

The worst-case scenario in nonlinear matrix equations

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Abstract—The worst situation in computing the solution X of a matrix equation $F(X) = 0$ arising in Markov models is the close-to-null-recurrent case, which occurs when the derivative of F at X is near to a singular matrix. When the derivative of F at X is singular (null recurrent case), the problem is ill-conditioned and the convergence of the algorithms based on matrix iterations is slow; however, there exist some techniques to remove the singularity and restore well-conditioning and fast convergence. This phenomenon is partially shown also in the close-to-null-recurrent case, but the techniques used for the null recurrent case cannot be applied to this setting.

Two methods to accelerate the convergence and amend the conditioning in close-to-null-recurrent cases for certain matrix equations are presented. The numerical experiments confirm the efficiency of the new methods.

Index Terms—nonsymmetric algebraic Riccati equation, unilateral quadratic matrix equation, shift technique, close-to-null-recurrent case, Möbius transform

I. INTRODUCTION

In certain Markov models the computation of the stationary probability is reduced to the solution of a nonlinear matrix equation. For instance, the computation of the stationary probability of a M/G/1 queue with a finite number of states is reduced to the solution of a Unilateral Matrix Equation (UME)

$$\sum_{i=0}^k A_i X^i = 0, \quad (1)$$

where, setting $B_1 = A_1 + I$ and $B_i = A_i$ for $i \neq 1$, one has that $B_i \in \mathbb{C}^{n \times n}$ have nonnegative elements and $\sum_{i=0}^k B_i$ is a stochastic matrix, in particular for $k = 2$ one has a QBD model (see [1], [2]).

Another important example arises in the study of fluid queues where the equation to be solved is a Nonsymmetric Algebraic Riccati Equation (NARE)

$$XCX - AX - XD + B = 0, \quad (2)$$

where $X, B \in \mathbb{C}^{m \times n}$, $A \in \mathbb{C}^{m \times m}$, $C \in \mathbb{C}^{n \times m}$, $D \in \mathbb{C}^{n \times n}$, and

$$M = \begin{bmatrix} D & -C \\ -B & A \end{bmatrix}$$

is either a nonsingular or a singular irreducible M-matrix (see [3]).

The solutions of these equations can be put in correspondence with the invariant subspaces of some matrix polynomial.

It is well known that the UME (1) is strictly related to the matrix polynomial $p(\lambda) = \sum_{i=0}^k A_i \lambda^i$. More precisely, the eigenvalues of any solution X of (1) are a subset of the roots of the matrix polynomial $p(\lambda)$, i.e., the solutions of the scalar equation $\det(p(\lambda)) = 0$, say $\lambda_1, \dots, \lambda_{kn}$, where some of the λ_i 's are set to ∞ if $\det(p(\lambda))$ has degree lower than kn . Moreover, there is a one-to-one correspondence between solutions of (1) and sets of linearly independent Jordan chains of $p(\lambda)$ (see [4]). In the M/G/1 queueing model the roots can be ordered by increasing modulus such that

$$|\lambda_0| \leq \dots \leq |\lambda_{n-1}| \leq \lambda_n \leq 1 \leq \lambda_{n+1} \leq |\lambda_{n+2}| \leq \dots, \quad (3)$$

that is, there are n roots inside the closed unit disk and the others are outside, and the *central eigenvalues*, λ_n and λ_{n+1} , are real [2]. We are interested in computing the solution whose eigenvalues have minimum modulus, which turns out to be the minimal element-wise nonnegative solution.

Similarly, the solutions of the NARE (2) are strictly related to the invariant subspaces of the matrix

$$H = \begin{bmatrix} D & -C \\ B & -A \end{bmatrix}. \quad (4)$$

More precisely, a matrix X is a solution of (2) if and only if the columns of $W = \begin{bmatrix} I \\ X \end{bmatrix}$ span an invariant subspace of H , in particular $HW = W(D - CX)$. In this case, the eigenvalues of $D - CX$ are a subset of the eigenvalues of H . In the fluid queueing models the eigenvalues can be ordered by decreasing real part such that

$$\operatorname{Re} \lambda_1 \geq \dots \geq \operatorname{Re} \lambda_{n-1} > \lambda_n \geq 0 \geq \lambda_{n+1} > \dots \geq \operatorname{Re} \lambda_{m+n},$$

that is, n eigenvalues belong to the closed left half plane and the others to the closed right half plane, and the *central eigenvalues*, λ_n and λ_{n+1} , are real and separated from the other eigenvalues. We are interested in computing the solution such that the eigenvalues of $D - CX$ are the leftmost eigenvalues of H . This solution turns out to be the minimal element-wise nonnegative solution (see [5]).

Equations (1) and (2) are usually solved by some matrix iteration, e.g., the Logarithmic Reduction (LR) [2], the Cyclic Reduction (CR) [6] or the Structure-preserving Doubling Algorithm (SDA) [7], [8], whose limit yields the required solution.

Both the conditioning of the equations and the convergence speed of the algorithms are strictly related to the gap between the central eigenvalues defined as $\text{gap}_p = |\lambda_n/\lambda_{n+1}| \leq 1$ for (1) — or for the associated matrix polynomial $p(\lambda)$ — and as $\text{gap}_H = \lambda_n - \lambda_{n+1}$ for equation (2) — or for the matrix H .

If $\text{gap}_p = 1$ — that is, in probabilistic terms, in the null recurrent case — then the minimal nonnegative solution of equation (1) is ill-conditioned and the convergence of iterations such as CR and SDA, which is quadratic in the generic case, turns to linear; the same happens to (2) if $\text{gap}_H = 0$. We speak of critical case, since in these cases the required solution is critical. In such critical cases the shift technique of [8], [9] restores quadratic convergence and reduces the ill-conditioning.

However, ill-conditioning and slow convergence appear also in the near-critical case, that is, in the close-to-null-recurrent case (weakly transient or weakly positive recurrent), or, in terms of the eigenvalues, when $\text{gap}_p \approx 1$ ($\text{gap}_H \approx 0$). This is the worst-case scenario in matrix equations since the numerical solution of the matrix equations is problematic and the shift technique cannot be used.

In this paper we present two techniques to handle the near-critical case. The first technique is applied to (1) when many eigenvalues are near to 1 and is based on the Möbius transform of the complex plane and aims to increase the gap. The second technique is applied to (2) when the central eigenvalues are well separated from the others and is based on the computation of the invariant subspace corresponding to both central eigenvalues and the accurate computation of their eigenvectors in this small subspace.

II. MÖBIUS TRANSFORMS APPLIED TO MATRIX POLYNOMIALS AND MATRICES

a) Analysis: We want to describe how to apply a linear rational function, also called Möbius transform, to the UME and how this can be used for computing the minimal solution.

Define the Möbius transform of parameters α, β, γ and δ — where we assume that $\alpha\delta - \beta\gamma \neq 0$ — as

$$\mathcal{M} : \mathbb{C} \rightarrow \mathbb{C}, \quad z \rightarrow \frac{\alpha + \beta z}{\gamma + \delta z}. \quad (5)$$

For $z \neq -\gamma/\delta$, \mathcal{M} is invertible and $\mathcal{M}^{-1}(z) = \frac{\alpha - \gamma z}{\delta z - \beta}$.

If a square matrix H has no eigenvalue equal to $-\gamma/\delta$, then the Möbius transform of H is $\mathcal{M}(H) = (\alpha I + \beta H)(\gamma I + \delta H)^{-1}$. The eigenvalues of $\mathcal{M}(H)$ are the images of the eigenvalues of H under the Möbius transform, thus no eigenvalue of $\mathcal{M}(H)$ can be β/δ . In the case of matrix polynomials the transform is more complicated.

Define \mathcal{P}_k as the quotient space of matrix polynomials of degree at most k modulo the following relation: $a(z), b(z) \in \mathcal{P}_k$ are equivalent if $a(z) = \tau b(z)$, for a nonzero constant τ . This is a meaningful setting since we are interested in the roots and the Jordan chains of a matrix polynomial, which do not change up to a multiplication of the polynomial by a nonzero constant.

The Möbius transform \mathcal{M} yields a map $\widehat{\mathcal{M}}$ from \mathcal{P}_k to \mathcal{P}_k : let $\varphi(z)$ be a matrix polynomial of degree k , then $\widehat{\mathcal{M}}(\varphi(z)) = (\delta z - \beta)^k \varphi(\mathcal{M}^{-1}(z))$. This function is well defined since $\widehat{\mathcal{M}}(k\varphi(z)) = k\widehat{\mathcal{M}}(\varphi(z))$.

Observe that

$$\begin{aligned} \widehat{\mathcal{M}}(A - \lambda I) &= (\delta \lambda - \beta) (A - \mathcal{M}^{-1}(\lambda)I) \\ &= (\gamma I + \delta A)\lambda - (\alpha I + \beta A) = (\mathcal{M}(A) - \lambda I)(-\gamma I - \delta A). \end{aligned}$$

The following result shows how the solutions of a UME change under a Möbius transform applied to the corresponding matrix polynomial.

Theorem 1. *Let $p(\lambda) = \sum_{i=0}^k A_i \lambda^i$ and $q(\lambda) = \widehat{\mathcal{M}}(p(\lambda)) = \sum_{i=0}^k B_i \lambda^i$. If $\sum A_i X^i = 0$, and $-\gamma/\delta$ is not an eigenvalue of X , then $\sum B_i \mathcal{M}(X)^i = 0$.*

Proof: Observe that $q(\lambda) = \sum_{i=0}^k B_i \lambda^i = \sum_{i=0}^k A_i (\mathcal{M}^{-1}(\lambda))^i (\delta \lambda - \beta)^k$ and thus $\sum_{i=0}^k B_i \mathcal{M}(X)^i = \left(\sum_{i=0}^k A_i X^i \right) (\delta \mathcal{M}(X) - \beta I)^k = 0$. Since β/δ cannot be an eigenvalue of $\mathcal{M}(X)$, the matrix $(\mathcal{M}(X) - \beta I)$ is invertible and the proof is completed. ■

b) QBD models: Now let us consider for simplicity the case which models QBD queues, in which the matrix polynomial has degree 2. Let $p(\lambda) := A\lambda^2 + B\lambda + C$ be a quadratic matrix polynomial whose ordered eigenvalues λ_i , $i = 1, \dots, 2n$, verify (3) and at least one between λ_n and λ_{n+1} is different from one (noncritical case).

For each $0 < a < 1$, there exists a unique Möbius transform $\mathcal{M}(z)$ which fixes the unit circle, for which the unit disk is invariant and such that $\mathcal{M}(a) = 0$, that is

$$\mathcal{M}(z) = \frac{z - a}{1 - az}. \quad (6)$$

On one hand, the function $\mathcal{M}(z)$ moves the points in a neighborhood of the point 1 far from the circle. On the other hand, $\mathcal{M}(z)$ moves the points in a neighborhood of the point -1 near to the circle. This can be used to let the gap of a quadratic matrix polynomial increase, when there are some roots near to 1 and no roots near to -1 , which is a typical situation in applications.

If $|\lambda_{n-1}| < \lambda_n$ and the eigenvalues outside the unit disk are not too near to the unit circle, then there exists $-1 < a < 1$ such that applying $\mathcal{M}(z)$ to $p(\lambda)$ yields a new quadratic matrix polynomial $q(\lambda) := \widehat{\mathcal{M}}(p(\lambda))$ such that

$$\text{gap}_q > \text{gap}_p,$$

where a can be relatively large if $\lambda_1, \dots, \lambda_{n-1}$ are well separated in modulus from λ_n or all the roots of $p(\lambda)$ have nonnegative real part.

It is easy to derive an expression for the polynomial q from the polynomial p for $-1 < a < 1$. Observe that $\mathcal{M}^{-1}(t) = \frac{t+a}{1+ta}$, so

$$q(\lambda) = (1 + \lambda a)^2 p(\mathcal{M}^{-1}(\lambda)) = (1 + \lambda a)^2 p((\lambda + a)/(1 + \lambda a));$$

- 1: Set $A_0 = A + aB + a^2C$, $B_0 = 2aA + (a^2 - 1)B - 2aC$,
 $C_0 = a^2A + aB + C$, $\widehat{B}_0 = B_0$;
- 2: **repeat** {CR step}
- 3: $A_{k+1} = -A_k B_k^{-1} A_k$
- 4: $B_{k+1} = B_k - A_k B_k^{-1} C_k - C_k B_k^{-1} A_k$
- 5: $C_{k+1} = -C_k B_k^{-1} C_k$
- 6: $\widehat{B}_{k+1} = \widehat{B}_k - A_k B_k^{-1} C_k$
- 7: **until** $\|A_{k+1}\| \leq \varepsilon$
- 8: Recover $X \approx -(\widehat{B}_k - aC_0)^{-1}(C_0 - a\widehat{B}_k)$.

Fig. 1. Algorithm 1: Solution of a near-critical UME

δ	gap	a	CR its, res	Algorithm 1 its, res
10^{-2}	0.970	0.5	11, 8.4e-16	9, 5.1e-16
10^{-3}	0.997	0.5	14, 7.5e-16	12, 8.5e-16
10^{-4}	0.999	0.5	17, 4.3e-16	15, 7.8e-16

Fig. 2. Number of iterations and relative residual for Algorithm 1 vs. CR on a random QBD

after some simple manipulations one has

$$q(\lambda) = (A + aB + a^2C)\lambda^2 + (2aA + (1 + a^2)B + 2aC)\lambda + a^2A + aB + C. \quad (7)$$

Any numerical algorithm like SDA or CR can be used after the Möbius transform. At the end, the solution of the original equation can be recovered. For the CR, one has Algorithm 1.

Using this technique to reduce the gap of a quadratic UME and then get a new equation with better conditioning has a drawback: since the solution of the well-conditioned transformed equation is $\mathcal{M}(X)$, in order to recover X from $\mathcal{M}(X)$, it is necessary to perform an inverse Möbius transform which may be very ill-conditioned. Fortunately, in some algorithms, like CR, there is no need to compute $\mathcal{M}(X)$ but the original solution can be obtained by a different, numerically stabler, formula (see line 8 of Algorithm 1).

The cost per step of Algorithm 1 is the same as the customary CR while the number of steps needed for convergence in the practical examples is reduced.

c) *Computational results:* We tested Algorithm 1 on a QBD described in [10] where A, M, C , are nonnegative matrices of size 32 such that $A + M + C$ is stochastic and $B = M - I$. The gap depends on the parameter δ used in [10]. We measured the residual of the computed solution and the number of CR iterations needed to get $\|A_{k+1}\|_1 \leq \varepsilon = 10^{-12}$ for certain values of δ . The results are reported in Figure 2.

III. A SHIFT TECHNIQUE FOR THE NONSINGULAR CASE

d) *Analysis:* In its original formulation [8], the shift technique for (2) relies on the fact that 0 is an eigenvalue of both M and H ; thus it can be applied only to critical problems. In the near-critical case, we have instead two small eigenvalues on the two sides of the imaginary axis. We shall describe a modification of the shift technique to compute the minimal solution to a NARE (2) in which the criticality is due only to a pair of eigenvalues very close to zero, which give rise to a very small $\text{gap}_H = \varepsilon$. In this case, we can

assume that all the other eigenvalues λ_i , $i \notin \{n, n+1\}$ satisfy $\|\lambda_i\| \geq |\text{Re}(\lambda_i)| \geq \delta$. A real-life example of this setting is the structured NARE appearing in transport theory [11], [12].

Let v_i (resp. u_i) be the right (resp. left) eigenvector associated with λ_i . Let VR_V (resp. UR_U) be a thin QR factorization (see [13, Chapter 5]) of the $(n+m) \times 2$ matrix $\begin{bmatrix} v_n & v_{n+1} \\ u_n & u_{n+1} \end{bmatrix}$ (resp. $\begin{bmatrix} u_n & u_{n+1} \end{bmatrix}$) with $\text{diag}(R_V) \geq 0$ ($\text{diag}(R_U) \geq 0$), such as the one produced by the Modified Gram-Schmidt algorithm [13, Algorithm 5.2.5].

Let $M = V^T H V$, and $\widetilde{H} = H + sVMU^T$ for a suitable real value $s > 0$ (the ‘‘shift’’). Let $(\widetilde{\lambda}_n, \widetilde{x}_n), (\widetilde{\lambda}_{n+1}, \widetilde{x}_{n+1})$ be the two eigenpairs of $V^T \widetilde{H} V = V^T H V + sMU^T V$. Direct computations using $\det(R_U) > 0, \det(R_V) > 0$ show that $\det(V^T \widetilde{H} V) \leq 0$, thus we may suppose that $\widetilde{\lambda}_n \geq 0$ and $\widetilde{\lambda}_{n+1} \leq 0$.

Let for brevity be $\widetilde{v}_i := V\widetilde{x}_i$ for $i \in \{n, n+1\}$. Then, one can see that the eigenpairs of \widetilde{H} are $(\widetilde{\lambda}_i, \widetilde{v}_i)$ for $i \in \{n, n+1\}$, plus (λ_i, v_i) for $i \notin \{n, n+1\}$. Similarly, the left eigenvectors of \widetilde{H} are $\widetilde{u}_i^T = \widetilde{y}_i^T U^T$, $i \in \{n, n+1\}$, where the y_i^T are the left eigenvectors of $U^T H U + sU^T V M$, plus all the left eigenvalues u_i^T of H , where $i \notin \{n, n+1\}$.

When s is large enough, $\widetilde{\lambda}_n$ and $\widetilde{\lambda}_{n+1}$ are larger than δ , therefore the gap of the NARE associated with \widetilde{H} is 2δ ; i.e., this NARE is not near-critical.

e) *Solution form:* From the minimal solution \widetilde{X} to the NARE associated with \widetilde{H} , we may compute the minimal solution X to the original critical NARE.

Theorem 2. *Let X be the minimal solution of the NARE associated with H , and \widetilde{X} the solution of the NARE associated with \widetilde{H} . Using the notation of the previous paragraphs, we have*

$$X = \widetilde{X} + r(\Delta v_2 - \widetilde{X} \Delta v_1) \widetilde{u}_n^T \widetilde{W}, \quad (8)$$

with

$$\widetilde{W} = \begin{bmatrix} I \\ \widetilde{X} \end{bmatrix}, \quad r = \left(1 + \widetilde{u}_n^T \widetilde{W} \Delta v_1\right)^{-1},$$

where $\Delta v := v_n - \widetilde{v}_n = [\Delta v_1^T \quad \Delta v_2^T]^T$.

Proof: The columns of the matrix \widetilde{W} form a basis of the stable space of \widetilde{H} , i.e., $\text{span}(v_1, \dots, v_n)$; what we need to build instead is a basis of the stable space of H , i.e., $\text{span}(v_1, \dots, v_{n-1}, v_n)$. Each column c_i of \widetilde{X} can be written as $c_i = \sum_{j=1}^{n-1} \alpha_j^{(i)} v_j + \alpha_n^{(i)} \widetilde{v}_n$. The left eigenvector \widetilde{u}_n^T of \widetilde{H} is such that $\widetilde{u}_n^T v_k = 0$ for $k = 1, \dots, n-1$ and $\widetilde{u}_n^T \widetilde{v}_n = 1$ (up to normalization), therefore $\widetilde{u}_n^T c_i = \alpha_n^{(i)}$. So $c_i + (\widetilde{u}_n^T c_i)(v_n - \widetilde{v}_n) = \sum_{j=1}^n \alpha_j^{(i)} v_j$ is a vector in the stable space of H .

It follows that the matrix

$$\widetilde{W} + (\Delta v) \widetilde{u}_n^T \widetilde{W}$$

is a matrix whose columns lie in the stable space of H . Let us suppose that its first block is nonsingular, so that it is indeed a basis. In order to compute the solution to the original equation X , we must invert the first block of this matrix, i.e.,

$$X = \left(\widetilde{X} + \Delta v_2 \widetilde{u}_n^T \widetilde{W} \right) \left(I + \Delta v_1 \widetilde{u}_n^T \widetilde{W} \right)^{-1}$$

- 1: Compute orthonormal bases U, V for the invariant subspaces corresponding to λ_n, λ_{n+1} , using an orthogonal subspace iteration on H^{-1}
- 2: Compute $\tilde{H} = H + s(VV^T H V U U^T)$
- 3: Solve the NARE associated with \tilde{H} , using SDA.
- 4: Compute $\tilde{u}_n, v_n, \tilde{v}_n$ by solving the two 2×2 eigenproblems $V^T \tilde{H} V, U^T \tilde{H} U$ and $V^T H V$.
- 5: Recover the solution to the original NARE X from the solution \tilde{X} using (8)

Fig. 3. Algorithm 2: solution of a near-critical NARE

We may find an explicit form for the inverse using the Sherman-Morrison formula; after some algebraic manipulations we obtain (8). ■

Therefore Algorithm 2 computes the solution to a near-critical NARE. Since the NARE associated with \tilde{H} is far from critical, we may expect that the number of SDA iterations needed in the solution of its associated NARE is lower than the number of iterations needed in the solution of the original NARE. The cost of the SDA in Step 3 is the dominant cost of the algorithm, since a step of subspace iteration costs $O((n+m)^2)$ arithmetic operations, and due to our assumptions on the localization of the central eigenvalues its convergence speed is controlled by $(\varepsilon/\delta)^k$ [13, Theorem 7.3.1].

f) Accuracy: Another crucial aspect of near-critical problems is the accuracy with which we can compute the solution. It is known [14] that the solution of a critical problem cannot be computed with better accuracy than $O(\sqrt{\mathbf{u}})$, where \mathbf{u} is the machine precision, while the solution of a non-critical one can be computed with precision $O(\mathbf{u})$. It is therefore to be expected that the constant hidden in the latter $O(\cdot)$ notation degrades as the problem approaches criticality. Where is this degradation to be expected in the above Algorithm 2?

Let us assume as a test case to have a perturbation of (2) such that $\lambda_n, \lambda_{n+1} \rightarrow 0$, while all the other eigenvalues satisfy $|\lambda_i| \geq \delta$. In this case, the computation of the orthogonal bases U and V stays tame, since the number of needed iterations is bounded. The NARE associated with \tilde{H} is far from critical, assuming a value s sufficiently large is chosen, in order to have $\tilde{\lambda}_n, \tilde{\lambda}_{n+1} > \delta$. Thus the only parts of the computation in which the ill-conditioning is reflected are the last two steps. As a result, in (8) the ill-conditioning appears only in the second summand. This allows more accurate computation of products in the form Xv , where v is a vector such that the second summand is very small. This is in contrast with the traditional algorithms, in which the solution is computed as a whole, and thus it is impossible to identify and compute the well-conditioned component of X along the subspaces orthogonal to the correction term.

In the case of a more general perturbation, the analysis is much more complicated, due to the fact that gap_H alone is not a good measure of the ill-conditioning of the problem, and more sophisticated notions of distance between subspaces are needed [13], [15].

n	c	α	SDA its	Algorithm 2 its
32	$1 - 10^{-3}$	10^{-3}	14	11
32	$1 - 10^{-6}$	10^{-8}	18	11
32	$1 - 10^{-12}$	10^{-12}	26	11
128	$1 - 10^{-3}$	10^{-3}	16	13
128	$1 - 10^{-6}$	10^{-8}	20	13

Fig. 4. Number of iterations for Algorithm 2 vs. SDA on the transport problem

g) Computational results: We tested Algorithm 2 on near-critical cases of the transport problem treated in [12], [11]. We measured the number of SDA iterations needed to get the relative residual below $\varepsilon = 10^{-12}$, for several matrix sizes $m = n$ and choices of the parameters c, α . We recall that the problem is critical for $(c, \alpha) = (1, 0)$. The results are reported in Figure 4.

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