



A Note on the Optimal Parameters of USSOR Method for Solving Linear Least Squares Problems

Peng-Bo Xu^a, Nai-Min Zhang^a

^aDepartment of Mathematics, Wenzhou University, Wenzhou, 325035, PR China

Abstract. For solving rank deficient linear least squares problems, unsymmetric successive overrelaxation (USSOR) type methods are investigated by some researchers recently. In this note, we continue to study the USSOR method for solving rank deficient linear least squares problems and obtain the optimal iteration parameters and the corresponding optimal convergence factors. Numerical experiments are given to examine the feasibility and effectiveness of the USSOR method with optimal parameters.

1. Introduction

Consider the least squares solution

$$\|q - By\|_2 = \min_{\hat{x} \in \mathbb{R}^n} \|q - B\hat{x}\|_2, \quad (1)$$

where $B \in \mathbb{R}_r^{m \times n}$, with $m \geq n$ and $\text{rank}(B) = r < n$, $q \in \mathbb{R}^m$.

It is well-known that the least square solution of minimal norm to (1) is B^+q , here B^+ is the Moore-Penrose generalized inverse of B , and y is the least squares solution to (1), if and only if

$$x = q - By, \quad (2)$$

satisfies

$$B^T x = 0, \quad (3)$$

where B^T denotes the transpose of the matrix B .

Without loss of generality, let B be the 2×2 block partitioned form

$$B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}, \quad (4)$$

where $B_{11} \in \mathbb{R}_r^{r \times r}$, $B_{12} \in \mathbb{R}^{r \times (n-r)}$, $B_{21} \in \mathbb{R}^{(m-r) \times r}$, $B_{22} \in \mathbb{R}^{(m-r) \times (n-r)}$.

2010 *Mathematics Subject Classification.* Primary 15A09; Secondary 65F10

Keywords. Optimal parameters, Least squares problems, USSOR method, Convergence, Rank deficient

Received: 11 March 2018; Revised: 06 February 2019; Accepted: 08 May 2019

Communicated by Predrag Stanimirović

Research supported by National Natural Science Foundation of China under grant No. 61572018

Email addresses: 2905423604@qq.com (Peng-Bo Xu), nmzhang@wzu.edu.cn (Nai-Min Zhang)

Let $y = (y_1^T, y_2^T)^T$, $x = (\delta_1^T, \delta_2^T)^T$, $q = (q_1^T, q_2^T)^T$, $y_1, q_1, \delta_1 \in \mathbb{R}^r$, $q_2, \delta_2 \in \mathbb{R}^{m-r}$, $y_2 \in \mathbb{R}^{n-r}$. It is easy to see that (2) and (3) can be written as the following consistent linear system:

$$\hat{B}\hat{z} = b, \tag{5}$$

where

$$\hat{B} = \begin{pmatrix} B_{11} & 0 & I_r & B_{12} \\ B_{21} & I_{m-r} & 0 & B_{22} \\ 0 & B_{21}^T & B_{11}^T & 0 \\ 0 & B_{22}^T & B_{12}^T & 0 \end{pmatrix}, \hat{z} = \begin{pmatrix} y_1 \\ \delta_2 \\ \delta_1 \\ y_2 \end{pmatrix}, b = \begin{pmatrix} q_1 \\ q_2 \\ 0 \\ 0 \end{pmatrix},$$

I_r and I_{m-r} are identity matrices with order r and $m - r$, respectively.

Notice (5) is equivalent to

$$\mathcal{A}X \equiv \begin{pmatrix} I_m & B \\ -B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} q \\ 0 \end{pmatrix} \equiv b, \tag{6}$$

where

$$\mathcal{A} = \begin{pmatrix} I_r & 0 & B_{11} & B_{12} \\ 0 & I_{m-r} & B_{21} & B_{22} \\ -B_{11}^T & -B_{21}^T & 0 & 0 \\ -B_{12}^T & -B_{22}^T & 0 & 0 \end{pmatrix}, X = \begin{pmatrix} \delta_1 \\ \delta_2 \\ y_1 \\ y_2 \end{pmatrix}.$$

For solving the rank deficient linear least squares problem (1), many authors studied overrelaxation-type methods. Miller and Neumann [8] first proposed a class of SOR method to solve (1). Tian et al. [7, 11] studied the AOR method. For rank deficient linear least squares problems, the symmetric SOR(SSOR) method is also studied, see, e.g. [3–5, 15]. Recently, Yun et al. [6, 13] proposed the unsymmetric SOR(USSOR) method to solve saddle point problems. And Song et al. [10] constructed the USSOR method to solve rank deficient linear least squares problems, which was based on the block consistent linear system (5).

In this note, we continue to study the USSOR method for solving rank deficient linear least squares problems and discuss its optimal parameters. The rest of this note is organized as follow. In Section 2, we introduce the USSOR method for solving the rank deficient linear least squares problem. In Section 3, we discuss the optimal iteration parameters and the corresponding optimal convergence factors. Numerical experiments are given to examine the feasibility and effectiveness of the USSOR method with optimal parameters in Section 4.

2. The USSOR method

According to the equation (6) and similar to [6], we consider the following splitting:

$$\mathcal{A} = M(\omega_1, \omega_2) - N(\omega_1, \omega_2), \tag{7}$$

where

$$M(\omega_1, \omega_2) = \frac{1}{\omega_1 + \omega_2 - \omega_1\omega_2} \begin{pmatrix} I_m & \omega_2 B \\ -\omega_1 B^T & -\omega_1\omega_2 B^T B + (1 - \omega_2)Q \end{pmatrix},$$

$$N(\omega_1, \omega_2) = \frac{1}{\omega_1 + \omega_2 - \omega_1\omega_2} \begin{pmatrix} (1 - \omega_1)(1 - \omega_2)I_m & (\omega_1\omega_2 - \omega_1)B \\ (\omega_2 - \omega_1\omega_2)B^T & -\omega_1\omega_2 B^T B + (1 - \omega_2)Q \end{pmatrix},$$

and ω_1, ω_2 are two positive parameters (relaxation factors) with $\omega_2 \neq 1$, $\omega_1 + \omega_2 - \omega_1\omega_2 \neq 0$. Here $Q \in \mathbb{R}^{n \times n}$ is the approximation of the Schur complement $B^T B$. Notice $B^T B$ is singular, it is more reasonable to choose

a singular matrix as its approximation, so, in this note Q is chosen by a symmetric positive semi-definite (and potentially singular) matrix. $M(\omega_1, \omega_2)$ will act as the preconditioner for (6). The coefficient matrix \mathcal{A} of (6) is singular, so, a singular matrix $M(\omega_1, \omega_2)$ may also be more reasonable to approximate \mathcal{A} .

The USSOR method can be derived from the splitting (7). On the other hand, we can also derive the USSOR method simply by the preconditioned system as follows. Notice when $\mathcal{N}(Q) \subseteq \mathcal{N}(B)$, where $\mathcal{N}(\cdot)$ denotes the null space of the corresponding matrix, then it is easy to see that the Moore-Penrose generalized inverse $M^\dagger(\omega_1, \omega_2)$ of $M(\omega_1, \omega_2)$ has the following expression:

$$M^\dagger(\omega_1, \omega_2) = (\omega_1 + \omega_2 - \omega_1\omega_2) \begin{pmatrix} I_m - \frac{\omega_1\omega_2}{1-\omega_2} BQ^\dagger B^T & \frac{-\omega_2}{1-\omega_2} BQ^\dagger \\ \frac{\omega_1}{1-\omega_2} Q^\dagger B^T & \frac{1}{1-\omega_2} Q^\dagger \end{pmatrix}.$$

Now we obtain the preconditioned system through multiplying both sides of (6) by $M^\dagger(\omega_1, \omega_2)$:

$$M^\dagger(\omega_1, \omega_2)\mathcal{A}X = M^\dagger(\omega_1, \omega_2)b, \tag{8}$$

It is known that the solution sets of (6) and (8) are identical so long as the condition $\mathcal{N}(M^\dagger(\omega_1, \omega_2)\mathcal{A}) = \mathcal{N}(\mathcal{A})$ holds. In fact, when $\mathcal{N}(Q) \subseteq \mathcal{N}(B)$, then [6] we have $\mathcal{N}(M^\dagger(\omega_1, \omega_2)\mathcal{A}) = \mathcal{N}(\mathcal{A})$.

From (8) we obtain the fixed point system

$$X = (I - M^\dagger(\omega_1, \omega_2)\mathcal{A})X + M^\dagger(\omega_1, \omega_2)b, \tag{9}$$

which reduces to the following general stationary iteration, i.e., the USSOR iteration:

$$X_{k+1} = H(\omega_1, \omega_2)X_k + M^\dagger b, \quad k = 0, 1, 2, \dots, \tag{10}$$

or

$$\begin{pmatrix} x_{k+1} \\ y_{k+1} \end{pmatrix} = H(\omega_1, \omega_2) \begin{pmatrix} x_k \\ y_k \end{pmatrix} + M^\dagger(\omega_1, \omega_2) \begin{pmatrix} q \\ 0 \end{pmatrix}, \quad k = 0, 1, 2, \dots, \tag{11}$$

where $H(\omega_1, \omega_2) = I - M^\dagger(\omega_1, \omega_2)\mathcal{A}$ is the iteration matrix and satisfies $H(\omega_1, \omega_2) = (\omega_1 + \omega_2 - \omega_1\omega_2) \times$

$$\begin{pmatrix} (\frac{1}{\omega_1 + \omega_2 - \omega_1\omega_2} - 1)I + \frac{(\omega_1 - 1)\omega_2}{1 - \omega_2} BQ^\dagger B^T & \frac{\omega_1\omega_2}{1 - \omega_2} BQ^\dagger B^T B - B \\ \frac{1 - \omega_1}{1 - \omega_2} Q^\dagger B^T & \frac{1}{\omega_1 + \omega_2 - \omega_1\omega_2} I - \frac{\omega_1}{1 - \omega_2} Q^\dagger B^T B \end{pmatrix}. \tag{12}$$

3. Optimal parameters of the USSOR method

In this section, we study the optimal parameters of the USSOR method (10). First, we introduce the pseudo-spectral radius $\nu(H(\omega_1, \omega_2))$ as follows:

$$\nu(H(\omega_1, \omega_2)) = \max\{|\lambda| : \lambda \in \sigma(H(\omega_1, \omega_2)), \lambda \neq 1\}, \tag{13}$$

where $\sigma(H(\omega_1, \omega_2))$ is the spectrum of $H(\omega_1, \omega_2)$.

We say the iteration (10) is semi-convergent if, for any initial guess X_0 , the iteration sequence X_k produced by (10) converges to a solution of (6). It is well known [1] that the sufficient and necessary conditions for the semi-convergence of (10) are: (i) $\mathcal{N}(M^\dagger(\omega_1, \omega_2)\mathcal{A}) = \mathcal{N}(\mathcal{A})$; (ii) $\text{rank}(I - H(\omega_1, \omega_2)) = \text{rank}(I - H(\omega_1, \omega_2))^2$; (iii) $\nu(H(\omega_1, \omega_2)) < 1$. Fan et al. [6] studied these conditions and obtained the semi-convergence results for USSOR by follows.

Theorem 3.1. ([6]) *Let Q be symmetric positive semi-definite with $\mathcal{N}(Q) \subseteq \mathcal{N}(B)$, and ρ be the spectral radius of $Q^\dagger B^T B$. Then USSOR is semi-convergent if ω_1 and ω_2 satisfy the following conditions*

$$0 < \omega_2 < \frac{4}{3 + \sqrt{1 + 4\rho}}, \tag{14}$$

and

$$0 < \omega_1 < \frac{1}{1 - \omega_2} \left(\frac{4}{1 + \sqrt{1 + 4\rho(1 - \omega_2)^{-1}}} - \omega_2 \right). \tag{15}$$

Corollary 3.2. ([6]) Let ρ be the spectral radius of $Q^\dagger B^T B$. Then USSOR semi-converges if ω_1 and ω_2 satisfy the following conditions

$$\omega_2 < 1, \text{ and } -\frac{\omega_2}{1 - \omega_2} < \omega_1 < \frac{1}{1 - \omega_2} \left(\frac{4}{1 + \sqrt{1 + 4\rho(1 - \omega_2)^{-1}}} - \omega_2 \right). \tag{16}$$

Remark 3.3. From the above Corollary we see that when ω_1 and ω_2 satisfy (16), then $v(H(\omega_1, \omega_2)) < 1$ holds true. Moreover, we consider the problem of how to choose the optimal ω_1 and ω_2 which minimize $v(H(\omega_1, \omega_2))$. Generally, we find it is very complicated to determine the optimal parameters when $\omega_1 \geq 1$. So, in this note we discuss the local optimal parameters, that is, we assume $\omega_1 < 1$, and together with (16), it holds $0 < (1 - \omega_1)(1 - \omega_2) < 1$.

We need the following lemmas to find the optimal parameters.

Lemma 3.4. Let Q be symmetric positive semi-definite with $\mathcal{N}(Q) \subseteq \mathcal{N}(B)$. For any $\lambda \in \sigma(H(\omega_1, \omega_2))$ and $\lambda \neq (1 - \omega_1)(1 - \omega_2)$, the μ which satisfies

$$\lambda^2 - \left(1 + (1 - \omega_1)(1 - \omega_2) + \frac{((1 - \omega_1)(1 - \omega_2) - 1)^2}{\omega_2 - 1} \mu \right) \lambda + (1 - \omega_1)(1 - \omega_2) = 0, \tag{17}$$

is the eigenvalue of $Q^\dagger B^T B$. On the contrary, for any $\mu \in \sigma(Q^\dagger B^T B)$, if $\lambda \neq (1 - \omega_1)(1 - \omega_2)$ and λ satisfies (17), then $\lambda \in \sigma(H(\omega_1, \omega_2))$.

Proof. We can rewrite the equation (17) as follows:

$$(\omega_2 - 1)(\lambda^2 - ((1 - \omega_1)(1 - \omega_2) + 1)\lambda + (1 - \omega_1)(1 - \omega_2)) = ((1 - \omega_1)(1 - \omega_2) - 1)^2 \mu \lambda, \tag{18}$$

Suppose that λ and $\xi = \begin{pmatrix} u \\ v \end{pmatrix}$ are the eigenvalue and eigenvector of $H(\omega_1, \omega_2)$, respectively, i.e.,

$$Hx = \lambda x.$$

By (12), after some algebra, we can rewrite this equation as:

$$\begin{aligned} ((1 - \omega_1)(1 - \omega_2) - \lambda)u &= (\omega_1 + \lambda\omega_2 - \omega_1\omega_2)Bv, \\ (1 - \lambda)((1 - \omega_2)Qv - \omega_1\omega_2B^T Bv) &= (-\lambda\omega_1 - \omega_2 + \omega_1\omega_2)B^T u, \end{aligned}$$

or

$$\begin{aligned} \frac{1 - \omega_1}{1 - \omega_2} Q^\dagger B^T u + \frac{1}{\omega_1 + \omega_2 - \omega_1\omega_2} v - \frac{\omega_1}{1 - \omega_2} Q^\dagger B^T Bv \\ = \frac{1}{\omega_1 + \omega_2 - \omega_1\omega_2} \lambda v, \end{aligned} \tag{19}$$

$$\begin{aligned} \left(\frac{1}{\omega_1 + \omega_2 - \omega_1\omega_2} - 1 \right) u + \frac{(\omega_1 - 1)\omega_2}{1 - \omega_2} BQ^\dagger B^T u + \frac{\omega_1\omega_2}{1 - \omega_2} BQ^\dagger B^T Bv - Bv \\ = \frac{1}{\omega_1 + \omega_2 - \omega_1\omega_2} \lambda u. \end{aligned} \tag{20}$$

Notice $((1 - \omega_1)(1 - \omega_2) - \lambda)u = (\omega_1 + \lambda\omega_2 - \omega_1\omega_2)Bv$ and ξ is an eigenvector. Then $v \neq 0$ and $u = \frac{\omega_1 + \lambda\omega_2 - \omega_1\omega_2}{1 - \lambda + \omega_1\omega_2 - \omega_1 - \omega_2}Bv$.

Substituting

$$u = \frac{\omega_1 + \lambda\omega_2 - \omega_1\omega_2}{1 - \lambda + \omega_1\omega_2 - \omega_1 - \omega_2}Bv$$

into the equation (19), and let $t = \frac{\omega_1 + \lambda\omega_2 - \omega_1\omega_2}{1 - \lambda + \omega_1\omega_2 - \omega_1 - \omega_2}$, then it holds

$$t \frac{1 - \omega_1}{1 - \omega_2} Q^+ B^T B v + \left(\frac{1}{\omega_1 + \omega_2 - \omega_1\omega_2} - \frac{\omega_1}{1 - \omega_2} Q^+ B^T B \right) v = \frac{\lambda}{\omega_1 + \omega_2 - \omega_1\omega_2} v.$$

After some algebra, this equation can be written as

$$Q^+ B^T B v = \frac{(\lambda - 1)((1 - \omega_1)(1 - \omega_2) - \lambda)(1 - \omega_2)}{(\omega_1 + \omega_2 - \omega_1\omega_2)((\omega_1 + \lambda\omega_2 - \omega_1\omega_2)(1 - \omega_1) - \omega_1((1 - \omega_1)(1 - \omega_2) - \lambda))} v. \tag{21}$$

Let $\mu = \frac{(\lambda - 1)((1 - \omega_1)(1 - \omega_2) - \lambda)(1 - \omega_2)}{(\omega_1 + \omega_2 - \omega_1\omega_2)((\omega_1 + \lambda\omega_2 - \omega_1\omega_2)(1 - \omega_1) - \omega_1((1 - \omega_1)(1 - \omega_2) - \lambda))}$. Then it is easy to see that μ is an eigenvalue of $Q^+ B^T B$ which satisfies (17). The proof of the second assertion of Lemma 3.4 can be given analogously. \square

Lemma 3.5. Let Q be symmetric positive semi-definite with $\mathcal{N}(Q) \subseteq \mathcal{N}(B)$. Assume $\lambda \in \sigma(H(\omega_1, \omega_2))$ and $\mu \in \sigma(Q^+ B^T B)$. Then λ and μ satisfy:

- (1) if $\mu = 0$, then $\lambda = 1$ or $\lambda = (1 - \omega_1)(1 - \omega_2)$,
- (2) if $\lambda = 1$, or $\lambda = (1 - \omega_1)(1 - \omega_2)$, then $\mu = 0$.

Proof. Making use of the equation (17), then the conclusions can be obtained easily. \square

According to Lemma 3.4, for any $\mu \in \sigma(Q^+ B^T A^{-1} B)$, the two roots of (17) or the two eigenvalues of the iteration matrix $H(\omega_1, \omega_2)$ are given by

$$\lambda_1(\omega_1, \omega_2, \mu) = \frac{1}{2} \left[f(\omega_1, \omega_2, \mu) + \sqrt{f^2(\omega_1, \omega_2, \mu) - 4(1 - \omega_1)(1 - \omega_2)} \right], \tag{22}$$

$$\lambda_2(\omega_1, \omega_2, \mu) = \frac{1}{2} \left[f(\omega_1, \omega_2, \mu) - \sqrt{f^2(\omega_1, \omega_2, \mu) - 4(1 - \omega_1)(1 - \omega_2)} \right], \tag{23}$$

where

$$f(\omega_1, \omega_2, \mu) = 1 + (1 - \omega_1)(1 - \omega_2) + \frac{((1 - \omega_1)(1 - \omega_2) - 1)^2}{\omega_2 - 1} \mu. \tag{24}$$

Lemma 3.6. Let Q be symmetric positive semi-definite with $\mathcal{N}(Q) \subseteq \mathcal{N}(B)$. Assume that μ_1 and μ_2 be the solutions of the equations $f(\omega_1, \omega_2, \mu) = 2\sqrt{(1 - \omega_1)(1 - \omega_2)}$ and $f(\omega_1, \omega_2, \mu) = -2\sqrt{(1 - \omega_1)(1 - \omega_2)}$, respectively. Let

$$\begin{cases} \lambda_1(\mu_1, \mu_2) = \frac{(\sqrt{\mu_2 - \mu_{\min}} + \sqrt{\mu_1 - \mu_{\min}})^2}{(\sqrt{\mu_1} + \sqrt{\mu_2})^2}, \\ \lambda_2(\mu_1, \mu_2) = \frac{(\sqrt{\mu_{\max} - \mu_1} + \sqrt{\mu_{\max} - \mu_2})^2}{(\sqrt{\mu_1} + \sqrt{\mu_2})^2}. \end{cases}$$

Then

$$v(H(\omega_1, \omega_2)) = \begin{cases} \lambda_1(\mu_1, \mu_2), \mu_1 + \mu_2 \geq \mu_{\min} + \mu_{\max}, \\ \lambda_2(\mu_1, \mu_2), \mu_1 + \mu_2 < \mu_{\min} + \mu_{\max}, \end{cases}$$

where $\mu_{\min} = \min\{\mu \mid \mu \in \sigma(Q^+ B^T B) \setminus \{0\}\}$ and $\mu_{\max} = \max\{\mu \mid \mu \in \sigma(Q^+ B^T B) \setminus \{0\}\}$.

Proof. Let

$$\lambda(\omega_1, \omega_2, \mu) = \max\{|\lambda_1(\omega_1, \omega_2, \mu)|, |\lambda_2(\omega_1, \omega_2, \mu)|\}. \tag{25}$$

Consider the following two cases:

(1) When $\Delta = f^2(\omega_1, \omega_2, \mu) - 4(1 - \omega_1)(1 - \omega_2) \leq 0$, then

$$|\lambda_1(\omega_1, \omega_2, \mu)| = |\lambda_2(\omega_1, \omega_2, \mu)| = \sqrt{(1 - \omega_1)(1 - \omega_2)}. \tag{26}$$

(2) When $\Delta > 0$, then

$$\lambda(\omega_1, \omega_2, \mu) = \begin{cases} \lambda_1(\omega_1, \omega_2, \mu), & \text{if } f(\omega_1, \omega_2, \mu) > 0, \\ -\lambda_2(\omega_1, \omega_2, \mu), & \text{if } f(\omega_1, \omega_2, \mu) \leq 0. \end{cases}$$

Together with the equation (17), it holds

$$\lambda_1(\omega_1, \omega_2, \mu)\lambda_2(\omega_1, \omega_2, \mu) = (1 - \omega_1)(1 - \omega_2).$$

Notice $0 < (1 - \omega_1)(1 - \omega_2) < 1$. Then

$$\lambda(\omega_1, \omega_2, \mu) \geq \sqrt{(1 - \omega_1)(1 - \omega_2)} > (1 - \omega_1)(1 - \omega_2). \tag{27}$$

By equations (25), (26), (27) and Lemma 3.5, it is easy to see that, to investigate the optimal parameters which minimize $v(H(\omega_1, \omega_2))$, it suffices to consider the case of $\Delta = f^2(\omega_1, \omega_2, \mu) - 4(1 - \omega_1)(1 - \omega_2) > 0$. So, from now on, we always assume $\Delta > 0$.

Let

$$\lambda_i(\omega_1, \omega_2) = \max_{\mu \in \sigma(Q^+ B^T B) \setminus \{0\}} \{|\lambda_i(\omega_1, \omega_2, \mu)|\}, \quad i = 1, 2. \tag{28}$$

Then

$$v(H(\omega_1, \omega_2)) = \max\{\lambda_1(\omega_1, \omega_2), \lambda_2(\omega_1, \omega_2)\}. \tag{29}$$

Together with equations (22) and (23), it holds:

When $\Delta > 0$ and $f(\omega_1, \omega_2, \mu) > 0$, i.e., $f(\omega_1, \omega_2, \mu) > 2\sqrt{(1 - \omega_1)(1 - \omega_2)}$, then

$$|\lambda_1(\omega_1, \omega_2, \mu)| \geq |\lambda_2(\omega_1, \omega_2, \mu)|.$$

When $\Delta > 0$ and $f(\omega_1, \omega_2, \mu) \leq 0$, i.e., $f(\omega_1, \omega_2, \mu) < -2\sqrt{(1 - \omega_1)(1 - \omega_2)}$, then

$$|\lambda_1(\omega_1, \omega_2, \mu)| \leq |\lambda_2(\omega_1, \omega_2, \mu)|.$$

Noticing $\frac{((1 - \omega_1)(1 - \omega_2) - 1)^2}{\omega_2 - 1} < 0$, then together with equations (22), (23), (24) and (28) we have

$$\begin{cases} \lambda_1(\omega_1, \omega_2) = \frac{1}{2} \left[f(\omega_1, \omega_2, \mu_{min}) + \sqrt{f^2(\omega_1, \omega_2, \mu_{min}) - 4(1 - \omega_1)(1 - \omega_2)} \right], \\ \lambda_2(\omega_1, \omega_2) = \frac{1}{2} \left[-f(\omega_1, \omega_2, \mu_{max}) + \sqrt{f^2(\omega_1, \omega_2, \mu_{max}) - 4(1 - \omega_1)(1 - \omega_2)} \right]. \end{cases} \tag{30}$$

Since $\frac{((1 - \omega_1)(1 - \omega_2) - 1)^2}{\omega_2 - 1} < 0$, there exist two variables μ_1 and μ_2 ($0 \leq \mu_1 \leq \mu_2$) satisfying the following equations:

$$1 + (1 - \omega_1)(1 - \omega_2) + \frac{((1 - \omega_1)(1 - \omega_2) - 1)^2}{\omega_2 - 1} \mu_1 = 2\sqrt{(1 - \omega_1)(1 - \omega_2)}, \tag{31}$$

$$1 + (1 - \omega_1)(1 - \omega_2) + \frac{((1 - \omega_1)(1 - \omega_2) - 1)^2}{\omega_2 - 1} \mu_2 = -2\sqrt{(1 - \omega_1)(1 - \omega_2)}. \tag{32}$$

We declare $\mu_1, \mu_2 \in [\mu_{min}, \mu_{max}]$. In fact, if $\mu_1 < \mu_{min}$ or $\mu_2 > \mu_{max}$, then $-2\sqrt{(1-\omega_1)(1-\omega_2)} < f(\omega_1, \omega_2, \mu) < 2\sqrt{(1-\omega_1)(1-\omega_2)}$, in other word, $\Delta < 0$, which is in contradiction with $\Delta > 0$. Making use of equations (31) and (32), after some algebra, it holds

$$\sqrt{(1-\omega_1)(1-\omega_2)} = \frac{\sqrt{\mu_2} - \sqrt{\mu_1}}{\sqrt{\mu_2} + \sqrt{\mu_1}}, \tag{33}$$

$$\omega_2 = 1 - \frac{4\mu_1\mu_2}{(\sqrt{\mu_1} + \sqrt{\mu_2})^2}. \tag{34}$$

Then we can rewrite $f(\omega_1, \omega_2, \mu)$, $\lambda_1(\omega_1, \omega_2)$ and $\lambda_2(\omega_1, \omega_2)$ as follows:

$$f(\omega_1, \omega_2, \mu) = \frac{2(\mu_1 + \mu_2 - 2\mu)}{(\sqrt{\mu_1} + \sqrt{\mu_2})^2}, \tag{35}$$

$$\begin{cases} \lambda_1(\omega_1, \omega_2) = \frac{(\sqrt{\mu_1 - \mu_{min}} + \sqrt{\mu_2 - \mu_{min}})^2}{(\sqrt{\mu_1} + \sqrt{\mu_2})^2}, \\ \lambda_2(\omega_1, \omega_2) = \frac{(\sqrt{\mu_{max} - \mu_1} + \sqrt{\mu_{max} - \mu_2})^2}{(\sqrt{\mu_1} + \sqrt{\mu_2})^2}. \end{cases} \tag{36}$$

For convenience, we denote $\lambda_1(\omega_1, \omega_2) \equiv \lambda_1(\mu_1, \mu_2)$ and $\lambda_2(\omega_1, \omega_2) \equiv \lambda_2(\mu_1, \mu_2)$. Easily, we see

$$\begin{cases} \lambda_1(\mu_1, \mu_2) = \lambda_2(\mu_1, \mu_2), & \mu_1 + \mu_2 = \mu_{min} + \mu_{max}, \\ \lambda_1(\mu_1, \mu_2) > \lambda_2(\mu_1, \mu_2), & \mu_1 + \mu_2 > \mu_{min} + \mu_{max}, \\ \lambda_1(\mu_1, \mu_2) < \lambda_2(\mu_1, \mu_2), & \mu_1 + \mu_2 < \mu_{min} + \mu_{max}. \end{cases} \tag{37}$$

Together with (29), (37) it holds

$$v(H(\omega_1, \omega_2)) = \begin{cases} \lambda_1(\mu_1, \mu_2), & \mu_1 + \mu_2 \geq \mu_{min} + \mu_{max}, \\ \lambda_2(\mu_1, \mu_2), & \mu_1 + \mu_2 < \mu_{min} + \mu_{max}, \end{cases} \tag{38}$$

which finishes the proof. \square

Theorem 3.7. Let Q be symmetric positive semi-definite with $\mathcal{N}(Q) \subseteq \mathcal{N}(B)$. Then the optimal parameters of the USSOR method are given by

$$\omega_{1opt} = 1 - \frac{(\sqrt{\mu_{max}} - \sqrt{\mu_{min}})^2}{4\mu_{max}\mu_{min}}, \quad \omega_{2opt} = 1 - \frac{4\mu_{max}\mu_{min}}{(\sqrt{\mu_{max}} + \sqrt{\mu_{min}})^2},$$

where $\mu_{min} = \min\{\mu \mid \mu \in \sigma(Q^\dagger B^T B) \setminus \{0\}\}$, $\mu_{max} = \max\{\mu \mid \mu \in \sigma(Q^\dagger B^T B) \setminus \{0\}\}$, and the corresponding optimal convergence factor of the USSOR method is

$$v(H(\omega_{1opt}, \omega_{2opt})) = \frac{\sqrt{\mu_{max}} - \sqrt{\mu_{min}}}{\sqrt{\mu_{max}} + \sqrt{\mu_{min}}}.$$

Proof. Notice

$$\begin{aligned} & \frac{\partial \lambda_1(\mu_1, \mu_2)}{\partial \mu_1} \\ &= \frac{\sqrt{\mu_2 - \mu_{min}} + \sqrt{\mu_1 - \mu_{min}}}{\sqrt{\mu_1} + \sqrt{\mu_2}} \frac{\sqrt{\mu_1\mu_2} + \mu_{min} - \sqrt{(\mu_1 - \mu_{min})(\mu_2 - \mu_{min})}}{\sqrt{\mu_1(\mu_1 - \mu_{min})(\sqrt{\mu_1} + \sqrt{\mu_2})^2}}, \end{aligned} \tag{39}$$

and

$$\begin{aligned} & \frac{\partial \lambda_2(\mu_1, \mu_2)}{\partial \mu_1} \\ &= -\frac{\sqrt{\mu_{\max} - \mu_1} + \sqrt{\mu_{\max} - \mu_2}}{\sqrt{\mu_1} + \sqrt{\mu_2}} \frac{\sqrt{\mu_1 \mu_2} + \mu_{\max} - \sqrt{(\mu_{\max} - \mu_1)(\mu_{\max} - \mu_2)}}{\sqrt{\mu_1(\mu_{\max} - \mu_1)}(\sqrt{\mu_1} + \sqrt{\mu_2})^2}. \end{aligned} \tag{40}$$

Then it is easy to see

$$\frac{\partial \lambda_1(\mu_1, \mu_2)}{\partial \mu_1} > 0, \quad \frac{\partial \lambda_2(\mu_1, \mu_2)}{\partial \mu_1} < 0.$$

Similarly, it also holds

$$\frac{\partial \lambda_1(\mu_1, \mu_2)}{\partial \mu_2} > 0 \quad \text{and} \quad \frac{\partial \lambda_2(\mu_1, \mu_2)}{\partial \mu_2} < 0.$$

By the same technique of Theorem 2.5 in [2], the rest proof can be completed, here omitted. \square

4. Numerical experiments

In this section, we give some examples to illustrate the theoretical results of the USSOR method as a solver and a preconditioner by comparing its iteration steps (denoted as "IT"), elapsed CPU time in seconds (denoted as "CPU") and relative residual error (denoted as "RES") with GSSOR method and MSSOR method. All the computations are implemented in MATLAB 2012b on a PC computer with Intel (R) Core (TM) i7-6700HQ CPU @2.60 GHz 2.60 GHz, and 8.00 GB memory.

In our experiments, all runs with respect to each method are started from the zero initial guess.

Example 4.1. This example is similar to the example 4.1 in [9]. Consider the linear system $Bx = q$ with

$$B = \begin{pmatrix} B_{11} & 0 \\ B_{21} & 0 \end{pmatrix} \in \mathbb{R}^{m \times n},$$

where $B_{11} \in \mathbb{R}^{l \times l}$ is nonsingular, $0 \neq B_{21} \in \mathbb{R}^{(m-l) \times l}$, $m > n$. B_{11} and B_{21} are random matrices which can be generated by MATLAB function **rand**.

In Table 1, for various m and n , we list the theoretical optimal iteration parameters w_{opt} , w_{1opt} and w_{2opt} as well as the corresponding pseudo-spectral radii $\nu(H(\omega_{opt}))$ and $\nu(H(\omega_{1opt}, \omega_{2opt}))$, respectively. It is clear to see that the pseudo-spectral radii of the GSSOR [2] and the USSOR method are the same, and less than that of the MSSOR [12] method when the optimal parameters are employed. We find that the numerical efficiency of the GSSOR method and the USSOR method are quite close.

Example 4.2. In this example we test the USSOR method as a preconditioner to accelerate GMRES. Consider the linear system $Bx = q$, where B is the (2,1)-block matrix of the example 4.1 in [14], which comes from the discretization of Navier-Stokes equations by IFISS software with uniform grids. We perform GMRES, USSOR-preconditioned GMRES (abbreviated as "USSOR-GMRES"), GSSOR-preconditioned GMRES (abbreviated as "GSSOR-GMRES"), and MSSOR-GMRES (abbreviated as "MSSOR-GMRES"), respectively. In Table 2, after taking the optimal iteration parameters, we list numerical results with different grids, respectively. We see that the GSSOR-GMRES and USSOR-GMRES always outperform the MSSOR-GMRES.

Acknowledgements

The authors would like to thank the referees for their very detailed comments which greatly improved the presentation of this paper.

Table 1: Computational results for Example 4.1

| $rank(B_{11})$ | | 100 | 300 | 500 |
|----------------|--|----------|----------|----------|
| m | | 500 | 1000 | 3000 |
| n | | 300 | 800 | 2000 |
| MSSOR | ω_{opt} | 0.0649 | 0.0513 | 0.0265 |
| | $\nu(H(\omega_{opt}))$ | 0.9935 | 0.9949 | 0.9974 |
| | IT | 1615 | 4724 | 5812 |
| | CPU | 6.3106 | 78.1760 | 721.1901 |
| | $RES(10^{-6})$ | 9.9918 | 9.9810 | 9.9860 |
| GSSOR | ω_{1opt} | 0.0468 | 0.0287 | 0.0164 |
| | ω_{2opt} | 1.8840 | 1.1874 | 1.0673 |
| | $\nu(H(\omega_{1opt}, \omega_{2opt}))$ | 0.9763 | 0.9855 | 0.9918 |
| | IT | 1276 | 2179 | 4827 |
| | CPU | 3.3111 | 18.5150 | 268.9314 |
| USSOR | $RES(10^{-6})$ | 9.9849 | 9.9581 | 9.9926 |
| | ω_{1opt} | -37.3864 | -39.1191 | -62.9318 |
| | ω_{2opt} | 0.9752 | 0.9758 | 0.9918 |
| | $\nu(H(\omega_{1opt}, \omega_{2opt}))$ | 0.9763 | 0.9855 | 0.9918 |
| | IT | 1511 | 2561 | 4903 |
| | CPU | 4.4420 | 27.3290 | 432.5890 |
| | $RES(10^{-6})$ | 9.976 | 9.9997 | 9.7846 |

Table 2: Computational results for Example 4.2

| Method | Grid | 16×16 | 32×32 | 64×64 |
|-------------|----------------|----------------|----------------|----------------|
| GMRES | IT | 175 | 394 | 788 |
| | CPU | 0.4301 | 0.8312 | 3.0642 |
| | $RES(10^{-9})$ | 9.7559 | 9.9962 | 9.9598 |
| MSSOR-GMRES | IT | 33 | 53 | 95 |
| | CPU | 0.0728 | 0.2210 | 12.3814 |
| | $RES(10^{-9})$ | 4.8525 | 7.7510 | 702730 |
| GSSOR-GMRES | IT | 29 | 48 | 93 |
| | CPU | 0.1474 | 0.2253 | 11.1726 |
| | $RES(10^{-9})$ | 6.7965 | 9.9686 | 7.1364 |
| USSOR-GMRES | IT | 29 | 48 | 94 |
| | CPU | 0.0642 | 0.2123 | 10.2316 |
| | $RES(10^{-9})$ | 8.2702 | 8.9315 | 7.3399 |

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