Approximating Splitting Pseudo-Iterations numerically must behave similar to both "orthodox" and regularization methods while approximating solutions respectively of well- and ill-conditioned problems.

5 An important particular case: the conditionedness-free Pseudo-Iterated Tikhonov's Regularization

Notice that, according to the Iterated Tikhonov's Regularization properties proved in [10], an interesting class of Approximating Splitting Pseudo-Iterations -Pseudo-Iterated Tikhonov's Regularization- can be derived from (15) if and are assumed to be there respectively

$$x^{[0]} = 0$$

and

$$P \mid P'P = 2\lambda D'D + A'A, \lambda \in \mathbb{R}, \lambda > 0$$

where P is either the identity matrix (regularization in standard form) or some real discretized differential operator-matrix [6, 7, 8, 11] (regularization in general form), which satisfies

$$\text{Null}(D) \cap \text{Null}(A) = \{0\}$$

and the regularization parameter λ [7, 8, 11] can be found by means of any of the procedures described therein.

Therefore, \widehat{x}^* can be viewed as a conditionedness-free regularized minimal norm least squares approximate of a certain unknown discretized function [6, 7, 8, 11].

Finally notice that, if the Number of Pseudo-Iterates τ were chosen as computed with (19), an important conditionedness-free particular case of Pseudo-Iterated Tikhonov's Regularization would be issued.

Numerical simulation experiments. The figures 1 and 2 illustrate the results of the numerical experiments performed with the conditionedness-free Pseudo-Iterated Tikhonov's Regularization (PITR) in standard form as a particular case of Approximating Splitting Pseudo-Iteration and compare these results with results of other well-known methods. They show the plots of the approximates resulting from the simulations made on the well-conditioned ($\kappa = 5, \text{cond} \approx 2.5387$) and the ill-conditioned ($\kappa = 1, \text{cond} \approx 7.3793 \times 10^{23}$) "Heat" test problems (discretized heat equation inverse problems) from Regutool [8]. Both test problems were constructed with the same arbitrary, previously chosen exact solution and right-hand sides were produced by post-multiplying the discretized operator-matrix on the given solution. Noise was generated assuming an uncorrelated unbiased gaussian distribution with variance $\sigma = 0.0049$ and $\sigma = 0.0015$ respectively for the well- and ill-conditioned cases.

The regularization parameter λ was chosen according to the Generalized Cross-Validation (GCV) rule [8, 11].

In both figures, dashed lines correspond to the exact solution plot; the two first row plots correspond to PITR, the two second ones, to the Pseudo-Inverse method (PINV) and the third two ones, to the known Tikhonov's Regularization method (TR) in standard form. Furthermore, the three left column plots correspond to cases without noise, while the three right ones correspond to cases with noise.

In both well-conditioned cases (with and without noise), the average Number of Pseudo-Iterates resulted in 27. In the ill-conditioned cases, an average of 2 was obtained for the noiseless case. When noise was added, the average number became 3.6667.

Finally, notice that if $x^{[0]}$ were assumed to be $x^{[0]} \neq 0$ and P , some real non-singular discretized differential operator-matrix, then, according to (4), \widehat{x}^* could be viewed as that approximate, whose plot sinuosity (maxima and minima points, convexity change points, etc.) would be the most smoothly similar to the one of the preliminary approximate $x^{[0]}$ [6, 10].

6 Conclusions

In this paper, a new direct method for approximating linear least squares solutions, named Approximating Splitting Pseudo-Iterations, was derived and formulated as a regularizing non-iterated variant of the Approximating Splitting Iteration method with a certain previously chosen number of iterates, named Number of Pseudo-Iterates.

Furthermore, a heuristic formula was developed for the a priori numerical estimation of the number of an iterate, at which Approximating Splitting Iteration sequences would reach a good trade-off between numerical accuracy and stability. This formula was discussed as a parameter estimator of the Number of Pseudo-Iterates for the new method.

By estimating that way the Number of Pseudo-Iterates, the general formula of a conditionedness-free regularizing method was derived for approximating solutions of linear least squares problems from the general Approximating Splitting Pseudo-Iteration formula Number of Pseudo-Iterates.

The results of several numerical simulation experiments with the conditionedness-free version of the Approximating Splitting Pseudo-Iteration method with distinct well-conditioned enough matrices V demonstrated that well-conditioned problem matrices provide large Numbers of Pseudo-Iterates, while ill-conditioned problem matrices provide small ones. For that reason, the new method numerically behaves similar to both "orthodox" and regularization methods while approximating solutions respectively of well- and ill-conditioned linear least squares problems.

At the end of the paper, the formula of the conditionedness-free Pseudo-Iterated Tikhonov's Regularization method in standard form was derived as an important particular case of conditionedness-free Approximating Splitting Pseudo-Iterations.

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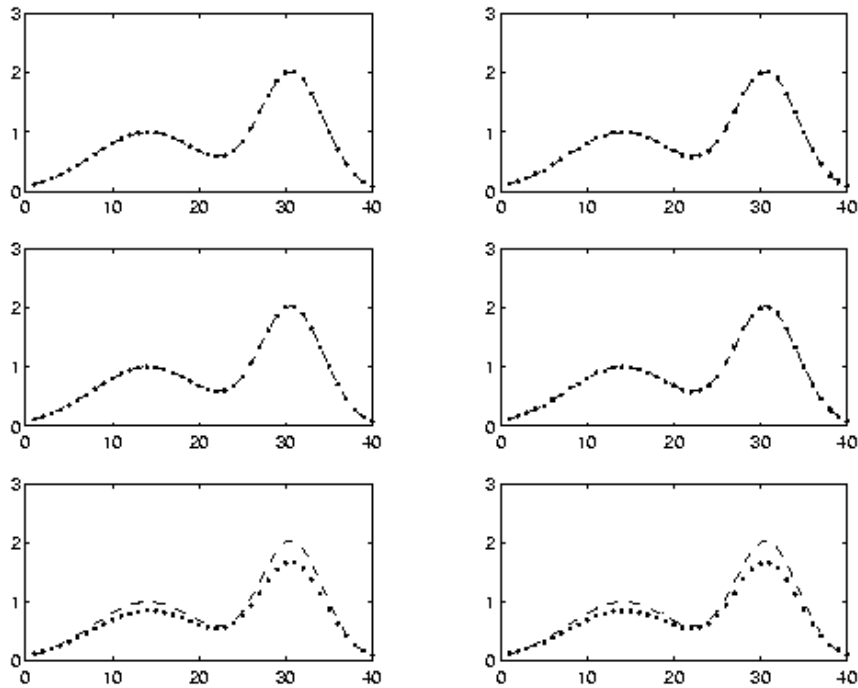


Fig. 1: This figure shows the results of the numerical simulations with the conditionedness-free Pseudo-Iterated Tikhonov's Regularization (PITR), in standard form, the Pseudo-Inverse method (PINV) and the Tikhonov's Regularization method (TR) in standard form in approximating solutions of a well-conditioned discretized heat equation inverse problem ($\text{cond} = 2.5387$). Dashed lines correspond to the exact solution plot. The two first row plots correspond to PITR, the two second ones, to PINV and the two third ones, to TR. Furthermore, the three left column plots correspond to cases without noise, while the three right ones, to cases with noise (uncorrelated, unbiased gaussian noise with 0.0049 variance). The average Number of Pseudo-Iterates resulted in 27.

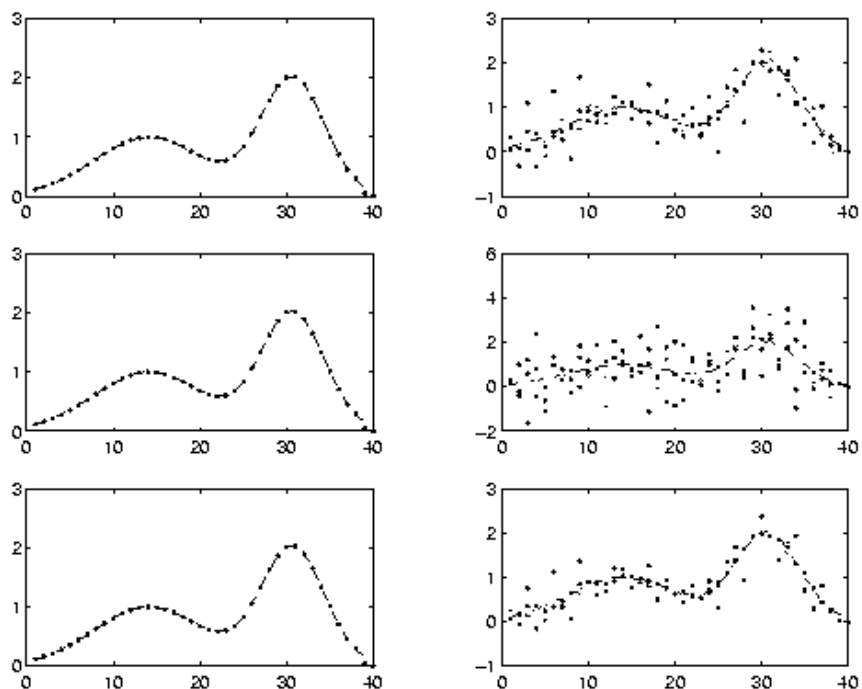


Fig. 2: This figure shows the results of the numerical simulations with the conditionedness-free Pseudo-Iterated Tikhonov's Regularization method (PITR) in standard form, the Pseudo-Inverse method (PINV) and the Tikhonov's Regularization method in standard form in approximating solutions of an ill-conditioned discretized heat equation inverse problem ($\text{cond} = 7.3793e+23$). Dashed lines correspond to the exact solution plot. The two first row plots correspond to PITR, the two second ones, to PINV and the two third ones, to TR. Furthermore, the three left column plots correspond to cases without noise, while the three right ones, to cases with noise (uncorrelated, unbiased gaussian noise with 0.0015 variance). The average Number of Pseudo-Iterates resulted 2 in the case without noise and 3.6667, with it.