A New Iterative Refinement of the Solution of Ill-Conditioned Linear System of Equations

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Abstract

In this paper, a new iterative refinement of the solution of an ill-conditioned linear system of equations are given. The convergence properties of the method are studied. Some numerical experiments of the method are given and compared with that of two of the available methods.

Keywords: linear system of equations, iterative refinement, ill-conditioned, Cholesky, convergence.

1. Introduction

Consider the linear system of equations

$$Ax = b, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$ is symmetric positive definite (SPD) and $x, b \in \mathbb{R}^n$. We assume that the matrix A is rather ill-conditioned. The matrix A is called ill-conditioned if its *condition number*, i.e.,

$$\mathrm{cond(A)} = \|\mathrm{A}\|\|\mathrm{A}^{-1}\|,$$

is very large, where $\|.\|$ is matrix norm. There are various direct and iterative methods to solve such systems. Unfortunately, direct solvers such as Gaussian elimination method may lead to an inaccurate solution of Eq. (1). Some methods have been proposed to overcome on this problem in the literature. One approach is to use the scaling strategy, but scaling of the equations and unknowns must proceed on a problem-by-problem basis. Hence, general scaling strategy are unreliable [3, 8, 10]. Another approach, which we focus our attention on it, is to use an iterative refinement of the solution obtained by a direct solver. Since A is an SPD matrix then it can be decomposed as $A = LL^T$ where L is lower triangular matrix with positive diagonal entries. This decomposition is known as the Cholesky factorization of A. Hence a common direct method for solving (1) is to solve $Ly = b$ for a vector y and then $L^T x = y$. A popular method of the iterative refinement is the well-known Wilkinson's iterative refinement [6, 7]. This method may be run as following.

Algorithm 1. `Wilkinson's iterative refinement`

1. Set $x_0 = 0$ and compute the Cholesky factor L of A
2. For $m = 0, 1, \ldots,$ until convergence Do
3. $\quad r_m = b - Ax_m$
4. $\quad$ Solve $LL^T y_m = r_m$ for y_m
5. $\quad x_{m+1} = x_m + y_m$
6. EndDo

In the absence of rounding errors, the process would stop at the first step, yielding the exact solution. Since rounding errors are also made in the iterative refinement it is by no means obvious that the successive x_m will be improved solutions. However, the convergence properties of the method can be improved by computing the residual in double precision, while computing the other quantities in single precision [5, 7].

A more efficient iterative refinement procedure has been presented by Wu et al. in [11]. Their proposed method, which call it as Wu's method, is as following

$$\begin{aligned} y_m &= (uI + A)^{-1}(b - Ax_m) \\ x_{m+1} &= x_m + y_m, \end{aligned}$$

where $u \geq 0$ is parameter and I is the identity matrix. Since A is SPD, $uI + A$ is also SPD. Hence the computation of y_m can be done by using Cholesky decomposition of $uI + A$. It can be easily seen that this iterative method unconditionally converges to the solution of (1). An strategy to choose a good value of u also proposed in [11]. Numerical experiments presented in [11] show that the method is more effective than the Wilkinson's method.

In this paper, a new two-step iterative refinement procedure is proposed and its properties are studied. Some numerical experiments are given to compare the results of the new method with that of the Wilkinson and Wu's methods.

This paper is organized as follows. In section 2, the new method and its properties are given. Numerical experiments are given in section 3. Section 4, is devoted to some concluding remarks.

2. New method

We write Eq. (1) in the following form

$$\alpha x + \beta x + Ax = (\alpha + \beta)x + b, \tag{2}$$

where $\alpha, \beta \in \mathbb{R}$. Then we define the following iterative procedure

$$(\alpha I + A)x_{m+1} = (\alpha + \beta)x_m - \beta x_{m-1} + b, \quad m = 1, 2, \ldots. \tag{3}$$

Let $\alpha \geq 0$. In this case $\alpha I + A$ is SPD and therefore Eq. (3) is written in the form

$$x_{m+1} = (\alpha I + A)^{-1}((\alpha + \beta)x_m - \beta x_{m-1} + b), \quad m = 1, 2, \ldots. \tag{4}$$

Similar to the Wu's method the $(m+1)$-th iteration of this procedure can be written as following

$$\begin{aligned} y_m &= (\alpha I + A)^{-1}[(\beta I - A)x_m - \beta x_{m-1} + b], \\ x_{m+1} &= x_m + y_m, \end{aligned}$$

which is equivalent to

$$\begin{aligned} y_m &= (\alpha I + A)^{-1}[r_m + \beta(x_m - x_{m-1})], \\ x_{m+1} &= x_m + y_m, \end{aligned}$$

where $r_m = b - Ax_m$. Obviously, if $\beta = 0$ then the new method is equivalent to the Wu's method. Next, we give some conditions for the convergence of the method. To do this we first recall the next theorem.

Theorem 1. (Axelsson [1]) *The second-degree equation $z^2 - rz + s = 0$, where r and s are real, has roots z_1 and z_2 with maximum moduli $z_0 = \max\{|z_1|, |z_2|\} < 1$ if and only if $|s| < 1$ and $|r| < 1 + s$.*

Now we state and prove the following theorem.

Theorem 2. *Let A be an SPD matrix, $\lambda_{\min}$ be its smallest eigenvalue and $\alpha \geq 0$. Then the iterative method defined by (4) is convergent with any initial guesses x_0 and x_1 if and only if*

$$-(\alpha + \frac{1}{2}\lambda_{\min}) < \beta < \alpha + \lambda_{\min}. \tag{5}$$

Proof. Let $e_i = x_i - x^*$ where $x^* = A^{-1}b$. From (2) and (4) we have

$$\begin{aligned} e_{m+1} &= (\alpha I + A)^{-1}((\alpha + \beta)e_m - \beta e_{m-1}) \\ &= (\alpha + \beta)(\alpha I + A)^{-1}e_m - \beta(\alpha I + A)^{-1}e_{m-1}. \end{aligned} \tag{6}$$

Let

$$w_{m+1} = \begin{pmatrix} e_{m+1} \\ e_m \end{pmatrix}.$$

It follows from (6) that

$$w_{m+1} = \mathcal{A}w_m, \quad m = 0, 1, \ldots,$$

where

$$\mathcal{A} = \begin{pmatrix} (\alpha + \beta)(\alpha I + A)^{-1} & -\beta(\alpha I + A)^{-1} \\ I & 0 \end{pmatrix}.$$

The characteristic polynomial of $\mathcal{A}$ is

$$\prod_{i=1}^{n} \det \begin{pmatrix} \frac{\alpha+\beta}{\alpha+\lambda_i} - \mu & -\frac{\beta}{\alpha+\lambda_i} \\ 1 & -\mu \end{pmatrix} = 0,$$

where $\lambda_i,\ i = 1, 2, \ldots, n$ are the eigenvalues of A. Thus the eigenvalues of the matrix $\mathcal{A}$ are given by equations with the following form

$$\mu^2 - \gamma\mu + \delta = 0,$$

where

$$\gamma = \frac{\alpha + \beta}{\alpha + \lambda}, \quad \delta = \frac{\beta}{\alpha + \lambda},$$

in which λ is an eigenvalue of A. From Theorem 1 the new method is convergent ($|\mu| < 1$) if and only if $|\delta| < 1$ and $|\gamma| < 1 + \delta$. It is easy to see that

$$|\delta| < 1 \Longleftrightarrow \lambda > |\beta| - \alpha \quad \text{or} \quad \lambda < -|\beta| - \alpha.$$

The inequality $\lambda < -|\beta| - \alpha$ can not hold, since $\lambda > 0$ and $\alpha \geq 0$. Therefore, we consider $\lambda > |\beta| - \alpha$. The two following cases are investigated.

Case 1: Let $\beta \geq 0$. Hence, $\lambda > \beta - \alpha$. Therefore,

$$|\gamma| = \mid \frac{\alpha+\beta}{\alpha+\lambda} \mid = \frac{\alpha+\beta}{\alpha+\lambda} = \frac{\alpha}{\alpha+\lambda} + \frac{\beta}{\alpha+\lambda} < 1+\delta.$$

Hence, in this case the condition $\lambda > \beta - \alpha$ guarantees the convergence of the method. On the other hand, this condition is equivalent to

$$\beta < \alpha + \lambda_{\min}, \tag{7}$$

which gives the right inequality in Eq. (5).

Case 2: Let $\beta < 0$. Obviously, we have $|\delta| < 1$. On the other hand, $|\gamma| < 1 + \delta$ if and only if $|\alpha + \beta| < \alpha + \lambda + \beta$, which is equivalent to

$$-(\alpha + \lambda + \beta) < \alpha + \beta < \alpha + \lambda + \beta. \tag{8}$$

The right inequality of (8) always holds. The left inequality is equivalent to $\lambda > -2(\alpha + \beta)$ which is itself equivalent to

$$\beta > -(\alpha + \frac{1}{2}\lambda_{\min}). \tag{9}$$

Eq. (7) together with (8) complete the proof. $\square$

For the implementation of the proposed method, x_1 is computed by the Wu's method and then x_m, $m \geq 2$ are computed by the proposed method. Hence the new method can be summarized as following.

Algorithm 2. `Two-step method`

1. `Set` $x_0 = 0$, `and choose parameters` α `and` β
2. `Compute` x_1 `by the Wu's method`
3. `Compute the Cholesky factor` L `of` $\alpha I + A$
4. `For` $m = 1, 2, \ldots,$ `until convergence Do`
5. $\quad r_m = b - Ax_m$
6. $\quad$ `Solve` $LL^T y_m = r_m + \beta(x_m - x_{m-1})$ `for` y_m
7. $\quad x_{m+1} = x_m + y_m$
8. `EndDo`

3. Illustrative examples

In this section, some numerical experiments are given to show the efficiency of the proposed method and comparing it with the Wilkinson and Wu's method. To do so, we give four examples, which the first three of them are from [11]. All of the numerical results were computed in double precision using some MATLAB codes. The stopping criterion

$$\|x_{m+1} - x_m\|_2 < 5 \times 10^{-6},$$

is always used and the maximum number of iterations is 100000. Additionally, for all of the examples we set $u = \alpha = 10^{-5}$ and $\beta = 10^{-6}$.

Example 1. We consider the well-known ill-conditioned system of linear equations

$$H_n x = b,$$

where H_n is the Hilbert matrix $H_n = (h_{ij}) = (\frac{1}{i+j-1})$ and $b = (b_1, b_2, \ldots, b_n)^T$ with $b_i = \sum_{j=1}^{n} h_{ij}$, $i = 1, \ldots, n$. Obviously, $x^* = (1, 1, \ldots, 1)^T$ is the exact solution of the system. The obtained numerical results by the Wilkinson's method (WILKM), Wu's method (WUM) and the proposed method (PM) are given in Table 1. For each method, the number of iterations for the convergence and the relative error

$$RE = \frac{\|x_m - x^*\|_2}{\|x^*\|_2}$$

are given. In this table, a † shows that the method fails. As we observe the results of the proposed method are better than that of the other two methods.

Table 1. Number of iteration of computed solutions for Example 1.

	n			
Method	12	20	50	90
WILKM	3724	†	†	†
	3.06e-4	-	-	-
WUM	74	93	137	157
	1.10e-4	1.12e-4	1.04e-4	9.74e-5
PM	69	87	133	150
	1.09e-4	1.10e-4	9.94e-5	9.45e-5

Example 2. We consider the previous example with the right hand side $b = (b_1, b_2, \dots, b_n)^T$ with $b_i = \sum_{j=1}^{n} h_{ij} \times j$, $i = 1, \dots, n$. Therefore the exact solution of the system is $x^* = (1, 2, \dots, n)^T$. All of the assumptions are as before. Our numerical results are given in Table 2.

Table 2. Number of iteration of computed solutions for Example 2.

	n			
Method	12	20	50	90
WILKM	942 1.86e-1	† -	† -	† -
WUM	1687 2.61e-4	2080 2.80e-4	4225 2.48e-4	11206 1.50e-4
PM	1603 2.50e-4	1941 2.78e-4	4101 2.42e-4	10620 1.47e-4

Example 3. In this example, we consider the ill-conditioned system of linear equations

$$Ax = b,$$

where $A = (a_{ij}) \in \mathbb{R}^{n\times n}$ with

$$a_{ij} = \begin{cases} 1 & i \neq j; \\ 1 + p^2, & i = j, \end{cases}$$

and $b = (b_1, b_2, \dots, b_n)^T$ with $b_i = \sum_{j=1}^{n} a_{ij} \times j$, $i = 1, 2, \dots, n$. Obviously, the exact solution is $x^* = (1, 2, \dots, n)^T$. In this case, the spectral condition number of A is [11, 9]

$$\kappa(A) = \frac{n + p^2}{p^2},$$

which is large for small enough p. For $p = 5 \times 10^{-4}$ the numerical results are given in Table 3. In this table, “No Conv.” means that the method is not convergent in 100000 iterations. We see that the results of the proposed method are better than that of the other two methods.

Table 3. Number of iteration of computed solutions for Example 3.

	n			
Method	120	150	170	200
WILKM	No Conv. -	No Conv. -	No Conv. -	No Conv. -
WUM	586 2.61e-7	599 1.90e-7	603 1.74e-7	615 1.35e-7
PM	531 2.32e-7	542 1.74e-7	550 1.39e-7	559 1.16e-7

Example 4. Consider the matrix $A = B^T B$, where $B = (b_{ij})$ is a symmetric matrix of order n with $b_{ij} = i/j$, for $i \geq j$. The right hand side $b = (b_1, b_2, \ldots, b_n)^T$ is chosen such a way that $b_i = \sum_{j=1}^{n} a_{ij} \times j$, $i = 1, 2, \ldots, n$. Obviously, the exact solution is $x^* = (1, 2, \ldots, n)^T$. Numerical results for four values of n are given in Table 4. All of the notations and assumptions are as before. As we observe the results for three values $n = 100, 105, 110$ of the WU's method and the proposed method are comparable. For $n = 115$, we see that the proposed method converges in 81 iterations, whereas the Wu's method is convergent in 274 iterations.

Table 4. Number of iteration of computed solutions for Example 4.

	n			
Method	100	105	110	115
WILKM	2 9.13e-9	4 9.14e-9	788 1.19e-8	No Conv. -
WUM	9 8.14e-9	10 8.38e-9	19 9.12e-09	274 1.32e-8
PM	7 7.29-9	8 8.53e-9	19 1.07e-8	81 1.37e-8

4. Conclusion

In this paper, a new two step iterative method for refining a solution of an SPD linear system of equations was presented. Convergence properties of the method was discussed and comparison results of the proposed method with that of the Wu's method and the Wilkinson's were also given. Numerical results show that our method often gives better results that the two other methods. An observation which can be posed here is that the parameter $\beta = 0.1\alpha$, when is in the convergence range presented in Theorem 2, usually gives good results.

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