Quadratic Vector Equations

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1 Introduction

In this paper, we aim to study in an unified fashion several quadratic vector and matrix equations with nonnegativity hypotheses. Specific cases of such problems have been studied extensively in the past by several authors. For references to the single equations and results, we refer the reader to the following sections, in particular section 3. Many of the results appearing here have already been proved for one or more of the single instances of the problems, resorting to specific characteristics of the problem. In some cases the proofs we present here are mere rewritings of the original proofs with a little change of notation to adapt them to our framework, but in some cases we are effectively able to remove some hypotheses and generalize the results by abstracting the specific aspects of each problem.

It is worth noting that Ortega and Rheinboldt [19, Chapter 13], in a 1970 book, treat a similar problem in a far more general setting, assuming only the monotonicity and operator convexity of the involved operator. Since their hypotheses are far more general than the ones of our problem, the obtained results are less precise than the one we are reporting here. Moreover, all of their proofs have to be adapted to our case, since the operator $F(x)$ we are dealing with is operator concave instead of convex.

Useful results In the following, $A \geq B$ (resp. $A > B$) means $A_{ij} \geq B_{ij}$ (resp. $A_{ij} > B_{ij}$) for all i, j. A real square matrix Z is said *Z-matrix* if $Z_{ij} \leq 0$ for all $i \neq j$. A Z-matrix is said an M-matrix if it can be written in the form $sI - P$, where $P \geq 0$ and $s \leq \rho(P)$ and $\rho(\cdot)$ denotes the spectral radius.

The following results are classical, see e.g. [3].

Theorem 1. *The following facts hold.*

1. *If Z is a Z-matrix and there exists a vector $v > 0$ such that $Zv \geq 0$, then Z is an M-matrix;*

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2. *If Z is a Z-matrix and $Z \geq M$ for an M-matrix $M \neq Z$, then Z is a nonsingular M-matrix.*

3. *A nonsingular Z-matrix Z is an M-matrix if and only if $Z^{-1} \geq 0$.*

2 General problem

We are interested in solving the equation

$$Mx = a + b(x, x) \tag{1}$$

(quadratic vector equation, QVE) where $M \in \mathbb{R}^{n \times n}$ is a nonsingular M-matrix, $a, x \in \mathbb{R}^n$, $a, x \geq 0$, and b is a nonnegative vector bilinear form, i.e., a map $b : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ such that

1. $b(v, \cdot)$ and $b(\cdot, v)$ are linear maps for each $v \in \mathbb{R}^n$ (bilinearity);

2. $b(x, y) \geq 0$ for all $x, y \geq 0$ (nonnegativity).

The map b can be represented by a tensor B_{ijk}, in the sense that $b(x, y)_k = \sum_{i,j=1}^{n} B_{ijk} x_i y_j$. It is easy to prove that $x \leq y$, $z \leq w$ implies $b(x, z) \leq b(y, w)$. If N is a nonsingular M-matrix, $N^{-1}B$ will denote the tensor representing the map $(x, y) \mapsto N^{-1}b(x, y)$. Note that, here and in the following, we do not require that b be symmetric (that is, $b(x, y) = b(y, x)$ for all x, y): while in the equation only the quadratic form associated to b is used, in the solution algorithms there are often terms of the form $b(x, y)$ with $x \neq y$. Since there are multiple ways to extend the quadratic form $b(x, x)$ to a bilinear map $b(x, y)$, this will leave more freedom in defining the actual solution algorithms.

We are only interested in nonnegative solutions $x^* \geq 0$; in the following, when referring to solutions of (1) we shall always mean *nonnegative* solutions only. A solution x^* of (1) is said *minimal* if $x^* \leq y^*$ for any other solution y^*.

Later on, we will give a necessary and sufficient condition for (1) to have a minimal solution.

3 Concrete cases

E1: Markovian binary trees in [2, 11], the equation

$$x = a + b(x, x),$$

with the assumption that $e = (1, 1, \ldots, 1)^T$ is a solution, arises from the study of Markovian binary trees.

E2: Lu's simple equation in [18, 17], the equation

$$\begin{cases} u = u \circ (Pv) + e, \\ v = v \circ (\tilde{P}u) + e, \end{cases}$$

where $u, v \in \mathbb{R}^m$ are the unknowns, e is as above, P and $\tilde{P}$ are two given nonnegative $m \times m$ matrices, and $a \circ b$ denotes the Hadamard (component-wise) product, arises as a special form of a Riccati equation appearing in a neutron transport problem. By setting $w := [u^T \, v^T]^T$, the equation takes the form (1).

E3: Nonsymmetric algebraic Riccati equation in [10], the equation

$$XCX + B - AX - XD = 0,$$

where $X, B \in \mathbb{R}^{m_1 \times m_2}$, $C \in \mathbb{R}^{m_2 \times m_1}$, $A \in \mathbb{R}^{m_1 \times m_1}$, $D \in \mathbb{R}^{m_2 \times m_2}$, and

$$\mathcal{M} = \begin{bmatrix} D & -C \\ -B & A \end{bmatrix} \tag{2}$$

is a nonsingular or singular irreducible M-matrix, is studied. Vectorizing everything, we get

$$(I \otimes A + D^T \otimes I) \operatorname{vec}(X) = \operatorname{vec}(B) + \operatorname{vec}(XCX),$$

which is in the form (1) with $n = m_1 m_2$.

E4: Unilateral quadratic matrix equation in several queuing problems [7], the equation

$$X = A + BX + CX^2,$$

with $A, B, C, X \in \mathbb{R}^{m \times m}$, $A, B, C \geq 0$, and $(A + B + C)e = e$, is considered. Vectorizing everything, we fall again in the same class of equations, with $n = m^2$: in fact, since $Be \leq e$, $(I - B)e \geq 0$ and thus $I - B$ is an M-matrix.

To ease the notation in the cases E3 and E4, in the following we shall set $x_k = \operatorname{vec}(X_k)$, and for E3 also $m = \max(m_1, m_2)$.

4 Minimal solution

Existence of the minimal solution It is clear by considering the scalar case ($n = 1$) that (1) may have no real solutions. The following additional condition will allow us to prove their existence.

Condition A1 There are a positive linear functional $l : \mathbb{R}^n \to \mathbb{R}^m$ and a vector $z \in \mathbb{R}^m$, $z \geq 0$ such that for any $x \geq 0$, it holds that $l(x) \leq z$ implies $l(M^{-1}(a + b(x, x))) \leq z$.

Theorem 2. *Equation* (1) *has at least one solution if and only if A1 holds. Among its solutions, there is a minimal one.*

Proof. Let us consider the iteration

$$x_{k+1} = M^{-1}\left(a + b(x_k, x_k)\right), \tag{3}$$

starting from $x_0 = 0$. Since M is an M-matrix, we have $x_1 = M^{-1}a \geq 0$. It is easy to see by induction that $x_k \leq x_{k+1}$:

$$x_{k+1} - x_k = M^{-1}(b(x_k, x_k) - b(x_{k-1}, x_{k-1})) \geq 0$$

since b is nonnegative. We will now prove by induction that $l(x_k) \leq z$. The base step is clear: $l(0) = 0 \leq z$; the inductive step is simply A1. Thus the sequence x_k is nondecreasing and bounded from above by $l(Mx_k) \leq z$, and therefore it converges. Its limit x^* is a solution to (1).

On the other hand, if (1) has a solution s, then we may choose $l = I$ and $z = s$; now, $x \leq s$ implies $M^{-1}(a + b(x, x)) \leq M^{-1}(a + b(s, s)) = s$, thus A1 is satisfied with this choices.

For any solution s, we may prove by induction that $x_k \leq s$:

$$s - x_{k+1} = a + b(s, s) - a - b(x^k, x^k) \geq 0.$$

Therefore, passing to the limit, $x^* \leq s$. □

Taylor expansion Let $F(x) := Mx - a - b(x, x)$. Since the equation is quadratic, the following expansion holds.

$$F(y) = F(x) + F'_x(y - x) + \frac{1}{2}F''_x(y - x, y - x), \tag{4}$$

where $F'_x(w) = Mw - b(x, w) - b(w, x)$ is the (Fréchet) derivative of F and $F''_x(w, w) = -2b(w, w) \leq 0$ is its second (Fréchet) derivative. Notice that F''_x is nonpositive and does not depend on x.

The following theorem is a straightforward extension to our setting of the argument in [10, Theorem 3.2].

Theorem 3. *If* $x^* > 0$, *then* F'_{x^*} *is an M-matrix.*

Proof. Let us consider the fixed point iteration (3). By a theorem on fixed-point iterations [15],

$$\limsup \sqrt[k]{\|x^* - x_k\|} \leq \rho(\mathcal{G}'_{x^*}), \tag{5}$$

where $\mathcal{G}'_{x^*}$ is the Fréchet derivative of the iteration map

$$\mathcal{G}(x) := M^{-1}(a + b(x, x)),$$

that is

$$\mathcal{G}'_{x^*}(y) = M^{-1}(b(x^*, y) + b(y, x^*)).$$

In fact, if $x^* > 0$, equality holds in (5). Let $e_k := x^* - x_k$. We have $e_{k+1} = P_k e_k$, where

$$P_k := M^{-1}(b(x^*, \cdot) + b(\cdot, x_k))$$

are nonnegative matrices. The matrix sequence P_k is nondecreasing and $\lim_{k\to\infty} P_k = \mathcal{G}'_{x^*}$. Thus for any $\varepsilon > 0$ we may find an integer l such that

$$\rho(P_m) \geq \rho(\mathcal{G}_{x^*}) - \varepsilon, \quad \forall m \geq l$$

We have

$$\begin{aligned}\limsup \sqrt[k]{\|x^* - x_k\|} &= \limsup \sqrt[k]{\|P_{k-1} \dots P_l \dots P_0 x^*\|} \\ &\geq \limsup \sqrt[k]{\left\|P_l^{k-l} P_0^l x^*\right\|}.\end{aligned}$$

Since $x^* > 0$, $P_0^l x^* > 0$ and thus $P_0^l x^* > c_l e$ for a suitable constant c_l. Also, $\left\|P_l^{k-l}\right\| = \left\|P_l^{k-l} v_{k,l}\right\|$ for a suitable $v_{k,l} \geq 0$ with $\|v_{k,l}\| = 1$, so

$$\begin{aligned}\limsup \sqrt[k]{\|x^* - x_k\|} &= \limsup \sqrt[k]{c_l \left\|P_l^{k-l} e\right\|} \\ &\geq \limsup \sqrt[k]{c_l \left\|P_l^{k-l} v_{k,l}\right\|} \\ &= \limsup \sqrt[k]{c_l \left\|P_l^{k-l}\right\|} \\ &= \rho(P_l) \geq \rho(\mathcal{G}_{x^*}) - \varepsilon\end{aligned}$$

Since ε is arbitrary, this shows that equality holds in (5).

From the convergence of the sequence x_k, we get thus

$$\rho(M^{-1}(b(x^*, \cdot) + b(\cdot, x^*))) \leq 1,$$

which implies that

$$M - b(x^*, \cdot) - b(\cdot, x^*)$$

is an M-matrix. □

Corollary 4. From point 2 of Theorem 1, we promptly obtain that $F'(x)$ is an M-matrix for all $x \leq x^*$.

Concrete cases We may prove A1 for all the examples E1–E4. E1 is covered by the following observation.

Lemma 5. If there is a vector $y \geq 0$ such that $F(y) \geq 0$, then A1 holds.

Proof. In fact, we may take the identity map as l and y as z. Clearly $x \leq y$ implies $M^{-1}(a + b(x, x)) \leq M^{-1}(a + b(y, y)) \leq y$ □

As for E2, it follows from the reasoning in [18] that a solution to the specific problem is $u = Xq + e$, $v = X^T q + e$, where X is the solution of an equation of the form E3; therefore, E2 follows from E3 and lemma 5. An explicit but rather complicate bound to the solution is given in [13].

The case E3 is treated in [8, Theorem 3.1]. Since $\mathcal{M}$ in (2) is a nonsingular or singular M-matrix, there are vectors $v_1, v_2 > 0$ and $u_1, u_2 \geq 0$ such that $Dv_1 - Cv_2 = u_1$ and $Av_2 - Bv_1 = u_2$. Let us set $l(x) = Xv_1$ and $z = v_2 - A^{-1}u_2$. We have

$$\begin{aligned}(AX_{k+1} + X_{k+1}D)v_1 =& (X_k C X_k + B)v_1 \\ \leq& X_k C v_2 + Av_2 - u_2 \leq XDv_1 + Av_2 - u_2.\end{aligned}$$

Since $X_{k+1}Dv_1 \geq X_k D v_1$ (monotonicity of the iteration), we get $X_{k+1}v_1 \leq v_2 - A^{-1}u_2$, which is the desired result.

The case E4 is similar. It suffices to set $l(x) = \text{vec}^{-1}(x)e$ and $z = e$:

$$X_{k+1}e = (I - B)^{-1}(A + CX_k^2)e \leq (I - B)^{-1}(Ae + Ce) \leq e,$$

since $(A + C)e = (I - B)e$

5 Functional iterations

5.1 Definition and convergence

We may define a functional iteration for (1) by choosing a splitting $b = b_1 + b_2$ such that $b_i \geq 0$ and a splitting $M = N - P$ such that N is an M-matrix and $P \geq 0$. We then have the iteration

$$(N - b_1(\cdot, x_k))x_{k+1} = a + Px_k + b_2(x_k, x_k). \tag{6}$$

Theorem 6. *Suppose that the equation* (1) *has a minimal solution* $x^* > 0$*. Let* x_0 *be such that* $0 \leq x_0 \leq x^*$ *and* $F(x_0) \leq 0$ *(e.g.* $x_0 = 0$*). Then:*

1. $N - b_1(\cdot, x_k)$ *is nonsingular for all* k*, i.e., the iteration* (6) *is well-defined.*

2. $x_k \leq x_{k+1} \leq x^*$*, and* $x_k \to x^*$ *as* $k \to \infty$*.*

3. $F(x_k) \leq 0$ *for all* k*.*

Proof. Let $J(x) := N - b_1(\cdot, x)$ and $g(x) := a + Px + b_2(x,x)$. It is clear from the nonnegativity constraints that J is nonincreasing (i.e., $x \leq y \Rightarrow J(x) \geq J(y)$) and g is nondecreasing (i.e., $x \leq y \Rightarrow g(x) \leq g(y)$).

The matrix $J(x)$ is a Z-matrix for all $x \geq 0$. Moreover, since $J(x^*)x^* = g(x^*) \geq 0$, $J(x^*)$ is an M-matrix by Theorem 1 and thus, by the same theorem, $J(x)$ is a nonsingular M-matrix for all $x \leq x^*$.

We shall first prove by induction that $x_k \leq x^*$. This shows that the iteration is well-posed, since it implies that $J(x_k)$ is an M-matrix for all k. Since $g(x^*) = J(x^*)x^* \leq J(x_k)x^*$ by inductive hypothesis, (6) implies

$$J(x_k)(x^* - x_{k+1}) \geq g(x^*) - g(x_k) \geq 0,$$

thus, since $J(x_k)$ is an M-matrix by inductive hypothesis, $x^* - x_{k+1} \geq 0$.

We will now prove by induction that $x_k \leq x_{k+1}$. For the base step, since we have $F(x_0) \leq 0$, and $J(x_0)x_0 - g(x_0) \leq 0$, thus $x_1 = J(x_0)^{-1}g(x_0) \geq x_0$. For $k \geq 1$,

$$J(x_{k-1})(x^{k+1} - x_k) \geq J(x_k)x_{k+1} - J(x_{k-1})x_k = g(x_k) - g(x_{k-1}) \geq 0.$$

thus $x_k \leq x_{k+1}$. The sequence x_k is monotonic and bounded above by x^*, thus it converges. Let x be its limit; by passing (6) to the limit, we see that x is a solution. But since $x \leq x^*$ and x^* is minimal, it must be the case that $x = x^*$.

Finally, for each k we have

$$F(x_k) = J(x_k)x_k - g(x_k) \leq J(x_k)x_{k+1} - g(x_k) = 0. \qquad \square$$

Theorem 7. *Let f be the map defining the functional iteration* (6), *i.e.* $f(x_k) = J(x_k)^{-1}g(x_k) = x_{k+1}$. *Let $\hat{J}$, $\hat{g}$, $\hat{f}$ be the same maps as J, g, f but for the special choice $b_2 = 0$, $P = 0$. Then $\hat{f}^k(x) \geq f^k(x)$, i.e., the functional iteration with $b_2 = 0$, $P = 0$ has the fastest convergence among all those defined by* (6)*.*

Proof. It suffices to prove that $\hat{f}(y) \geq \hat{f}(x)$ for all $y \geq x$, which is obvious from the fact that $\hat{J}$ is nonincreasing and $\hat{g}$ is nondecreasing, and that $\hat{f}(x) \geq f(x)$, which descends from the fact that $\hat{J}(x) \leq J(x)$ and $\hat{g}(x) \geq g(x)$. $\square$

Corollary 8. Let

$$x_{k+1}^{GS} = J(y_k)^{-1}g_k, \tag{7}$$

where y_k is a vector such that $x_k \leq y_k \leq x_{k+1}$, and g_k a vector such that $g(x_k) \leq g_k \leq g(x_{k+1})$. It can be proved with the same arguments that $x_{k+1} \leq x_{k+1}^{GS} \leq x^*$. This implies that we can perform the iteration in a "Gauss-Seidel" fashion: if in some place along the computation an entry of x_k is needed, and we have already computed the same entry of x_{k+1}, we can use that entry instead. It can be easily shown that $J(x_k)^{-1}g(x_k) \leq J(y_k)^{-1}g_k$, therefore the Gauss-Seidel version of the iteration converges faster than the original one.

Remark 9. The iteration (6) depends on b as a bilinear form, while Equation (1) and its solution depend only on b as a quadratic form. Therefore, different choices of the bilinear form b lead to different functional iterations for the same equation. Since for each iterate of each functional iteration both $x_k \leq x^*$ and $F(x_k) \leq 0$ hold (thus x_k is a valid starting point for a new functional iteration), we may safely switch between different functional iterations at every step.

Concrete cases For E1, the algorithm called *depth* in [2] is given by choosing $P = 0.b_2 = 0$. The algorithm called *order* in the same paper is obtained with the same choices, but starting by the bilinear form $\tilde{b}(x, y) := b(y, x)$ obtained by switching the arguments of b. The algorithm called *thicknesses* in [11] is given by performing alternately one iteration of each of the two above methods.

For E2, Lu's simple iteration [18] and the algorithm NBJ in [1] can be seen as the basic iteration (3) and $P = 0, b_2 = 0$. The algorithm NBGS in the same paper is a Gauss-Seidel-like variant.

For E3, the fixed point iterations in [10] are given by $b_2 = b$ and different choices of P. The iterations in [14] are the one given by $b_2 = 0, P = 0$ and a Gauss-Seidel-like variant.

For E4, the iterations in [7, chapter 6] can also be reinterpreted in our framework.

6 Newton's method

6.1 Definition and convergence

We may define the Newton method for the equation (1) as

$$F'_{x_k}(x_{k+1} - x_k) = -F(x_k). \tag{8}$$

Alternatively, we may write

$$F'_{x_k} x_{k+1} = a - b(x_k, x_k).$$

Also notice that

$$-F(x_k) = b(x_{k+1} - x_k, x_{k+1} - x_k). \tag{9}$$

Theorem 10. *If $x^* > 0$, the Newton method (8) starting from $x_0 = 0$ is well-defined, and the generated sequence x_k converges monotonically to x^*.*

Proof. First notice that since F'_{x^*} is an M-matrix by Theorem 3, F'_x is a nonsingular M-matrix for all $x \leq x^*$, $x \neq x^*$.

We shall prove by induction that $x_k \leq x_{k+1}$. We have $x_1 = M^{-1}a \geq 0$, so the base step holds. From (9), we get

$$F'_{x_{k+1}}(x_{k+2} - x_{k+1}) = b(x_{k+1} - x_k, x_{k+1} - x_k) \geq 0,$$

thus, since $F'_{x_{k+1}}$ is a nonsingular M-matrix, $x_{k+2} \geq x_{k+1}$, which completes the induction proof.

Moreover, we may prove by induction that $x_k < x^*$. The base step is obvious, the induction step is

$$\begin{aligned} F'_{x_k}(x^* - x_{k+1}) =& Mx^* - b(x_k, x^*) - b(x^*, x_k) - a + b(x_k, x_k) \\ =& b(x^* - x_k, x^* - x_k) > 0. \end{aligned}$$

The sequence x_k is monotonic and bounded from above by x^*, thus it converges; by passing (8) to the limit we see that its limit must be a solution of (1), hence x^*. □

6.2 Concrete cases

Newton methods for E1, E2, and E3 appear respectively in [11], [17] and [10], with more restrictive hypotheses which hold true in the special applicative cases. In particular, in [10] (and later [8]) the authors impose that $x_1 > 0$; [11] impose that F'_{x^*} is an M-matrix, which is true in their setting because of probabilistic assumptions; and in the setting of [17], $x_1 > 0$ is obvious. The Newton method is usually not considered for E4 due to its high computational cost.

As far as we know, the more general hypothesis $x^* > 0$ first appeared here.

7 Modified Newton method

Recently Hautphenne and Van Houdt [12] proposed a different version of Newton's method for E1 that has a better convergence rate than the traditional one. Their idea is to apply the Newton method to the equation

$$G(x) = x - (M - b(\cdot, x))^{-1}a, \tag{10}$$

which is equivalent to (1).

7.1 Theoretical properties

Let us set for the sake of brevity $R_x := M - b(\cdot, x)$. The Jacobian of G is

$$G'_x = I - R_x^{-1} b(R_x^{-1}a, \cdot).$$

As for the original Newton method, it is a Z-matrix, and a nonincreasing function of x. It is easily seen that G'_{x^*} is an M-matrix. The proof in

Hautphenne and Van Houdt [12] is of probabilistic nature and cannot be extended to our setting; we shall provide here a different one. We have

$$G'(x^*) = R_{x^*}^{-1}\left(M - b(\cdot, x^*) - b(R_{x^*}^{-1}a, \cdot)\right) = R_{x^*}^{-1}\left(M - b(\cdot, x^*) - b(x^*, \cdot)\right);$$

the quantity in parentheses is F'_{x^*}, an M-matrix, thus there is a vector $v > 0$ such that $F'_{x^*}v \geq 0$, and therefore $G'_{x^*}v = R_{x^*}^{-1}F'_{x^*}v \geq 0$. This shows that G'_x is an M-matrix for all $x \leq x^*$ and thus the modified Newton method is well-defined. The monotonic convergence is easily proved in the same fashion as for the traditional method.

The following result holds.

Theorem 11. *[12] Let $\tilde{x}_k$ be the iterates of the modified Newton method and x_k those of the traditional Newton method, starting from $\tilde{x}_k = x_k = 0$. Then $\tilde{x}_k - x_k \geq 0$.*

The proof in Hautphenne and Van Houdt [12] can be adapted to our setting with minor modifications.

7.2 Concrete cases

Other than for E1, its original setting, the modified Newton method is useful for the other concrete cases of quadratic vector equations.

For E2, let us choose the bilinear map b as

$$b([u_1 v_1], [u_2 v_2]) := [u_1 \circ (P v_2), v_1 \circ (\tilde{P} u_2)].$$

This way, it is easily seen that $b(\cdot, x)$ is a diagonal matrix and $b(x, \cdot)$ has the same structure that allowed a fast (with $O(n^2)$ operations per step) implementation of the traditional Newton's method in Bini *et al.* [5]. Therefore the modified Newton method can be implemented with a negligible overhead ($O(n)$ ops per step on an algorithm that takes $O(n^2)$ ops per step) with respect to the traditional one, and increased convergence rate.

We have performed some numerical experiments on the modified Newton method for E2; as can be seen in Figure 1, the modified Newton method does indeed converge faster to the minimal solution, and this allows one to get better approximations to the solution with the same number of steps.

For E3 and E4, the modified Newton method leads to similar equations to the traditional one (continuous- and discrete-time Sylvester equations), but requires additional inversions and products of $m \times m$ matrices; that is, the overhead is of the same order of magnitude $O(m^3)$ of the cost of the Newton step. Therefore it is not clear whether the improved convergence rate makes up for the increase in the computational cost.

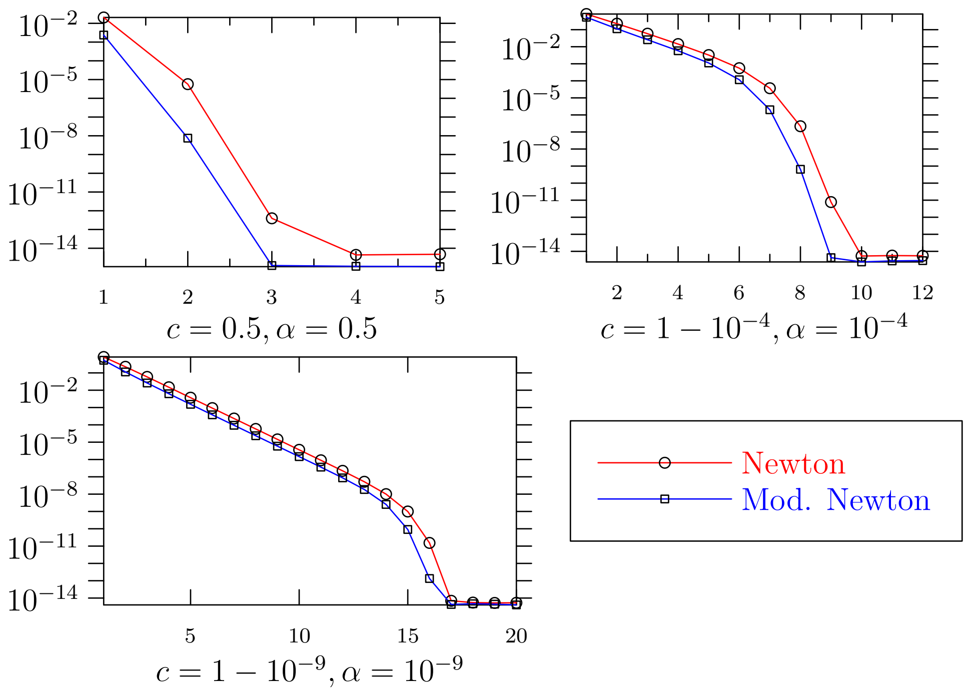

Figure 1: Convergence history of the two Newton methods for E2 for several values of the parameters α and c. The plots show the residual Frobenius norm of Equation (1) vs. the number of iterations

8 Newton method and Cyclic/Logarithmic Reduction

8.1 Recall of Logarithmic and Cyclic Reduction

Cyclic and Logarithmic Reduction [7] are two closely related methods for solving E4, which have quadratic convergence and a lower computational cost than Newton's method. Both are based on specific properties of the problem and cannot be extended in a straightforward way to any quadratic vector equation.

Logarithmic Reduction (LR) is based on the fact that if X solves

$$X = B_{-1} + B_1 X^2,$$

then it can be shown with algebraic manipulations that $Y = X^2$ solves the equation

$$Y = (I - B_{-1}B_1 - B_1 B_{-1})^{-1} (B_{-1})^2 + (I - B_{-1}B_1 - B_1 B_{-1})^{-1} (B_1)^2 Y^2, \quad (11)$$

with the same structure. Therefore we may start from an approximation $X_1 = B_{-1}$ to the solution and refine it with a term $B_1 Y$, where Y is (an approximation to) the solution of (11). Such an approximation is computed with the same method, and refined successively by applying the same method recursively. The resulting algorithm is reported here as Algorithm 1 An

Algorithm 1 Logarithmic Reduction for E4 [7]

{Input: A, B, C}
{Output: a solution X to $X = A + BX + CX^2$}
$B_{-1} \leftarrow (I - B)^{-1}A$
$B_1 \leftarrow (I - B)^{-1}C$
$X \leftarrow B_{-1}$
$U \leftarrow B_1$
while stopping criterion is not satisfied **do**
  $C \leftarrow I - B_1B_{-1} - B_{-1}B_1$
  $B_{-1} \leftarrow C^{-1}B_{-1}^2$
  $B_1 \leftarrow C^{-1}B_1^2$
  $X \leftarrow X + UB_{-1}$
  $U \leftarrow UB_1$
end while
return X

alternative interpretation of LR [7] arises by defining the matrix-valued function $f : \mathbb{C} \to \mathbb{C}^{m\times m}$ as $f(z) = B_{-1} - z + B_1z^2$ and applying the Graeffe iteration $f \mapsto f(z)f(-z)$, which yields a quadratic polynomial in z^2 with the same roots of $f(z)$ plus some additional ones.

Cyclic Reduction (CR) is a similar algorithm, which is connected to LR by simple algebraic relations (see the Bini *et al.* book [7] for more detail). We shall report it here as Algorithm 2.

Algorithm 2 Cyclic Reduction for E4 [7]

{Input: A, B, C}
{Output: a solution X to $X = A + BX + CX^2$}
$R \leftarrow I - B$
$S \leftarrow I - B$
$A_0 \leftarrow A$
while stopping criterion is not satisfied **do**
  $S \leftarrow R - CR^{-1}A$
  $X \leftarrow S^{-1}A_0$
  $R' \leftarrow R - AR^{-1}C - CR^{-1}A$
  $A' \leftarrow AR^{-1}A$
  $C' \leftarrow CR^{-1}C$
  $R, A, C \leftarrow R', A', C'$
end while
return X

8.2 Generalization attempts

We may attempt to produce algorithms similar to LR and CR for a generic quadratic vector equation. Notice that we cannot look for an equation in X^2 in our vector setting, since x^2 for a vector x has not a clear definition — using e.g. the Hadamard (component-wise) product does not lead to a simple equation. Nevertheless, we may try to find an equation in $b(x,x)$, which is the only quadratic expression that makes sense in our context.

We will look for an expression similar to the Graeffe iteration. If x solves $0 = F(x) = Mx - a - b(x,x)$, then it also solves $b(F(x), F(-x)) + b(F(-x), F(x)) = 0$ (notice that a symmetrization is needed), that is,

$$
\begin{aligned}
b(x - M^{-1}a - M^{-1}b(x,x), x + M^{-1}a + M^{-1}b(x,x)) + \\
b(x + M^{-1}a + M^{-1}b(x,x), x - M^{-1}a - M^{-1}b(x,x)) = 0.
\end{aligned}
$$

If we set $v_1 = M^{-1}b(x,x)$ and exploit the bilinearity of $b(\cdot,\cdot)$, the above equation reduces to

$$
-b(M^{-1}a, M^{-1}a) + \left(M - b(M^{-1}a, \cdot) - b(\cdot, M^{-1}a)\right) v_1 - b(v_1, v_1) = 0, \quad (12)
$$

which is suitable to applying the same process again. A first approximation to x is given by $M^{-1}a$; if we manage to solve (even approximately) (12), this approximation can be refined as $x = M^{-1}a + v_1$. We may apply this process recursively, getting an algorithm similar to Logarithmic Reduction. The algorithm is reported here as Algorithm 3. It is surprising to see that

Algorithm 3 A Cyclic Reduction-like formulation of Newton's method for a quadratic vector equation

$x \leftarrow 0$, $\tilde{M} \leftarrow M$, $\tilde{a} \leftarrow a$
while stopping criterion is not satisfied **do**
  $w \leftarrow \tilde{M}^{-1}\tilde{a}$
  $x \leftarrow x + w$
  $\tilde{a} \leftarrow b(w,w)$
  $\tilde{M} \leftarrow \tilde{M} - b(w,\cdot) - b(\cdot,w)$
end while
return x

this algorithm turns out to be equivalent to Newton's method. In fact, it is easy to prove by induction the following proposition.

Theorem 12. *Let x_k be the iterates of Newton's method on* (1) *starting from $x_0 = 0$. At the kth iteration of the **while** cycle in Algorithm 3, $x = x_k$, $w = x_{k+1} - x_k$, $\tilde{M} = F'_{x_k}$, $\tilde{a} = -F(x_k)$.*

The modified Newton method discussed in section 7 can also be expressed in a form that looks very similar to LR/CR. We may express all the computations of step $k+1$ in terms of $R_{x_k}^{-1} b$ and $R_{x_k}^{-1} a$ only: in fact,

$$R_{x_{k+1}} = R_{x_k} - b(\cdot, x_{k+1} - x_k) = R_{x_k} \left(I - R_{x_k}^{-1} b(\cdot, x_{k+1} - x_k) \right),$$

and thus

$$R_{x_{k+1}}^{-1} R_{x_k} = \left(I - R_{x_k}^{-1} b(\cdot, x_{k+1} - x_k) \right)^{-1}.$$

The resulting algorithm is reported here as Algorithm 4.

Algorithm 4 A Cyclic Reduction-like formulation of the modified Newton method for a quadratic vector equation

$x \leftarrow 0$, $\tilde{a} \leftarrow a$, $\tilde{b} \leftarrow b$, $\tilde{w} \leftarrow 0$
while stopping criterion is not satisfied **do**
  $\tilde{a} \leftarrow (I - \tilde{b}(\cdot, w))^{-1} \tilde{a}$
  $\tilde{b} \leftarrow (I - \tilde{b}(\cdot, w))^{-1} \tilde{b}$
  $w \leftarrow (I - \tilde{b}(\tilde{a}, \cdot))^{-1} (\tilde{a} - x)$
  $x \leftarrow x + w$
end while
return x

The similarities between the two Newton formulations and LR are apparent. In all of them, only two variables (B_{-1} and B_1, $\tilde{a}$ and $\tilde{M}$, $\tilde{a}$ and $\tilde{b}$) are stored and used to carry on the successive the iteration, and some extra computations and variables are needed to extract from them the approximation of the solution (X, x) which is refined at each step with a new additive term.

It is a natural question whether there are algebraic relations among LR and Newton methods, or if LR can be interpreted as an inexact Newton method (see e.g. Ortega and Rheinboldt [19]), thus providing an alternative proof of its quadratic convergence. However, we were not able to find an explicit relation among the two classes of methods. This is mainly due to the fact that the LR and CR methods are based upon the squaring $X \mapsto X^2$, which we have no means to translate in our vector setting. To this regard we point out that we cannot invert the matrix C, since in many applications it is strongly singular.

9 Positivity of the minimal solution

9.1 Role of the positivity

In many of the above theorems, the hypothesis $x^* > 0$ is required. Is it really necessary? What happens if it is not satisfied?

In all the algorithms we have exposed, we worked with only vectors x such that $0 \leq x \leq x^*$. Thus, if x^* has some zero entry, we may safely replace the problem with a smaller one by projecting the problem on the subspace of all vectors that have the same zero pattern as x^*: i.e., we may replace the problem with the one defined by

$$\hat{a} = \Pi a,\ \hat{M} = \Pi M \Pi^T,\ \hat{b}(x,y) = \Pi b(\Pi^T x, \Pi^T y),$$

where Π is the orthogonal projector on the subspace

$$W = \{x \in \mathbb{R}^n : x_i = 0 \text{ for all } i \text{ such that } x_i^* = 0\}, \tag{13}$$

i.e. the linear operator that removes the entries known to be zero from the vectors. Performing the above algorithms on the reduced vectors and matrices is equivalent to performing them on the original versions, provided the matrices to invert are nonsingular. Notice, though, that both functional iterations and Newton-type algorithms may break down when the minimal solution is not strictly positive. For instance, consider the problem

$$a = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix},\ M = I_2,\ b\left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}\right) = \begin{pmatrix} \frac{1}{2}x_1 y_1 \\ K x_1 y_2 \end{pmatrix},\ x^* = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

For suitable choices of the parameter K, the matrices to be inverted in the functional iterations (excluding obviously (3)) and Newton's methods are singular; for large values of K, none of them are M-matrices. However, the nonsingularity and M-matrix properties still hold for their restrictions to the subspace W defined in (13). It is therefore important to consider the positivity pattern of the minimal solution in order to get working algorithms.

9.2 Computing the positivity pattern

By considering the functional iteration (3), we may derive a method to infer the positivity pattern of the minimal solution in time $O(n^3)$. Let us denote by e_t the t-th vector of the canonical basis, and $e_S = \sum_{s \in S} e_s$ for any set $S \in \{1, \dots, n\}$. Algorithm 5 is reported here.

Theorem 13. *The above algorithm runs in at most $O(n^3)$ operations and computes the set $\{h \in \{1, \dots, n\} : x_h^* > 0\}$*

Proof. For the implementation of the sets, we shall use the simple approach to keep in memory two vectors $S, T \in \{0,1\}^n$ and set to 1 the components relative to the indices in the sets. With this choice, insertions and membership tests are $O(1)$, loops are easy to implement, and retrieving an element of the set costs at most $O(n)$.

Let us first prove that the running time of the algorithm is at most $O(n^3)$. If we precompute a PLU factorization of M, each subsequent operation $M^{-1}v$, for $v \in \mathbb{R}^n$, costs $O(n^2)$. The first **for** loop runs in at most $O(n)$ operations. The body of the **while** loop runs at most n times, since an element can be inserted into S and T no more than once (S never decreases).

Algorithm 5 Compute the positivity pattern of the solution x^*

Require: a, M, b
  $S \leftarrow \emptyset$ {entries known to be positive}
  $T \leftarrow \emptyset$ {entries to check}
  $a' \leftarrow M^{-1}a$
  for $i = 1$ to n **do**
    if $a'_i > 0$ **then**
      $T \leftarrow T \cup \{i\}$; $S \leftarrow S \cup \{i\}$
    end if
  end for
  while $T \neq \emptyset$ **do**
    $t \leftarrow$ some element of T
    $T \leftarrow T \setminus \{t\}$
    $u \leftarrow M^{-1}(b(e_S, e_t) + b(e_t, e_S))$ {or only its positivity pattern}
    for $i \in \{1, \dots, n\} \setminus S$ **do**
      if $u_i > 0$ **then**
        $T \leftarrow T \cup \{i\}$; $S \leftarrow S \cup \{i\}$
      end if
    end for
  end while
  return S

Each of its iterations costs $O(n^2)$, since evaluating $b(e_t, e_S)$ is equivalent to computing the matrix-vector product between the matrix $(B_{tij})_{i,j=1,\dots,n}$ and e_S, and similarly for $b(e_S, e_t)$.

The fact that the algorithm computes the right set may not seem obvious at first sight. Since the sequence x_k is increasing, if one entry in x_k is positive, then it is positive for all iterates x_h, $h > k$. When does an entry of x_k become positive? The positive entries of x_1 are those of $M^{-1}a$; then, an entry t of x_{k+1} is positive if either the corresponding entry of x_k was positive or two entries r, s of x_k were positive and $B_{rst} > 0$. Thus, an entry in x^* is positive if and only if we can find a sequence S_i of subsets of $\{1, \dots, n\}$ such that:

- $S_0 = \{h \in \{1, \dots, n\} : (M^{-1}a)_h > 0\}$;
- $S_{i+1} = S_i \cup \{t_i\}$, and there are two elements $r, s \in S_i$ such that $B_{rst_i} > 0$.

For each element u of $\{h \in \{1, \dots, n\} : x^*_h > 0\}$, we may prove by induction on the length of its minimal sequence S_i that it eventually gets into S (and T). In fact, suppose the last element of the sequence is S_l. Then, by inductive hypothesis, all the elements of S_{l-1} eventually get into S and T. All of them are removed from T at some step of the algorithm. When the last one is removed, the **if** condition triggers and the element u is inserted into T. Conversely, if u is an element that gets inserted into S, then by considering the values of S at the successive steps of the algorithm we get a valid sequence $\{S_i\}$. □

It is a natural question to ask whether for the cases E3 and E4 it is possible to use the special structure of M and b in order to develop a similar algorithm with running time $O(m^3)$, that is, the same as the cost per step of the basic iterations. Unfortunately, we were unable to go below $O(m^4)$. It is therefore much less appealing to run this algorithm as a preliminary step before, since its cost is likely to outweigh the cost of the actual solution. However, we remark that the strict positiveness of the coefficients is usually a property of the problem rather than of the specific matrices involved, and can often be solved in the model phase before turning to the actual computations. An algorithm such as the above one would only be needed in an "automatic" subroutine to solve general instances of the problems E3 and E4.

10 Other concrete cases

In Bini *et al.* [6], the matrix equation

$$X + \sum_{i=1}^{d} A_i X^{-1} D_i = B - I$$

appears, where $B, A_i, D_i \geq 0$ and the matrices $B + D_j + \sum_{i=1}^{d} A_i$ are stochastic. The solution $X = T - I$, with $T \geq 0$ minimal and sub-stochastic, is sought. Their paper proposes a functional iteration and Newton's method. By setting $Y = -X^{-1}$ and multiplying both sides by Y, we get

$$(I - B)Y = I + \sum A_i Y D_i Y,$$

which is again in the form (1). It is easy to see that Y is nonnegative whenever T is substochastic, and Y is minimal whenever T is.

The paper considers two functional iteration and the Newton method; all these algorithm are expressed in terms of X instead of Y, but they essentially coincide with those exposed in the present paper.

11 Research lines

There are many open questions that could yield a better theoretical understanding of this class of equations or better solution algorithms.

- Is there a way to translate to our setting the spectral theory of E4 (see e.g. Bini *et al.* [7, chapter 3])?

- The shift technique [7, chapter 3] is a method to transform a singular problem (i.e. one in which F'_{x^*} is singular) of the kind E4 (or also E3, see e.g. [9, 4]) to a nonsingular one. Is there a way to adapt it to a generic quadratic vector equation? Is there a similar technique for near-to-singular problems, which are the most difficult to solve in the applications?

- As we discussed in the section 8: is there an explicit algebraic relation among Newton's method and Logarithmic/Cyclic Reduction, or an interpretation of the latter as an inexact Newton method?

- Is there a way to determine the optimal splitting to use in the functional iteration (6)? We proved that $P = b_3 = 0$ is optimal, but it is an open question how to divide b into b_1 and b_2 to obtain the fastest convergence. Also, is there a relation between the *thicknesses* method of Hautphenne *et al.* [11] and the symmetrized functional iteration $b_1 = b_2 = \frac{1}{2}b$ for E1?

- Can this approach be generalized to the positive definite ordering on symmetric matrices ($A \geq B$ if $A - B$ is positive semidefinite)? This would lead to the further unification of the theory of a large class of equations, including the algebraic Riccati equations appearing in control theory [16]. A lemma proved by Ran and Reurings [20, theorem 2.2] could replace the first point of Theorem 1 in an extension of the results of this paper to the positive definite ordering.

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