An Iterative Method for Symmetric Positive Semidefinite Linear System of Equations

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Abstract

In this paper, a new two-step iterative method for solving symmetric positive semidefinite linear system of equations is presented. A sufficient condition for the semiconvergence of the method is also given. Some numerical experiments are presented to show the efficiency of the proposed method.

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1. Introduction

Consider the linear system of equations

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

where $A \in \mathbb{R}^{n\times n}$ is singular and $x, b \in \mathbb{R}^n$ with b known and x unknown. We assume that the system (1) is solvable, i.e., it has at least one solution. We frequently meet these kind of linear systems when we solve the actual problems in statistics, economics, differential equations, image and signal processing. For example, finite difference formulations of the Neumann problem and those for elastic bodies with free surfaces and Poisson's equation on a sphere and with periodic boundary conditions result in singular linear system of equations [2]. Also, the stationary probability distribution vector of a finite homogeneous Markov chain is a solution of a singular linear system of equations [10, 2]. Motivated by work in this area, we focus our attention on linear system of equations with symmetric positive semidefinite coefficient matrix and propose a two-step stationary iterative method for solving (1).

If A is split into $A = M - N$, where M is nonsingular, then a stationary iterative method for solving (1) can be described as follows

$$x_{m+1} = M^{-1}Nx_m + M^{-1}b, \quad m = 0, 1, \ldots. \tag{2}$$

Here the matrix $T = M^{-1}N$ is called the iteration matrix of the method. It is well known that for nonsingular systems the iterative method (2) is convergent if the spectral radius of T is less than 1, i.e., $\rho(T) < 1$. In this case, for any initial guess x_0 the method converges to the exact solution of (1) [1, 2, 6, 7, 12]. For singular systems the method is called semiconvergent if (2) converges to a solution of (1) for every initial guess x_0. By [2], it is well known that the iterative method (2) is semiconvergent if and only if

- $\rho(T) = 1$;
- index$(I - T) = 1$, which means that
  $\text{rank}(I - T) = \text{rank}(I - T)^2$;
- If $\mu \in \sigma(T)$ with $|\mu| = 1$, then $\mu = 1$, i.e.,
  $\upsilon(T) = \{|\mu|, \mu \in \sigma(T), \mu \neq 1\} < 1$,
  where $\sigma(T)$ is spectrum of T.

The semiconvergence of the the iterative method (2) has been investigated in many papers (from example see [3, 5, 11, 15]). Several theorems concerning semiconvergence of (2) have been presented by Song in [11]. Also, semiconvergence of extrapolated iterative methods have been discussed in [9, 10, 15].

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

2. New method and its semiconvergence properties

Let A be a symmetric positive semidefinite matrix. We write Eq. (1) in the following form

$$\alpha x + \beta x + Ax = (\alpha + \beta)x + b,$$

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

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

where x_0 and x_1 are two initial guesses and I is the identity matrix of order n. Let $\alpha > 0$. In this case, the matrix $\alpha I + A$ is symmetric positive definite and therefore, (3) can be written in the form

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

By some simple manipulation it can be seen that the $(m+1)$-th iteration of this procedure can be written as

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

which is equivalent to

$$\begin{cases} y_m = (\alpha I + A)^{-1}(r_m + \beta(x_m - x_{m-1})), \\ x_{m+1} = x_m + y_m, \end{cases} \tag{5}$$

where $r_m = b - Ax_m$. In [8], Salkuyeh and Fahim have used this procedure for refining an approximate solution of a symmetric positive definite linear system of equations. Next, we discuss the semiconvergence of the proposed method for solving (1) with symmetric positive semidefinite coefficient matrix A. We first present the following lemma which is similar to Lemma 5.8 in [1].

Lemma 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 $z_0 = \max\{|z_1|, |z_2|\} \le 1$ if and only if $|s| \le 1$ and $|r| \le 1 + s$.*

Proof. Assume first that $z_0 \le 1$. Then, from $z_1 z_2 = s$ we have

$$|s| = |z_1||z_2| \le z_0^2 \le 1.$$

Now we consider two following cases:

`Case 1`. If $r^2 < 4s$, then

$$|r| < 2\sqrt{s} \le 1 + s.$$

`Case 2`. If $r^2 \ge 4s$, then

$$z_0 = \frac{1}{2}|r| + \frac{1}{2}|r^2 - 4s|^{\frac{1}{2}}.$$

We claim that $|r| \le 1 + s$. Otherwise $|r| > 1 + s$, and we have

$$\begin{aligned} z_0 &= \frac{1}{2}|r| + |(\frac{r}{2})^2 - s|^{\frac{1}{2}} \\ &> \frac{1}{2}(1+s) + |(\frac{1+s}{2})^2 - s|^{\frac{1}{2}} \\ &= 1, \end{aligned}$$

which is a contradiction.

Conversely, assume that $|s| \le 1$ and $|r| \le 1+s$. Then

$$
\begin{aligned}
z_0 &= \frac{1}{2}|r| + |(\frac{r}{2})^2 - s|^{\frac{1}{2}} \\
&\le \frac{1}{2}(1+s) + |(\frac{1+s}{2})^2 - s|^{\frac{1}{2}} \\
&= \frac{1}{2}(1+s) + \frac{1}{2}|1-s| \\
&= 1.
\end{aligned}
$$

So the proof is completed. $\square$

Now, we state and prove the following theorem.

Theorem 1. *Let A be a symmetric positive semidefinite matrix and $\alpha > 0$. Then the iterative method defined by (5) is semiconvergent with any initial guesses x_0 and x_1 if $|\beta| < \alpha$.*

Proof. Consider the iterative method (5) and suppose that

$$
w_{m+1} = \begin{pmatrix} x_{m+1} \\ x_m \end{pmatrix}.
$$

Then, we have

$$
w_{m+1} = \begin{pmatrix} (\alpha+\beta)(\alpha I_n + A)^{-1} & -\beta(\alpha I_n + A)^{-1} \\ I_n & 0 \end{pmatrix} w_m + \begin{pmatrix} (\alpha I_n + A)^{-1} b \\ 0 \end{pmatrix},
$$

or

$$
w_{m+1} = \mathcal{A} w_m + \mathcal{C}, \quad m = 0, 1, \ldots, \tag{6}
$$

where

$$
\mathcal{A} = \begin{pmatrix} (\alpha+\beta)(\alpha I_n + A)^{-1} & -\beta(\alpha I_n + A)^{-1} \\ I_n & 0 \end{pmatrix}, \quad \mathcal{C} = \begin{pmatrix} (\alpha I_n + A)^{-1} b \\ 0 \end{pmatrix},
$$

in which I_n is the identity matrix of order n. It is easy to see that characteristic polynomial of $\mathcal{A}$ can be written as

$$
\prod_{\lambda \in \sigma(A)} \det \begin{pmatrix} \frac{\alpha+\beta}{\alpha+\lambda} - \mu & -\frac{\beta}{\alpha+\lambda} \\ 1 & -\mu \end{pmatrix} = 0,
$$

where $\mu \in \sigma(\mathcal{A})$ (see [1], page 173). This relation shows that for every $\lambda \in \sigma(A)$ we have

$$
\mu^2 - \gamma\mu + \delta = 0, \tag{7}
$$

where

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

Since the eigenvalues of A are nonnegative, from $|\beta| < \alpha$ we obtain

$$|\delta| = \frac{|\beta|}{\alpha+\lambda} < \frac{\alpha}{\alpha+\lambda} \leq 1,$$

and

$$|\gamma| = |\frac{\alpha+\beta}{\alpha+\lambda}| \leq \frac{\alpha+\beta}{\alpha+\lambda} = \frac{\alpha}{\alpha+\lambda} + \frac{\beta}{\alpha+\lambda} \leq 1+\delta,$$

Hence, according to Lemma 1, we have

$$\max\{|\mu_1|, |\mu_2|\} \leq 1, \tag{8}$$

where μ_1 and μ_2 are the roots of (7). Now, let

$$\mu = e^{i\theta} = \cos\theta + i\sin\theta$$

be a root of (7) where i is the imaginary unit. Substituting this into Eq. (7), yields

$$\sin 2\theta - \gamma\sin\theta = 0, \tag{9}$$

and

$$\cos 2\theta - \gamma\cos\theta + \delta = 0, \tag{10}$$

where $0 \leq \theta < 2\pi$. From (9), it follows that

$$\sin\theta = 0, \quad \text{or} \quad \cos\theta = \frac{\gamma}{2}.$$

If $\cos\theta = \frac{\gamma}{2}$, then from (10) we see that

$$2\cos^2\theta - 1 - \gamma\cos\theta + \delta = 0 \Rightarrow \delta = 1.$$

But, δ cannot be equal to 1, since from $|\beta| < \alpha$ and $\lambda \geq 0$, we have

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

Now let $\sin\theta = 0$. In this case $\mu = \cos\theta = \pm 1$. If $\mu = -1$, then from (7), we have $1+\gamma+\delta = 0$, which is impossible, since $\gamma \geq 0$ and $\delta \geq 0$. Therefore, $\rho(\mathcal{A}) = 1$ and if $|\mu| = 1$, then $\mu = 1$, i.e., $\upsilon(\mathcal{A}) < 1$.

Now, it is enough to show that $index(I - \mathcal{A}) = 1$, or equivalently $rank(I - \mathcal{A}) = rank(I - \mathcal{A})^2$. Let $p = 2n$. We have

$$
\begin{aligned}
I_p - \mathcal{A} &= \begin{pmatrix} I_n - (\alpha+\beta)(\alpha I_n + A)^{-1} & \beta(\alpha I_n + A)^{-1} \\ -I_n & I_n \end{pmatrix} \\
&= \begin{pmatrix} (\alpha I_n + A)^{-1}(A - \beta I_n) & \beta(\alpha I_n + A)^{-1} \\ -I_n & I_n \end{pmatrix} \\
&= \begin{pmatrix} (\alpha I_n + A)^{-1} & 0 \\ 0 & I_n \end{pmatrix} \begin{pmatrix} A - \beta I_n & \beta I_n \\ -I_n & I_n \end{pmatrix},
\end{aligned} \tag{11}
$$

where I_r is the identity matrix of order r. Let

$$
\mathcal{S} = \begin{pmatrix} (\alpha I_n + A)^{-1} & 0 \\ 0 & I_n \end{pmatrix}, \qquad \mathcal{T} = \begin{pmatrix} A - \beta I_n & \beta I_n \\ -I_n & I_n \end{pmatrix}.
$$

Since $\mathcal{S}$ is a nonsingular matrix, from (11) we have

$$
\begin{aligned}
rank(I_p - \mathcal{A}) &= rank(\mathcal{S}\mathcal{T}) \\
&= rank \begin{pmatrix} A - \beta I_n & \beta I_n \\ -I_n & I_n \end{pmatrix} \\
&= rank \begin{pmatrix} A & \beta I_n \\ 0 & I_n \end{pmatrix} \\
&= n + rank(A).
\end{aligned}
$$

On the other hand,

$$
rank(I - \mathcal{A})^2 = rank(\mathcal{S}\mathcal{T}\mathcal{S}\mathcal{T}) = rank(\mathcal{T}\mathcal{S}\mathcal{T}).
$$

Straightforward computation reveals that

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

Since $A - \beta I_n$ commutes with $(\alpha I_n + A)^{-1}$, it follows that

$$
\begin{aligned}
\mathcal{T}\mathcal{S}\mathcal{T} &= \begin{pmatrix} (\alpha I_n + A)^{-1}(A - \beta I_n)^2 - \beta I_n & \beta(\alpha I_n + A)^{-1}(A - \beta I_n) + \beta I_n \\ -(\alpha I_n + A)^{-1}(A - \beta I_n) - I_n & -\beta(\alpha I_n + A)^{-1} + I_n \end{pmatrix} \\
&= \begin{pmatrix} (\alpha I_n + A)^{-1} & 0 \\ 0 & (\alpha I_n + A)^{-1} \end{pmatrix} \\
&\quad \times \begin{pmatrix} (A - \beta I_n)^2 - \beta(\alpha I_n + A) & \beta(A - \beta I_n) + \beta(\alpha I_n + A) \\ -(A - \beta I_n) - (\alpha I_n + A) & -\beta + (\alpha I_n + A) \end{pmatrix}
\end{aligned}
$$

$$= \begin{pmatrix} (\alpha I_n + A)^{-1} & 0 \\ 0 & (\alpha I_n + A)^{-1} \end{pmatrix}$$
$$\times \begin{pmatrix} A^2 - 3\beta A + \beta(\beta-\alpha)I_n & 2\beta A + \beta(\alpha-\beta)I_n \\ -2A + (\beta-\alpha)I_n & A + (\alpha-\beta)I_n \end{pmatrix}$$

Assume that R_i and C_i denote the ith block-row and block-column of the matrix $\mathcal{A}$, respectively. Then, we have

$$\begin{aligned}
rank(\mathcal{TST}) &= rank \begin{pmatrix} A^2 - 3\beta A + \beta(\beta-\alpha)I_n & 2\beta A + \beta(\alpha-\beta)I_n \\ -2A + (\beta-\alpha)I_n & A + (\alpha-\beta)I_n \end{pmatrix} \xrightarrow{R_1 := R_1 - \beta R_2} \\
&= rank \begin{pmatrix} A^2 - \beta A & \beta A \\ -2A + (\beta-\alpha)I_n & A + (\alpha-\beta)I_n \end{pmatrix} \xrightarrow{C_1 := C_1 + C_2} \\
&= rank \begin{pmatrix} A^2 & \beta A \\ -A & A + (\alpha-\beta)I_n \end{pmatrix} \xrightarrow{C_2 := C_1 + C_2} \\
&= rank \begin{pmatrix} A^2 & \beta A + A^2 \\ -A & (\alpha-\beta)I_n \end{pmatrix} \xrightarrow{C_1 := C_1 + \frac{1}{\alpha-\beta} A \times C_2} \\
&= rank \begin{pmatrix} A^2(\frac{\alpha}{\alpha-\beta} I_n + A) & \beta A + A^2 \\ 0 & (\alpha-\beta)I_n \end{pmatrix} \\
&= n + rank(A^2) \\
&= n + rank(A).
\end{aligned}$$

Here, it is mentioned that $rank(A) = rank(A^2)$ and $\alpha - \beta \neq 0$. Therefore, the proof of this theorem is completed. $\square$

For $\beta = 0$, Eq. (5) is reduced to

$$\begin{cases} y_m = (\alpha I + A)^{-1} r_m, \\ x_{m+1} = x_m + y_m. \end{cases} \tag{12}$$

which is equivalent to the method presented by Wu et al. in [13] for refining an approximate solution of ill-conditioned symmetric positive definite linear system of equation. According to Theorem 1, this method is semiconvergent with any initial guess x_0 for symmetric positive semidefinite linear system of equations. In practice, for an initial guess x_0, we first compute x_1 using (12) and then x_m, $m = 2, 3, \ldots$, are computed via (5). Moreover, the computation of y_m in (12) are done by the Cholesky factorization of $\alpha I + A$.

3. Numerical experiments

All the numerical results presented in this section were computed by a MATLAB code in double precision. We use

$$\frac{\|r_m\|_2}{\|r_0\|_2} < 10^{-10},$$

as the stopping criterion, where $r_k = b - Ax_k$. For each example, we report the forward stability factors (see [4], for more details) for the computed solutions x_m and the exact solution x_* to (1), i.e.

$$\eta_m = \frac{\|x_m - x_*\|_2}{\kappa(A)\|x_*\|_2},$$

where

$$\kappa(A) = \|A\|_2 \|A^\dagger\|_2, \tag{13}$$

in which $A^\dagger$ is the pseudoinverse (the Moore-Penrose inverse) of A [6].

Example 1. Consider the linear system of equations $Ax = b$, where

$$A = \begin{pmatrix} 3 & 1 & 0 & 0 & 1 \\ 1 & 4 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 3 \end{pmatrix}, \qquad b = \begin{pmatrix} 5 \\ 8 \\ 4 \\ 4 \\ 7 \end{pmatrix}.$$

The matrix A is symmetric positive semidefinite with $\kappa(A) = 9.90$ and $b = A(1,1,1,1,1)^T$. Hence, this system is solvable and $x_* = (1,1,1,1,1)^T$ is a solution of this system. Let x_0 be the zero vector, $\alpha = 0.5$ and $\beta = 0.1$. In this case, the method is semiconvergent in 17 iterations, and the approximate solution is

$$x_{17} = \begin{pmatrix} 0.99999999966640 \\ 1.00000000029093 \\ 0.99999999942429 \\ 0.99999999942429 \\ 1.00000000050225 \end{pmatrix}.$$

Here we have $\eta_{17} = 4.76 \times 10^{-11}$. For the same initial guess, $\alpha = 0.5$ and $\beta = 0$ the method is semiconvergent in 25 iterations,

$$x_{25} = \begin{pmatrix} 0.99999999965409 \\ 1.00000000030173 \\ 0.99999999940301 \\ 0.99999999940301 \\ 1.00000000052074 \end{pmatrix}.$$

and we have $\eta_{25} = 4.94 \times 10^{-11}$.

We now change the entry $(1,1)$ of A to 10^6. In this case, we have $\kappa(A) = 1.17 \times 10^6$. All of the other assumptions are as before. The method with $\alpha = 0.5$ and $\beta = 0.1$ is semiconvergent in 7 iterations, and the computed solution is

$$x_7 = \begin{pmatrix} 1.00000000004902 \\ 0.99998472311991 \\ 1.00004250039264 \\ 1.00004250039264 \\ 0.99996625348584 \end{pmatrix}.$$

Here, the forward stability factor is $\eta_7 = 2.70 \times 10^{-11}$. If we set $\alpha = 0.5$ and $\beta = 0$ then the method is semiconvergent in 9 iterations and we have $\eta_9 = 2.52 \times 10^{-11}$. Moreover, the provided approximate solution by the proposed method is

$$x_9 = \begin{pmatrix} 0.99999999995425 \\ 1.00001594593278 \\ 0.99996004378370 \\ 0.99996004378370 \\ 1.00002979926269 \end{pmatrix}.$$

An observation which can be posed here is that the computed solution for the latter system of linear equations is less accurate than the previous one, since it is more ill-conditioned.

Example 2. Consider the $n \times n$ matrix

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & \\ 1 & 2 & 2 & 1 & & & \\ 1 & 2 & 3 & 2 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 1 & 2 & 3 & 2 & 1 \\ & & & 1 & 2 & 3 & 2 \\ & & & & 1 & 2 & 2 \end{pmatrix}.$$

It can be seen that this matrix is symmetric positive semidefinite for every $n \in \mathbb{N}$. Let $b = A(1,1,\ldots,1)^T$. In this case, $x_* = (1,1,\ldots,1)^T$ is a solution of the system $Ax = b$. The condition number of A, number of iterations for the semiconvergence (denoted by "Iters"), and the corresponding forward stability factor of the proposed method with $(\alpha,\beta) = (0.5, 0.45)$ and $(\alpha,\beta) = (0.5, 0)$ for four values of n are given in Table 1. All of the assumptions are as the previous

Table 1: Numerical results for Example 2.

n	20	40	60	80
$\kappa(A)$	4.80×10^2	1.99×10^3	4.52×10^3	7.77×10^3
Iters ($\beta = 0$)	385	908	2649	4202
η_m	9.26×10^{-11}	9.71×10^{-11}	9.81×10^{-11}	9.86×10^{-11}
Iters ($\beta = 0.45$)	148	150	204	318
η_m	9.16×10^{-11}	2.03×10^{-11}	9.25×10^{-11}	9.66×10^{-11}

example. For $n = 40$, we have found that the system has an another solution of the form

$$\tilde{x}_* = \frac{1}{27} \begin{pmatrix} 26 & 27 & 28 & 26 & 27 & 28 & \dots & 26 & 27 & 28 & 26 \end{pmatrix}^T \in \mathbb{R}^{40},$$

and the method with the zero initial guess converges to it. Now let

$$x_0 = \begin{pmatrix} 0 & 1 & 0 & 1 & \dots & 0 & 1 \end{pmatrix}^T \in \mathbb{R}^{40}.$$

In this case, with $(\alpha, \beta) = (0.5, 0.45)$ the method converges to x_* in 186 iterations ($\eta_{186} = 3.83 \times 10^{-11}$) and with $(\alpha, \beta) = (0.5, 0)$ it converges in 1398 iterations ($\eta_{1398} = 4.86 \times 10^{-11}$). As we observe the proposed method is quite suitable for linear system of equations with symmetric positive semidefinite coefficient matrix. Moreover the proposed method is superior to the method proposed by Wu et al. in [13].

Example 3. Let

$$B = \begin{pmatrix} 0 & 1 & & & & \\ q & 0 & p & & & \\ 0 & q & 0 & p & & \\ & & \ddots & \ddots & \ddots & \\ & & & q & 0 & p \\ & & & & 1 & 0 \end{pmatrix} \in \mathbb{R}^{n \times n},$$

where $p, q > 0$ and $p + q = 1$. This matrix is singular (see [15]). We assume that $A = 10^6 e_1 e_1^T + B^T B$, where e_1 is the first column of the identity matrix of order n, $b = A(1, 1, \dots, 1)^T$, and $p = 0.5$. Therefore $x_* = (1, 1, \dots, 1)^T$ is a solution of this system. Obviously, A is symmetric positive semidefinite. Number of iterations ("Iters") for the semiconvergence with $\alpha = 0.5$ and three values of

Table 2: Numerical results for Example 3.

		Iters (η_m)		
n	$\kappa(A)$	$\beta = 0$	$\beta = 0.2$	$\beta = 0.4$
500	1.01×10^{11}	$215(4.34 \times 10^{-14})$	$129(4.35 \times 10^{-14})$	$42(4.41 \times 10^{-14})$
1000	4.05×10^{11}	$215(7.67 \times 10^{-15})$	$129(7.68 \times 10^{-15})$	$42(7.79 \times 10^{-15})$
1500	9.11×10^{11}	$215(2.78 \times 10^{-15})$	$129(2.78 \times 10^{-15})$	$42(2.83 \times 10^{-15})$
2000	1.62×10^{12}	$215(1.36 \times 10^{-15})$	$129(1.36 \times 10^{-15})$	$42(2.38 \times 10^{-15})$

β ($= 0, 0.2$ and 0.4) are given in Table 2. The condition number of the matrices and the forward stability factors (in parenthesis) are also presented in this table. As we see the systems of linear equations are very ill-conditioned and the method is quite suitable to solve them.

4. Conclusion

In this paper, we have presented a new two-step iterative method for solving system of linear equations with symmetric positive semidefinite coefficient matrix. The proposed method involves two parameters and we have found a region for the semiconvergence of the method. Numerical results presented in this paper show that the method is efficient.

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