

Newton Iterations in Implicit Time-Stepping Scheme for Differential Linear Complementarity Systems

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Abstract. We propose a generalized Newton method for solving the system of nonlinear equations with linear complementarity constraints in the implicit or semi-implicit time-stepping scheme for differential linear complementarity systems (DLCS). We choose a specific solution from the solution set of the linear complementarity constraints to define a locally Lipschitz continuous right-hand-side function in the differential equation. Moreover, we present a simple formula to compute an element in the Clarke generalized Jacobian of the solution function. We show that the implicit or semi-implicit time-stepping scheme using the generalized Newton method can be applied to a class of DLCS including the nondegenerate matrix DLCS and hidden Z-matrix DLCS, and has a superlinear convergence rate. To illustrate our approach, we show that choosing the least-element solution from the solution set of the Z-matrix linear complementarity constraints can define a Lipschitz continuous right-hand-side function with a computable Lipschitz constant.

Keywords: differential linear complementarity problem, least-norm solution, least-element solution, nondegenerate matrix, Z-matrix, generalized Newton method.

AMS Subject Classifications: 90C30, 90C33

1 Introduction

Given four matrices $A \in R^{m \times m}$, $B \in R^{m \times n}$, $N \in R^{n \times m}$, $M \in R^{n \times n}$, and two Lipschitz continuous functions $f : R \rightarrow R^m$ and $g : R \rightarrow R^n$, we consider the ordinary differential linear complementarity system (DLCS):

$$\begin{aligned} \dot{x}(t) &= Ax(t) + By(t) + f(t) \\ y(t) &\in \text{SOL}(Nx(t) + g(t), M) \\ x(0) &= x_0, \quad t \in [0, T], \end{aligned} \tag{1.1}$$

where $\text{SOL}(Nx(t) + g(t), M) \subseteq R^n$ is the solution set of the following linear complementarity problem (LCP):

$$0 \leq y(t) \perp Nx(t) + g(t) + My(t) \geq 0. \tag{1.2}$$

The nonnegativity notation and orthogonality notation in (1.2) express that for $i = 1, \dots, n$,

$$y_i(t) \geq 0, \quad (Nx(t) + g(t) + My(t))_i \geq 0, \quad y_i(t)(Nx(t) + g(t) + My(t))_i = 0.$$

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The DLCS (1.1) has wide applications in engineering and economics. In the last decade, numerous research articles on DLCS have been published in the areas of applied mathematics, operations research, civil engineering, electrical engineering, transportation sciences, etc. See [1, 4, 10, 12, 13, 14, 19, 21].

A popular numerical method for solving the DLCS is the time-stepping method, which uses a finite-difference formula to approximate the derivative \dot{x} . In particular, this method divides the time interval $[0, T]$ into N_h subintervals

$$0 = t_{h,0} < t_{h,1} < \cdots < t_{h,N_h} = T,$$

where $t_{h,i+1} - t_{h,i} = h = T/N_h$, $i = 0, \dots, N_h - 1$. Starting from $x^{h,0} = x^0 \in R^m$, we compute two finite sets of vectors

$$\{x^{h,1}, x^{h,2}, \dots, x^{h,N_h}\} \subset R^m \quad \text{and} \quad \{y^{h,1}, y^{h,2}, \dots, y^{h,N_h}\} \subset R^n$$

by the recursion: for $i = 0, 1, \dots, N_h - 1$,

$$\begin{aligned} x^{h,i+1} &= x^{h,i} + h [A(\theta x^{h,i} + (1 - \theta)x^{h,i+1}) + By^{h,i+1} + f(t_{h,i+1})], \\ y^{h,i+1} &\in \text{SOL}(Nx^{h,i+1} + g(t_{h,i+1}), M), \end{aligned} \quad (1.3)$$

where $\theta \in [0, 1]$ is a scalar to distinguish an explicit ($\theta = 1$), an implicit ($\theta = 0$), or a semi-implicit ($\theta \in (0, 1)$) scheme. In this paper, we consider the implicit scheme and semi-implicit scheme.

A critical part in numerical implementation of the time-stepping scheme is to find a good solution $y^{h,i+1}$ in the solution set $\text{SOL}(Nx^{h,i+1} + g(t_{h,i+1}), M)$. In many cases, the solution set $\text{SOL}(Nx^{h,i+1} + g(t_{h,i+1}), M)$ is neither convex nor bounded. Using some vector in the solution set can cause the numerical method unstable or make the linear complementary problem unsolvable in the next step. Moreover, at each time step of the implicit scheme or semi-implicit scheme, $x^{h,i+1}$ is a solution u^* of the following system of nonsmooth equations with linear complementarity constraints

$$\begin{aligned} u &= H(u) := (1 + h\theta A)x^{h,i} + h[(1 - \theta)Au + By(u) + f(t_{h,i+1})] \\ y(u) &\in \text{SOL}(Nu + g(t_{h,i+1}), M). \end{aligned} \quad (1.4)$$

This system has to be solved efficiently and accurately. A bad numerical solution of the nonsmooth equations (1.4) at one time step can cause the final numerical results failure. In this paper, we choose a solution from the solution set $\text{SOL}(Nu + g(t_{h,i+1}), M)$ to define a Lipschitz continuous solution function $y(\cdot)$. Moreover, we present a simple formula to compute an element in the Clarke generalized Jacobian of the solution function, which will be used for the generalized Newton method to solve the system of nonsmooth equations (1.4) at each time step of the implicit scheme and semi-implicit scheme.

In Section 2, we study how to choose a solution $y(q)$ from the solution set $\text{SOL}(q, M)$ such that y is locally Lipschitz with respect to q . By the Rademacher Theorem [7], a locally Lipschitz function is differentiable almost everywhere. Hence, we can define the Clarke generalized Jacobian [7]

$$\partial y(q) = \text{co}\{\lim y'(q^k) : q^k \rightarrow q, q^k \in \Omega_y\},$$

where Ω_y denotes the set of points at which y is differentiable, and “co” denotes the convex hull. To use the generalized Newton method for solving (1.4), we show that

$$-(I - D + DM)^{-1}D \in \partial y(q) \quad (1.5)$$

if $I - D + DM$ is nonsingular, where $D = \text{diag}(d_1, \dots, d_n)$ is a diagonal matrix with diagonals

$$d_i = \begin{cases} 1, & y_i(q) > 0 \\ 0, & \text{otherwise.} \end{cases}$$

It is easy to see that $-(I - D + DM)^{-1}$ is nonsingular if and only if the principal submatrix $M_{J,J}$ is nonsingular, where $J = \{i \mid y_i > 0\}$. Hence we can use (1.5) and the generalized Newton method to solve (1.4) if all principal minors of M are nonzero.

For a given matrix M , let $M_{J,K}$ be the submatrix of M whose entries of M are indexed by the sets $J, K \in \{1, \dots, n\}$. If $J = K$, the submatrix $M_{J,K}$ is called a principal submatrix of M . The determinant of a principal submatrix of M is called a principal minor of M .

A matrix M is called a *nondegenerate matrix* if all principal minors of M are nonzero [8]. A nondegenerate matrix is also called a nonzero principal minor matrix or principally nonsingular matrix [3, 17, 23]. A matrix M is called a P-matrix (N-matrix), if all principal minors of M are positive (negative). M is called an NP-matrix (PN-matrix) if each $k \times k$ principal minor of M has $\text{sign}(-1)^k ((-1)^{k+1})$ [17]. Obviously, the class of nondegenerate matrices includes the class of P-matrices, N-matrices, NP-matrices and PN-matrices. Such matrices have many applications in engineering and economics [3, 8, 9, 17]. It is worth noting that M is a P-matrix if and only if the matrix $I - D + DM$ is nonsingular for all $d_i \in [0, 1]$ [11]. A matrix M is a nondegenerate matrix if and only if the matrix $I - D + DM$ is nonsingular for all $d_i \in \{0, 1\}$.

In Section 3, we propose a generalized Newton method to solve (1.4) with a Lipschitz solution function $y(Nu + g(t_{h,i+1}))$ from $\text{SOL}(Nu + g(t_{h,i+1}), M)$, and an element from $\partial y(Nu + g(t_{h,i+1}))$ given in (1.5). We prove the generalized Newton method starting from $x^{h,i}$ is well-defined and superlinearly convergent. Moreover, we present an error bound of a numerical solution to the true solution of (1.4).

We use the class of Z-matrices to show that the implicit scheme and the semi-implicit scheme using Newton's method can be applied to the DLCS (1.1) without the non-singularity assumption on the matrix M . A matrix $M \in R^{n \times n}$ is called a *Z-matrix*, if its off-diagonal elements are non-positive. An M-matrix is a Z-matrix. The Z-matrix LCP arises from the finite element or finite difference discretization of free boundary problems, reaction-diffusion problems and journal bearing problems [2, 8, 9, 22, 24].

If M is a Z-matrix and the feasible set

$$\text{FEA}(q, M) = \{y \mid q + My \geq 0, y \geq 0\}$$

is nonempty, then the solution set $\text{SOL}(q, M)$ is nonempty [8], and there is a **least-element** solution in $\text{SOL}(q, M)$. A solution x^* of $\text{LCP}(q, M)$ is called a least-element solution if $x^* \leq x$ for all $x \in \text{SOL}(q, M)$, which can be obtained by solving the following linear programming

$$\begin{aligned} & \text{minimize} && e^T y \\ & \text{subject to} && q + My \geq 0, \quad y \geq 0, \end{aligned} \quad (1.6)$$

where $e \in R^n$ with $e_i = 1, i = 1, \dots, n$ [8]. We show that the least-element solution of $LCP(q, M)$ is global Lipschitz continuous with the following Lipschitz constant

$$\mathcal{L} = \max \left\{ \|M_{J,J}^{-1}\| \mid M_{J,J} \text{ is nonsingular for } J \subseteq \{1, \dots, n\} \right\}.$$

Moreover, we show that \mathcal{L}_∞ defined by the $\|\cdot\|_\infty$ is much smaller than the constant given by Mangasarian and Shiau [15].

In Section 4, we use the constant \mathcal{L} to derive a time interval $[0, T_0]$, such that the following least-element LCS has a unique solution (x^*, y^*) such that x^* is continuously differentiable and y^* is Lipschitz continuous on $[0, T_0]$.

Least-Element LCS

$$\begin{aligned} \dot{x}(t) &= Ax(t) + By(x(t)) + f(t) \\ y(x(t)) &= \operatorname{argmin} e^T v \\ &\text{subject to } v \in \operatorname{SOL}(Nx(t) + g(t), M) \\ x(0) &= x_0, \quad t \in [0, T]. \end{aligned} \tag{1.7}$$

Moreover, we show that the following implicit least-element time-stepping scheme converges to (x^*, y^*) linearly, and the generalized Newton method using (1.5) is well-defined and superlinearly converges to a solution u^* of (1.4) from $x^{h,i}$ on the interval $[0, T_0]$.

Implicit Least-Element Time-Stepping Scheme (ILETS scheme)

$$\begin{aligned} x^{h,i+1} &= x^{h,i} + h(Ax^{h,i+1} + By^{h,i+1} + f(t_{h,i+1})) \\ y^{h,i+1} &= \operatorname{argmin} \{ e^T v \mid 0 \leq v \perp Nx^{h,i+1} + g(t_{h,i+1}) + Mv \geq 0 \}. \end{aligned} \tag{1.8}$$

In [14], Han, Tiwari, Camlibel, and Pang, proposed the following scheme.

Implicit Least-Norm Time-Stepping Scheme (ILNTS scheme)

$$\begin{aligned} x^{h,i+1} &= x^{h,i} + h(Ax^{h,i+1} + By^{h,i+1} + f(t_{h,i+1})) \\ y^{h,i+1} &= \operatorname{argmin} \{ \|v\|_2 \mid 0 \leq v \perp Nx^{h,i+1} + g(t_{h,i+1}) + Mv \geq 0 \}. \end{aligned} \tag{1.9}$$

They showed that using such least-norm solutions of the discrete-time subproblems, an implicit Euler scheme is convergent for passive initial-value DLCS. Obviously, a least-element solution is a least-norm solution. Moreover, if M is a Z-matrix, then [8]

$$\operatorname{argmin} \{ e^T v \mid 0 \leq v \perp q + Mv \geq 0 \} = \operatorname{argmin} \{ e^T v \mid v \geq 0, q + Mv \geq 0 \}.$$

Hence, (1.8) can be considered as an implementation version of the implicit least-norm time-stepping scheme proposed in [14] for the Z-matrix DLCS.

Throughout this paper, we use $\|x\|$ to denote the maximum norm $\|x\| := \max_{t \in [0, T]} \|x(t)\|$ for a function x defined on $[0, T]$ or $\|x\| := \max_{1 \leq i \leq m} |x_i|$ for a vector $x \in R^m$. Let J^c denote the complementarity set of J . Let e denote the vector whose all entries are one. We say a function is differentiable if it is F-differentiable.

2 Solution function $y(q)$ of $LCP(q, M)$

Let $R_{LCP}(M)$ denote the LCP-Range of M which is the set of all vectors q such that $\operatorname{SOL}(q, M) \neq \emptyset$. M is called a Q-matrix if $R_{LCP}(M) = R^n$ [8, 16]. It is known that M

is a P-matrix if and only if $R_{LCP}(M) = R^n$ and $\text{SOL}(q, M)$ is singleton for any $q \in R^n$ [8]. However, in general, $\text{SOL}(q, M)$ can be empty or unbounded. Using some concepts, such as the least-norm solution and the least-element solution [6, 8, 14], we may define a single valued solution function $y(\cdot)$ on an open set Ω in $R_{LCP}(M)$. In this section, we first give a necessary and sufficient condition for a single valued solution function $y(\cdot)$ to be differentiable at $q \in \Omega$. Next, we present a simple formula to compute an element in the Clarke generalized Jacobian of $y(\cdot)$ at $q \in \Omega$ and give computable Lipschitz constants of $y(\cdot)$ in Ω for nondegenerate matrices and Z -matrices.

For a single valued solution function $y(q) \in \text{SOL}(q, M)$, we define the following index sets:

$$\begin{aligned} J_q &= \{i \mid y_i(q) > 0\} \\ I_q &= \{i \mid (My(q) + q)_i > 0\} \\ K_q &= \{i \mid (My(q) + q)_i = q_i = 0\}. \end{aligned}$$

We say $y(q)$ is nondegenerate if $K_q = \emptyset$. We define the diagonal matrix D_q whose diagonal elements are

$$(D_q)_{ii} = \begin{cases} 1, & i \in J_q \\ 0, & \text{otherwise.} \end{cases}$$

Lemma 2.1 *Suppose that $\Omega \subseteq R_{LCP}(M)$ is an open set. Let y be a continuous function defined on Ω such that $y(q) \in \text{SOL}(q, M)$ for $q \in \Omega$. Denote $J = J_q$ and $D = D_q$. Then y is differentiable at q if and only if $y(q)$ is nondegenerate and $M_{J,J}$ is nonsingular. In the case $y(\cdot)$ is differentiable at q , we have*

$$y'(q) = -(I - D + DM)^{-1}D. \quad (2.1)$$

Proof: Suppose that $y(q)$ is nondegenerate. By the continuity of y , there is a neighborhood of q such that for any p in the neighborhood, we have

$$y_J(p) > 0, \quad y_{J^c}(p) = 0, \quad (My(p) + p)_J = 0, \quad (My(p) + p)_{J^c} > 0.$$

Hence we obtain

$$(I - D)y(p) + D(My(p) + p) = 0.$$

If J is empty, then $D = 0$. This implies $y(p) \equiv 0$ in the neighborhood. If J is not empty and $M_{J,J}$ is nonsingular, then the matrix $I - D + DM$ is nonsingular. This implies that

$$y(p) = -(I - D + DM)^{-1}Dp$$

is the unique solution of $\text{SOL}(p, M)$ in the neighborhood. Hence in both cases, y is differentiable at q and (2.1) holds.

Conversely, we assume that y is differentiable at q . Let $G(y(p)) = \min(y(p), My(p) + p)$ for $p \in \Omega$. Since $G(y(p)) \equiv 0$, G is differentiable and $G'(y(p)) \equiv 0$. Moreover, we have

$$(My'(q) + I)_J = 0 \quad \text{and} \quad y'_{J^c}(q) = 0.$$

This implies

$$M_{J,J}y'_{J,J}(q) + I_{J,J} = 0 \quad \text{and} \quad M_{J,J}y'_{J,J^c}(q) = 0.$$

Hence $M_{J,J}$ is nonsingular, $y'_{J,J}(q) = -M_{J,J}^{-1}$ and $y'_{J,J^c}(q) = 0$. Moreover, $I - D + DM$ is nonsingular, and

$$(I - D + DM)y'(q) = -D.$$

We obtain (2.1). Now, we show $y(q)$ is nondegenerate. Suppose there is $i \in J^c$ such that

$$(My(q) + q)_i = y(q)_i = 0.$$

By the argument in the proof of Proposition 5.8.2 of [8], we have

$$(My(q) + q)'_i = y'(q)_i = 0,$$

which implies

$$M_{i,\cdot}y'_{\cdot,i}(q) + 1 = 0, \tag{2.2}$$

where $M_{i,\cdot}$ is the i th-row of M and $y'_{\cdot,i}(q)$ is the i th-column of $y'(q)$. By the argument above, $y'_{\cdot,i}(q) = 0$. This contradicts to (2.2). Hence $y(q)$ is nondegenerate. \blacksquare

2.1 Nondegenerate matrix

In this subsection, we consider the class of nondegenerate matrices [3, 8, 17, 23]. This class of matrices contains several classes of matrices characterized by the sign of the determinants of principal submatrices such as P-matrices whose principal minors are all positive.

Theorem 2.1 *Suppose that $\Omega \subseteq R_{LCP}(M)$ is an open set. Let y be a continuous function defined on Ω such that $y(q) \in SOL(q, M)$ for $q \in \Omega$. Assume that any principle submatrix $M_{J,J}$ of M is nonsingular then y is locally Lipschitz continuous in Ω with Lipschitz constant*

$$L = \max_{J \subseteq \{1, \dots, n\}} \|M_{J,J}^{-1}\|. \tag{2.3}$$

Moreover, the Clarke generalized Jacobian of y is defined by

$$\partial y(q) = \text{co}\{\lim y'(p) = -(I - D_p + D_p M)^{-1} D_p : p \rightarrow q, y(p) \text{ is nondegenerate}\}.$$

In addition,

$$-(I - D_q + D_q M)^{-1} D_q \in \partial y(q). \tag{2.4}$$

Proof: Take $q \in \Omega$. If $y(q)$ is nondegenerate, then by the first part of the proof for Lemma 2.1, we know that there is a neighborhood $\mathcal{N}_q \subseteq \Omega$ of q such that for any $p \in \mathcal{N}_q$,

$$y(p) = -(I - D_q + D_q M)^{-1} D_p.$$

Hence, y is differentiable and Lipschitz continuous in \mathcal{N}_q with Lipschitz constant

$$\|(I - D_q + D_q M)^{-1} D_q\| = \|M_{J_q, J_q}^{-1}\| \leq L.$$

Moreover, (2.4) holds with $\partial y(q) = \{y'(q)\}$.

For the case $y(q)$ is degenerate, there is a neighborhood $\mathcal{N}_q \subseteq \Omega$ of q such that for $p \in \mathcal{N}_q$,

$$J_q \subset J_p \quad \text{and} \quad I_q \subset I_p.$$

For $i \in K_q$, if $y_i(p) = 0$, then

$$(I(y(q) - y(p)))_i = 0.$$

If $y_i(p) > 0$, then $(My(q) + q)_i = (My(p) + p)_i = 0$, which gives

$$(M(y(q) - y(p)))_i = -(q - p)_i.$$

Hence for any $p \in \mathcal{N}_q$, we have

$$(I - D_{pq} + D_{pq}M)(y(q) - y(p)) = -D_{pq}(q - p),$$

where D_{pq} is a diagonal matrix with diagonals

$$(D_{pq})_{ii} = \begin{cases} 1, & i \in J_q \text{ and } i \in K_q \cap J_p \\ 0, & \text{otherwise.} \end{cases}$$

Hence, y is Lipschitz continuous in \mathcal{N}_q with Lipschitz constant L .

Therefore, y is locally Lipschitz continuous in Ω . By the Rademacher Theorem, y is almost everywhere differentiable in Ω . By Lemma 2.1, we obtain the Clarke Jacobian $\partial y(q)$.

In addition, it is easy to see that for any positive number ϵ , $y(q + \epsilon(I - D)e) = y(q)$ is a nondegenerate solution of $\text{LCP}(q + \epsilon(I - D_q)e, M)$. Hence y is differentiable at $q + \epsilon(I - D)e$ and $y'(q + \epsilon(I - D_q)e) = -(I - D_q + D_qM)^{-1}D_q$. This implies

$$\lim_{\epsilon \downarrow 0} y'(q + \epsilon(I - D_q)e) = -(I - D_q + D_qM)^{-1}D_q \in \partial y(q).$$

■

Corollary 2.1 *Suppose that M is a P-matrix. Then for any $p, q \in R^n$, we have*

$$\|y(q) - y(p)\| \leq L\|p - q\|, \quad (2.5)$$

where L is defined in (2.3).

Proof: It is known that for any $q \in R^n$, $\text{LCP}(q, M)$ has a unique solution $y(q)$ and $y(\cdot)$ is globally Lipschitz continuous in R^n [8]. By [7, Proposition 2.6.5], we have

$$y(p) - y(q) \in \text{co}\partial y([p, q])(p - q),$$

where $[p, q]$ is the segment between p and q . From Theorem 2.1, for any element $C \in \partial y([p, q])$, we have $\|C\| \leq L$. Hence (2.5) holds. ■

It was shown in [11] that M is a P-matrix if and only if $I - D + DM$ is nonsingular for any diagonal matrix D with diagonals $D_{ii} \in [0, 1]$. In [5], we showed that

$$\|y(q) - y(p)\| \leq \max_{D_{ii} \in [0, 1]} \|(I - D + DM)^{-1}D\| \|p - q\| \quad (2.6)$$

for M being a P-matrix. Obviously, we have

$$L = \max_{J \subseteq \{1, \dots, n\}} \|M_{J,J}^{-1}\| = \max_{D_{ii} \in \{0, 1\}} \|(I - D + DM)^{-1}D\| \leq \max_{D_{ii} \in [0, 1]} \|(I - D + DM)^{-1}D\|.$$

Hence the error bound (2.5) is sharper than (2.6). Furthermore, the error bound (2.5) can be used for a larger class of matrices than the class of the P-matrix. We use the following example to illustrate Theorem 2.1 and the new Lipschitz constant L .

Example 2.1 Consider the LCP(M, q) with a nondegenerate matrix $M = \begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix}$. The solution set has the following form

$$\begin{aligned} \text{SOL}(q, M) &= \emptyset, & \text{if } q_2 < 0; \\ \text{SOL}(q, M) &= \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ q_2 \end{pmatrix} \right\}, & \text{if } q_1 \geq 0, q_2 \geq 0; \\ \text{SOL}(q, M) &= \left\{ \begin{pmatrix} -q_1 \\ 0 \end{pmatrix}, \begin{pmatrix} \max(-q_1 - q_2, 0) \\ q_2 \end{pmatrix} \right\}, & \text{if } q_1 \leq 0, q_2 \geq 0. \end{aligned}$$

The matrix $I - D + DM$ is nonsingular if the diagonal matrix D having $D_{ii} \in \{0, 1\}$, but $I - D + DM$ may be singular for $D_{i,i} \in [0, 1]$, for instance, $D_{2,2} = 0.5$.

We can define a single valued solution function in $\text{SOL}(q, M)$ by the solution of the following optimization problem

$$y(q) = \operatorname{argmin}\{ \|Cv - b\|_2^2 : v \in \text{SOL}(q, M), q_2 \geq 0 \},$$

where $C \in R^{2 \times 2}$ is a positive semidefinite matrix and $b \in R^2$ is a vector. If we choose $C = I$ and $b = 0$, then it is the least-norm solution [8]. However, the least-norm solution is not unique in the region $\{q : q_1 < 0, q_2 \geq 0\}$. Let us choose $C = \text{diag}(0, 1)$ and $b = 0$. Then we have a piecewise linear single valued solution function

$$y(q) = \begin{cases} (0, 0)^T, & q_1 \geq 0, q_2 \geq 0 \\ (-q_1, 0)^T, & q_1 \leq 0, q_2 \geq 0 \end{cases}$$

in $\text{SOL}(q, M)$. The function $y(\cdot)$ is Lipschitz continuous with the Lipschitz constant $L = 1$ and it is continuously differentiable in the region $\{q \mid q_1 < 0, q_2 > 0\} \cup \{q \mid q_1 > 0, q_2 > 0\}$. Moreover the Clarke generalized Jacobian at q with $q_1 = 0$ and $q_2 > 0$ has the version

$$\partial y(q) = \left\{ \begin{pmatrix} -\alpha & 0 \\ 0 & 0 \end{pmatrix}, \alpha \in [0, 1] \right\}.$$

Remark 2.1 If M is a positive semi-definite matrix and the solution set $\text{SOL}(q, M)$ is nonempty, then the solution set $\text{SOL}(q, M)$ is convex and has a unique least-norm solution [8]. Hence we can define a single valued function by the least-norm solution. However, the least-norm solution is not necessarily Lipschitz continuous for M being positive semi-definite. See Example 3.4 in [15].

2.2 Z-matrix

Now we consider M is a Z-matrix. In this case, M can be singular and the solution set $\text{SOL}(q, M)$ can be nonempty or unbounded. It is known that if the feasible set $\text{FEA}(q, M)$ is not empty, then there is a unique least-element solution in the solution set $\text{SOL}(q, M)$ when M is a Z-matrix [8]. In the following, we denote the least-element solution by $y(q)$ if $\text{SOL}(q, M) \neq \emptyset$ and show the solution function is globally Lipschitz in $R_{LCP}(M)$ with a computable Lipschitz constant.

Lemma 2.2 Suppose that $M \in R^{n \times n}$ is a Z-matrix. If $q \in R_{LCP}(M)$, then for any $p \geq q$, we have $p \in R_{LCP}(M)$ and $y(p) \leq y(q)$.

Proof: It directly follows from that for any $q \in R_{LCP}(M)$, the least-element solution $y(q)$ of $LCP(q, M)$ is the solution of the linear program (1.6) and $FEA(q, M) \subseteq FEA(p, M)$. ■

Theorem 2.2 Let $M \in R^{n \times n}$ be a Z-matrix, $q \in R_{LCP}(M)$, and $y(q)$ be the least-element solution of $LCP(q, M)$. With the index set $J = J_q$ and diagonal matrix $D = D_q$, the following statements hold.

- (i) $M_{J,J}$ is nonsingular for $J \neq \emptyset$;
- (ii) $y(q) = -(I - D + DM)^{-1}Dq$;
- (iii) $\|(I - D + DM)^{-1}D\| \leq \mathcal{L} := \max\{\|M_{\alpha,\alpha}^{-1}\| \mid M_{\alpha,\alpha} \text{ is nonsingular for } \alpha \subseteq \{1, \dots, n\}\}$;
- (iv) There is a neighborhood \mathcal{N}_q of q such that $SOL(p, M) \neq \emptyset$ for any $p \in \mathcal{N}_q$. Thus, we have $-(I - D + DM)^{-1}D \in \partial y(q)$.

Proof: Note that we can choose a permutation matrix $U \in R^{n \times n}$ such that

$$UDU^T = \begin{pmatrix} I_{J,J} & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad UMU^T = \begin{pmatrix} M_{J,J} & M_{J,J^c} \\ M_{J^c,J} & M_{J^c,J^c} \end{pmatrix}.$$

Thus

$$U(I - D + DM)U^T = \begin{pmatrix} M_{J,J} & M_{J,J^c} \\ 0 & I \end{pmatrix}. \quad (2.7)$$

Since $LCP(Uq, UM)$ and $LCP(q, M)$ are equivalent, without loss of generality, we assume $U = I$ in (2.7), $J = \{1, 2, \dots, k\}$ and

$$M = \begin{pmatrix} M_{J,J} & M_{J,J^c} \\ M_{J^c,J} & M_{J^c,J^c} \end{pmatrix}, \quad y(q) = \begin{pmatrix} y_J(q) \\ 0 \end{pmatrix}, \quad q = \begin{pmatrix} q_J \\ q_{J^c} \end{pmatrix}.$$

Note that $y_J(q) > 0$. It follows $M_{J,J}y_J(q) + q_J = 0$. If $M_{J,J}$ is singular, then there exist a nonzero vector $x_0 \in R^{|J|}$ and a sufficiently small real positive number δ such that

$$M_{J,J}x_0 = 0, \quad y_J(q) \pm \delta x_0 > 0, \quad M_{J,J}(y_J(q) \pm \delta x_0) + q_J = 0.$$

Hence $y_J(q) \pm \delta x_0 \in FEA(q_J, M_{J,J})$ and $q_J \in R_{LCP}(M_{J,J})$. Since $M_{J,J}$ is also a Z-matrix, then there is a unique least-element solution $\bar{y}_J \in SOL(q_J, M_{J,J})$ such that

$$\min(\bar{y}_J, M_{J,J}\bar{y}_J + q_J) = 0, \quad \bar{y}_J \leq y_J(q) \quad \text{and} \quad \bar{y}_J \leq y_J(q) \pm \delta x_0. \quad (2.8)$$

From (2.8), we see that $\bar{y}_J \leq y_J(q)$ and $\bar{y}_J \neq y_J(q)$ due to that $x_0 \neq 0$. Let $\bar{y} = (\bar{y}_J^T, 0)^T$. Since $M_{J^c,J} \leq 0$ and

$$M_{J^c,J}\bar{y}_J + q_{J^c} \geq M_{J^c,J}y_J(q) + q_{J^c} \geq 0,$$

then it derives that $M\bar{y} + q \geq 0$. Therefore, $\bar{y} = (\bar{y}_J^T, 0)^T \in FEA(q, M)$ and $\bar{y} = (\bar{y}_J^T, 0)^T \geq y(q) = (y_J(q)^T, 0)^T$. It is a contradiction with $\bar{y}_J \leq y_J(q)$ and $\bar{y}_J \neq y_J(q)$. Hence $M_{J,J}$ is nonsingular.

(ii) From the nonsingularity of $M_{J,J}$, expression (2.7) with $U = I$ implies that $I - D + DM$ is nonsingular and

$$(I - D + DM)^{-1}D = \begin{pmatrix} M_{J,J} & M_{J,J^c} \\ 0 & I \end{pmatrix}^{-1} D = \begin{pmatrix} M_{J,J}^{-1} & 0 \\ 0 & 0 \end{pmatrix}. \quad (2.9)$$

From $(I - D)y(q) + D(My(q) + q) = 0$ and (2.9), we obtain the desired results.

(iii) This result is directly from (2.9).

(iv) If $y(q) > 0$, then by the discussion above, $D = I$ and M is nonsingular. Moreover from $y(q) = -M^{-1}q > 0$, there is a neighborhood of q such that for each point p in this neighborhood, the corresponding LCP(p, M) is solvable and $y(p) = -M^{-1}p > 0$. Hence $y(\cdot)$ is differentiable at q and $y'(q) = -M^{-1} = -(I - D + DM)^{-1}$ with $D = I$.

Now we consider the case that $y(q)$ has zero entries. Let us define

$$q(\epsilon) = q + \epsilon(I - D)e, \quad \text{for } \epsilon > 0$$

that is, $q_i(\epsilon) = q_i$ for $i \in J$ and $q_i(\epsilon) = q_i + \epsilon$ for $i \in J^c$.

By Lemma 2.2, $q(\epsilon) \in R_{LCP}(M)$ and $y(q(\epsilon)) \leq y(q)$. From the Lipschitz continuity of $y(\cdot)$, we have

$$q(\epsilon) \downarrow q, \quad y(q(\epsilon)) \uparrow y(q) \quad \text{as } \epsilon \downarrow 0.$$

This, together with $\min(y(q), My(q) + q) = 0$, derives that for all sufficiently small $\epsilon > 0$

$$y_J(q(\epsilon)) = -M_{J,J}^{-1}q_J(\epsilon) > 0, \quad y_{J^c}(q(\epsilon)) \equiv 0$$

$$(My(q(\epsilon)) + q(\epsilon))_{J^c} = M_{J^c,J}y_J(q(\epsilon)) + q_{J^c} + \epsilon e_{J^c} \geq M_{J^c,J}y_J(q) + q_{J^c} + \epsilon e_{J^c} > 0.$$

This implies that $y(q(\epsilon))$ is a strictly complementarity solution and the index sets of nonzero entries of $y(q)$ and $y(q(\epsilon))$ are identical. Furthermore, for each fixed $q(\epsilon)$, we can choose sufficiently small $\eta > 0$ such that for all $p \in \mathcal{B}(0, 1) := \{p \mid \|p\| \leq 1\}$,

$$\eta M_{J,J}^{-1}p_J < -M_{J,J}^{-1}q_J(\epsilon), \quad \eta M_{J^c,J}M_{J,J}^{-1}p_J - \eta p_{J^c} < q_{J^c}(\epsilon) - M_{J^c,J}M_{J,J}^{-1}q_J(\epsilon), \quad (2.10)$$

since $\mathcal{B}(0, 1)$ is a closed bounded compact set and

$$y_J(q(\epsilon)) = -M_{J,J}^{-1}q_J(\epsilon) > 0, \quad q_{J^c}(\epsilon) - M_{J^c,J}M_{J,J}^{-1}q_J(\epsilon) = (My(q(\epsilon)) + q(\epsilon))_{J^c} > 0. \quad (2.11)$$

Set $z \in R^n$ with $z_J = -M_{J,J}^{-1}(q(\epsilon) + \eta p)_J$ and $z_{J^c} = 0$. It is easy to verify from (2.11) that $z \in R_+^n$ and $z \in \text{FEA}(q(\epsilon) + \eta p, M)$.

Hence $q(\epsilon) + \eta p \in R_{LCP}(M)$ for all small η and $p \in \mathcal{B}(0, 1)$, that is, $q(\epsilon)$ is an interior point of $R_{LCP}(M)$. This, with that $y(q(\epsilon))$ is a strictly complementarity solution and $y(\cdot)$ is Lipschitz continuous, implies $y(\cdot)$ is differentiable at $q(\epsilon)$. Moreover, from (ii) of this theorem,

$$y'(q(\epsilon)) \equiv -(I - D + DM)^{-1}D$$

for all small $\epsilon > 0$, which implies $-(I - D + DM)^{-1}D \in \partial y(q)$.

In particular, for the case $J = \emptyset$, we have $q \geq 0$ and $y(q) = 0$. Choose $q(\epsilon) = q + \epsilon e$. Since $q(\epsilon) > 0$ for all $\epsilon > 0$, it is easy to verify that $q(\epsilon)$ is an interior point of $R_{LCP}(M)$. Note that $y(q(\epsilon)) \equiv 0$ and $My(q(\epsilon)) + q(\epsilon) > 0$. Thus y is differentiable at $q(\epsilon)$ and $y'(q(\epsilon)) \equiv 0$. This yields $0 \in \partial y(q)$. We complete the proof. \blacksquare

Theorem 2.3 *Suppose $M \in R^{n \times n}$ is a Z-matrix. Let $y(p)$ and $y(q)$ be the least-element solutions of LCP(p, M) and LCP(q, M), respectively, for any $p, q \in \text{LCP-Range}(M)$. Then we have*

$$\|y(p) - y(q)\| \leq \mathcal{L}\|p - q\|. \quad (2.12)$$

Proof: It is easy to see that for any $\lambda \in [0, 1]$, the feasible set $\text{FEA}(\lambda q + (1 - \lambda)p, M)$ is not empty and thus we have the least-element solution $y(\lambda q + (1 - \lambda)p)$ of $\text{LCP}(\lambda q + (1 - \lambda)p, M)$. From Theorem 2.2, we can see $y(\cdot)$ is Lipschitz continuous on the segment between p and q . Therefore, $y(\cdot)$ is almost everywhere differentiable on the segment between p and q , and we can write

$$y(p) - y(q) = \int_0^1 y'(\lambda q + (1 - \lambda)p)(p - q)d\lambda.$$

See [7, Proposition 2.6.5]. Moreover, if y is differentiable, then we have $y'(\lambda q + (1 - \lambda)p) = \partial y(\lambda q + (1 - \lambda)p)$. Hence by (iii) and (iv) of Theorem 2.2, we complete the proof. \blacksquare

In the following, we show that the Lipschitz constant \mathcal{L} is much smaller than the constant derived by Mangasarian and Shiau [15].

By Theorem 3.11.18 in [8], $y(p)$ and $y(q)$ are the unique solutions of the following linear programming problems, respectively,

$$\begin{aligned} & \text{maximize} && -e^T z & & \text{maximize} && -e^T z \\ & \text{subject to} && \begin{pmatrix} -M \\ -I \end{pmatrix} z \leq \begin{pmatrix} p \\ 0 \end{pmatrix}, & & \text{subject to} && \begin{pmatrix} -M \\ -I \end{pmatrix} z \leq \begin{pmatrix} q \\ 0 \end{pmatrix}. \end{aligned} \quad (2.13)$$

Hence, applying the perturbation error bound for linear programming problems in [15] yields

$$\|y(p) - y(q)\| \leq v_\infty(M)\|p - q\|, \quad (2.14)$$

where

$$v_\infty(M) = \sup_{u,v} \left\{ \|u\|_1 \mid \begin{array}{l} \|u^T P\|_1 = 1 \text{ and rows of } P := \begin{pmatrix} M \\ I \end{pmatrix} \text{ corresponding} \\ \text{to nonzero elements of } u \text{ are linearly independent} \end{array} \right\}.$$

Proposition 2.1 *For any matrix $M \in R^{n \times n}$, the following inequality holds*

$$\mathcal{L}_\infty \leq v_\infty(M). \quad (2.15)$$

Proof: Let $W = \text{diag}(U, U)$ be a block matrix, where $U \in R^{n \times n}$ is a permutation matrix. Then we have

$$\begin{aligned} \sup_{u \in R^{2n}} \{ \|u\|_1 \mid \|u^T P\|_1 = 1, u \in \mathcal{U} \} &= \sup_{u \in R^{2n}} \{ \|Wu\|_1 \mid \|(Wu)^T W P\|_1 = 1, u \in \mathcal{U} \} \\ &= \sup_{u \in R^{2n}} \{ \|Wu\|_1 \mid \|(Wu)^T W P U\|_1 = 1, u \in \mathcal{U} \}, \end{aligned}$$

where

$$\mathcal{U} = \{u \in R^{2n} \mid \text{rows of } P \text{ corresponding to nonzero elements of } u \text{ are linearly independent}\}.$$

Hence, we have

$$v_\infty(UMU^T) = v_\infty(M).$$

Then for any nonsingular principle submatrix $M_{J,J}$, without loss of generality, we assume

$$M = \begin{pmatrix} M_{J,J} & M_{J,J^c} \\ M_{J^c,J} & M_{J^c,J^c} \end{pmatrix} \quad \text{and} \quad I = \begin{pmatrix} I_{J,J} & 0 \\ 0 & I_{J^c,J^c} \end{pmatrix}.$$

Let $b \in R^{|J|}$ with $b_i = 1$ and $b_j = 0$ for $j \neq i, j = 1, \dots, |J|$ such that $\|M_{J,J}^{-T}b\|_1 = \|M_{J,J}^{-T}\|_1$.

Note that $\|M_{J,J}^{-T}\|_1 = \|M_{J,J}^{-1}\|_\infty$. Define $v = \begin{pmatrix} M_{J,J}^{-T}b \\ -M_{J^c,J}^T M_{J,J}^{-T}b \end{pmatrix} \in R^n$. Then

$$\|v^T \begin{pmatrix} M_{J,J} & M_{J,J^c} \\ 0 & I \end{pmatrix}\|_1 = \|b\|_1 = 1, \quad \text{rank} \begin{pmatrix} M_{J,J} & M_{J,J^c} \\ 0 & I \end{pmatrix} = n$$

and $\|v\|_1 \geq \|M_{J,J}^{-T}b\|_1 = \|M_{J,J}^{-1}\|_\infty$, which implies $v_\infty(M) \geq \mathcal{L}_\infty$. ■

Remark 2.2. The Lipschitz constant $v_\infty(M)$ is generally quite difficult to compute and it is often much larger than \mathcal{L}_∞ . Consider

$$M = \begin{pmatrix} 0 & 0 \\ -\tau & 0 \end{pmatrix}, \quad \tau > 0.$$

It is easy to find $\mathcal{L}_\infty = 0$ and $v_\infty(M) \geq \frac{1}{\tau} \rightarrow \infty$, as $\tau \rightarrow 0$.

Note that $\mathcal{L} = L$ if all principal submatrices of M are nonsingular.

3 Convergence of the generalized Newton method

In this section, we consider the convergence of the generalized Newton method for solving (1.4). We set $\theta = 0$, for the simplicity. Similar results hold for $\theta \in (0, 1)$.

We redefine the function $H : R^m \rightarrow R^m$ by

$$\begin{aligned} H(u) &= x^{h,i} + h[Au + By(u) + f(t_{h,i+1})] \\ y(u) &\in \text{SOL}(q(u), M), \end{aligned} \quad (3.1)$$

where

$$q(u) := Nu + g(t_{h,i+1}).$$

We show that for a certain time step size $h > 0$, $x^{h,i+1}$ is the unique solution of

$$F(u) = u - H(u) = 0 \quad (3.2)$$

near $x^{h,i}$, and the generalized Newton method

$$u^{k+1} = u^k - V_k^{-1}F(u^k) \quad (3.3)$$

converges to $x^{h,i+1}$ from the starting point $u^0 = x^{h,i}$, where

$$V_k = I - h[A - B(I - D_k + D_k M)^{-1}D_k N] \in \partial F(u^k) \quad \text{with} \quad D_k = D_{q(u^k)}.$$

Let

$$\kappa = \|A\| + \mathcal{L}\|B\|\|N\|.$$

We take $h < 1/\kappa$, and set

$$\gamma = \frac{h\|Ax^{h,i} + By^{h,i} + f(t_{h,i+1})\|}{1 - h\kappa}, \quad \mathcal{B}(x^{h,i}, \gamma) = \{z : \|z - x^{h,i}\| \leq \gamma\}.$$

Lemma 3.1 *Assume that M is nondegenerate matrix or a Z-matrix, and $q(z) \in R_{LCP}(M)$ for all $z \in \mathcal{B}(x^{h,i}, \gamma)$. Then (3.2) has a solution in $\mathcal{B}(x^{h,i}, \gamma)$.*

Proof: Suppose $u \in \mathcal{B}(x^{h,i}, \gamma)$. By Theorem 2.1 and Theorem 2.2, there is $v(u) \in \text{SOL}(Nu + g(t_{h,i+1}), M)$ such that

$$\begin{aligned} \|H(u) - x^{h,i}\| &\leq h(\|Ax^{h,i} + By^{h,i} + f(t_{h,i+1})\| + \|A(u - x^{h,i}) + B(v(u) - v(x^{h,i}))\|) \\ &\leq h(\|Ax^{h,i} + By^{h,i} + f(t_{h,i+1})\| + (\|A\| + \mathcal{L}\|B\|\|N\|)\gamma) \\ &= \gamma. \end{aligned}$$

This implies that $H(u) \in \mathcal{B}(x^{h,i}, \gamma)$. Hence H maps $\mathcal{B}(x^{h,i}, \gamma)$ into $\mathcal{B}(x^{h,i}, \gamma)$. Suppose that $u, w \in \mathcal{B}(x^{h,i}, \gamma)$. Using Theorem 2.1 and Theorem 2.2 again, we obtain

$$\|H(u) - H(w)\| = h\|A(u - w) + B(v(u) - v(w))\| \leq h\kappa\|u - w\|.$$

Hence $H : \mathcal{B}(x^{h,i}, \gamma) \rightarrow \mathcal{B}(x^{h,i}, \gamma)$ is a contraction mapping. By the Banach fixed point theorem [18], H has a fixed point in $\mathcal{B}(x^{h,i}, \gamma)$, which is the solution of (3.2) in $\mathcal{B}(x^{h,i}, \gamma)$. ■

Under the conditions of Lemma 3.1, we can choose $y(u)$ from $\text{SOL}(q(u), M)$ such that F is a Lipschitz continuous function in $\mathcal{B}(x^{h,i}, \gamma)$. By the Rademacher Theorem [7], F is differentiable almost everywhere. Therefore, we can define the Clarke generalized Jacobian

$$\partial F(x) = \text{co}\{\lim F'(x^k) : x^k \rightarrow x, x^k \in \Omega_F\},$$

where Ω_F denotes the set of points at which F is differentiable, and co denotes the convex hull.

From the convergence analysis of the generalized Newton method for nonsmooth equations in [20], we know that under the condition that F is well-defined in a domain containing $x^{h,i+1}$ and all matrices in $\partial F(x^{h,i+1})$ are nonsingular, there is a neighborhood of $x^{h,i+1}$ such that the generalized Newton method (3.3) converges to the fixed point $x^{h,i+1}$ of H superlinearly from any starting point in the neighborhood. However, it is too hard to find such neighborhood and too strong to assume all matrices in $\partial F(x^{h,i+1})$ are nonsingular for a Z-matrix DLCS.

In the following, we show that for certain small h , the generalized Newton method (3.3), with the starting point $u^0 = x^{h,i}$ and a special matrix V_k in the generalized Jacobian $\partial F(u^k)$, is well-defined and converges to $x^{h,i+1}$ superlinearly. Moreover, we give a method to compute the matrix $V_k \in \partial F(u^k)$.

The following theorem presents a nonsingular matrix in the generalized Jacobian $\partial F(u)$.

Theorem 3.1 *Let $J = J_q$ and $D = D_q$. Under the assumption of Lemma 3.1, we have*

$$V(u) = I - h[A - B(I - D + DM)^{-1}DN] \in \partial F(u).$$

Proof: To show $V(u) \in \partial F(u)$, it is sufficient to show that there is a sequence $\{u_k\}$ such that $u_k \rightarrow u$, $y'(q(u_k))$ is differentiable and

$$y'(q(u_k)) = -(I - D + DM)^{-1}DN,$$

since it implies that F is differentiable at u_k and

$$F'(u_k) = I - h[A - B(I - D + DM)^{-1}DN].$$

For sufficiently small $\epsilon > 0$, we set

$$q_\epsilon(u) = q(u) + \epsilon(I - D)e.$$

From the proof of Theorem 2.1 and Theorem 2.2, we see that $y(q_\epsilon(u)) = y(q(u))$ is a nondegenerate solution of $\text{LCP}(q_\epsilon(u), M)$. Hence y is differentiable at $q_\epsilon(u)$ and $q_\epsilon(u) + \eta p \in R_{\text{LCP}}(M)$ for all small η and $p \in \mathcal{B}(0, 1)$.

We choose a sequence of positive numbers ϵ_k with $\lim_{k \rightarrow \infty} \epsilon_k = 0$.

Case 1: $\text{rank}(N) = n$: Since N is of full row rank, for each ϵ_k , we set $u_k = u + \epsilon_k N^T (N N^T)^{-1} (I - D)e$. Then u_k is a solution of the linear equations

$$N u_k = N u + \epsilon_k (I - D)e \quad \text{and} \quad \lim_{k \rightarrow \infty} u_k = u.$$

Then y is differentiable at $q_{\epsilon_k}(u) = q(u) + \epsilon_k (I - D)e = q(u_k) = N u_k + g(t_{h,i+1})$ and $y'(q(u_k)) = -(I - D + D M)^{-1} D N$.

Case 2: $\text{rank}(N) < n$: Assume $n \leq m$. We choose a sequence of positive numbers η_ℓ with $\lim_{\ell \rightarrow \infty} \eta_\ell = 0$, and an $n \times n$ diagonal matrix

$$\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n), \quad (|\lambda_i| = 1, i = 1, 2, \dots, n)$$

such that $\Lambda u \geq 0$ and

$$\text{rank}(N + \eta_\ell N_1) = n, \quad \text{for } \ell = 1, 2, \dots,$$

where $N_1 := (\Lambda, 0) \in R^{n \times m}$, since the leading m th-order principle submatrix of N has at most n different eigenvalues.

Define $q^\ell(u) = (N + \eta_\ell N_1)u + g(t_{h,i+1})$. Since

$$q^\ell(u) \geq q(u) \quad \text{and} \quad \lim_{\ell \rightarrow \infty} q^\ell(u) = q(u),$$

by assumptions of this theorem, $\text{LCP}(q^\ell(u), M)$ has a solution $y(q^\ell(u))$, and

$$\lim_{\ell \rightarrow \infty} y(q^\ell(u)) = y(q(u)).$$

Define $D_\ell = \text{diag}(d_1^\ell, \dots, d_n^\ell)$ with

$$d_i^\ell = \begin{cases} 1, & y_i(q^\ell(u)) > 0 \\ 0, & \text{otherwise.} \end{cases}$$

Following the proof for Case 1, we have y is differentiable at

$$q^\ell(u_k) = q^\ell(u) + \epsilon_k (I - D_\ell)e$$

and

$$y'(q^\ell(u_k)) = -(I - D_\ell + D_\ell M)^{-1} D_\ell (N + \eta_\ell N_1).$$

Moreover, from the definition of $q^\ell(u_k)$, we have

$$\begin{aligned} \|q^\ell(u_k) - q(u)\| &\leq \|q^\ell(u_k) - q^\ell(u)\| + \|q^\ell(u) - q(u)\| \\ &\leq \epsilon_k n + \|q^\ell(u) - q(u)\| \rightarrow 0 \quad \text{as } k \rightarrow \infty, \ell \rightarrow \infty. \end{aligned}$$

Taking a subsequence $q^{\ell_i}(u_{k_i})$ of $q^\ell(u_k)$ and using

$$y'(q^{\ell_i}(u_{k_i})) = -(I - D_{\ell_i} + D_{\ell_i}M)^{-1}D_{\ell_i}(N + \eta_{\ell_i}N_1)$$

we obtain

$$\begin{aligned} & \lim_{\ell_i \rightarrow \infty} (I - h[A - B(I - D_{\ell_i} + D_{\ell_i}M)^{-1}D_{\ell_i}(N + \eta_{\ell_i}N_1)]) \\ &= I - h[A - B(I - D + DM)^{-1}DN] \in \partial F(u). \end{aligned}$$

Finally, we consider the case that $\text{rank}(N) < n$ and $n > m$. Let us consider the equivalent augmented LCP($\bar{N}\bar{u} + g(t_{h,i+1}), M$), where $\bar{N} = (N, 0) \in R^{n \times n}$ and $\bar{u} = (u^T, 0)^T \in R^n$, then LCP($\bar{N}\bar{u} + g(t_{h,i+1}), M$) and LCP($Nu + g(t_{h,i+1}), M$) have the same solutions. From the above proof for $\text{rank}(N) < n$ and $n \leq m$, we can get the generalized Jacobian of the augmented function. Note that the generalized Jacobian of the augmented function confined to R^m is the generalized Jacobian of the original function [7]. We complete the proof. ■

Now we present the convergence theorem of the generalized Newton method (3.3). Let

$$\gamma_1 = \frac{h\|Ax^{h,i} + By^{h,i} + f(t_{h,i+1})\|}{1 - 3h\kappa}, \quad \mathcal{B}(x^{h,i}, \gamma_1) = \{z : \|z - x^{h,i}\| \leq \gamma_1\}.$$

Theorem 3.2 *Under the assumptions of Lemma 3.1, if $3h\kappa < 1$, then the generalized Newton method (3.3) with the starting point $x^{h,i}$ converges to $x^{h,i+1}$ superlinearly.*

Proof: For $u \in \mathcal{B}(x^{h,i}, \gamma_1)$, we define

$$G(u) = u - V(u)^{-1}F(u),$$

where

$$V(u) = I - h[A - B(I - D_{q(u)} + D_{q(u)}M)^{-1}D_{q(u)}N].$$

Recall

$$\mathcal{L} = \max\{\|M_{\alpha,\alpha}^{-1}\| \mid M_{\alpha,\alpha} \text{ is nonsingular for } \alpha \subseteq \{1, \dots, n\}\} \quad \text{and} \quad \kappa = \|A\| + \mathcal{L}\|B\|\|N\|.$$

We obtain

$$\begin{aligned} \|A - B(I - D_{q(u)} + D_{q(u)}M)^{-1}D_{q(u)}N\| &\leq \|A\| + \|B\|\|(I - D_{q(u)} + D_{q(u)}M)^{-1}D_{q(u)}\|\|N\| \\ &\leq \|A\| + \mathcal{L}\|B\|\|N\| \\ &\leq \kappa. \end{aligned}$$

Hence, the assumption $3h\kappa < 1$ implies that $V(u)$ is nonsingular and

$$\|V(u)^{-1}\| \leq \frac{1}{1 - h\|A - B(I - D_{q(u)} + D_{q(u)}M)^{-1}D_{q(u)}N\|} \leq \frac{1}{1 - h\kappa}. \quad (3.4)$$

Similar to the proof of Lemma 3.1, we have

$$\|H(u) - x^{h,i}\| \leq h \left(\|Ax^{h,i} + By^{h,i} + f(t_{h,i+1})\| + \kappa\gamma_1 \right)$$

and thus

$$\begin{aligned}
\|G(u) - x^{h,i}\| &\leq \|V(u)^{-1}(V(u)(u - x^{h,i}) - u + H(u))\| \\
&\leq \|V(u)^{-1}\| \| (I - V(u))(u - x^{h,i}) \| + \|V(u)^{-1}\| \|H(u) - x^{h,i}\| \\
&\leq \frac{h\kappa\gamma_1}{1 - h\kappa} + \frac{h\|Ax^{h,i} + By^{h,i} + f(t_{h,i+i})\| + h\kappa\gamma_1}{1 - h\kappa} \\
&= \gamma_1.
\end{aligned} \tag{3.5}$$

Therefore, for any $u \in \mathcal{B}(x^{h,i}, \gamma_1)$, $G(u)$ is well-defined and $G(u) \in \mathcal{B}(x^{h,i}, \gamma_1)$. By the Banach fixed point theorem, G has a fixed point \hat{u} in $\mathcal{B}(x^{h,i}, \gamma_1)$. By the definition of G and (3.4), \hat{u} is also a fixed point of H in $\mathcal{B}(x^{h,i}, \gamma_1)$. Moreover, from

$$\|H(u) - H(w)\| \leq h\kappa\|u - w\|, \quad \text{for } u, w \in \mathcal{B}(x^{h,i}, \gamma_1),$$

H is a contraction mapping on $\mathcal{B}(x^{h,i}, \gamma_1)$. Hence \hat{u} is the unique fixed point of H in $\mathcal{B}(x^{h,i}, \gamma_1)$. We set $x^{h,i+1} = \hat{u}$.

Consequently, G has a unique fixed point $x^{h,i+1} \in \mathcal{B}(x^{h,i}, \gamma_1)$ and the generalized Newton method (3.3) with the starting point $x^{h,i}$ generates a sequence $\{u^k\}$ which satisfies $u^k = G(u^{k-1}) \in \mathcal{B}(x^{h,i}, \gamma_1)$ and converges to $x^{h,i+1}$. Furthermore, from Theorem 3.1, $x^{h,i+1} \in \mathcal{B}(x^{h,i}, \gamma) \subset \mathcal{B}(x^{h,i}, \gamma_1)$ and $\gamma < \gamma_1$, that is $x^{h,i+1}$ is an interior point of $\mathcal{B}(x^{h,i}, \gamma_1)$. Hence, from that V_k is in the generalized Jacobian of F , and F is semi-smooth [20], we deduce that the convergence is locally superlinear. \blacksquare

4 Least-element Z-matrix DLCS

How to choose a solution from the solution set $\text{SOL}(Nx + g(t), M)$ is very important for the existence of solutions of the differential system and convergence of a numerical scheme. In this section, we show that choosing the least-element solution from $\text{SOL}(Nx + g(t), M)$ for the Z-matrix DLCS is essential.

In Section 2, we show that the least-element solution $y(q)$ of the Z-matrix LCP(q, M) is Lipschitz continuous with respect to q and the Lipschitz constant \mathcal{L} is computable and smaller than the constant derived from [15]. Based on the Lipschitz continuity, we find a positive constant T_0 such that the least-element LCS (1.7) has a unique solution (x^*, y^*) such that x^* is continuously differentiable and y^* is Lipschitz continuous on $[0, T_0]$. Moreover, using the Lipschitz continuity, we can choose the time step size such that the implicit least-element time-stepping scheme (1.8) using Newton's method (3.3) converges to (x^*, y^*) .

Theorem 4.1 *Suppose that $M \in R^{n \times n}$ is a Z-matrix and at the initial point, there is $v \in R^n$ such that*

$$Nx(0) + g(0) + Mv > 0, \quad v > 0. \tag{4.1}$$

Then the following statements hold.

(i) *There are constants $T > 0$ and $\gamma > 0$ such that*

$$Nz + g(t) \in R_{LCP}(M), \quad \text{for } t \in [0, T], z \in \mathcal{B}(x_0, \gamma) = \{z : \|z - x_0\| \leq \gamma\}. \tag{4.2}$$

(ii) The least-element LCS (1.7) has a unique solution $(x^*, y^*) \in C^1[0, T_0] \times C[0, T_0]$, where

$$T_0 = \min\left\{T, \frac{\gamma}{c_0 + \kappa\gamma}\right\}, \quad c_0 = \|Ax_0 + By_0 + f\|, \quad \kappa = \|A\| + \mathcal{L}\|B\|\|N\|.$$

(iii) If the time step size $h < 1/3\kappa$, then the generalized Newton method (3.3) with the starting point $x^{h,i}$ converges to $x^{h,i+1}$ superlinearly, which is the unique fixed point of $H(u)$ defined by

$$\begin{aligned} H(u) &= x^{h,i} + h[Au + By(u) + f(t_{h,i+1})] \\ y(u) &= \operatorname{argmin}\{e^T v \mid v \in \operatorname{SOL}(q(u), M)\}. \end{aligned}$$

(iv) For the implicit least-element time-stepping scheme (1.8), we have the error bound

$$\|x^{h,i} - x(t_{h,i})\| \leq O(h). \quad (4.3)$$

Proof: (i) Let $x_0(t) \equiv x_0$. Condition (4.1) indicates that the feasible set $\operatorname{FEA}(Nx(0) + g(0), M)$ has an interior point v . Hence there are constants $T > 0$ and $\gamma > 0$ such that (4.2) holds.

(ii) From (4.2) the solution set $\operatorname{SOL}(Nx_0(t) + g(t), M) \neq \emptyset$ for all $t \in [0, T_0]$. Let

$$y(x_0(t)) = \operatorname{argmin}\{e^T v \mid Nx_0(t) + g(t) + Mv \geq 0, v \geq 0\}.$$

Then by Theorem 2.2, $y(x_0(\cdot))$ is Lipschitz continuous in $[0, T_0]$.

Now we define sequences $\{x_k\}$ and $\{y_k\}$ over $[0, T_0]$ by the following recursion, for $k = 1, 2, \dots$,

$$\begin{aligned} x_{k+1}(t) &= x_0(t) + \int_0^t (Ax_k(s) + By(x_k(s)) + f(s)) ds \\ y(x_{k+1}(t)) &= \operatorname{argmin}\{e^T v \mid Nx_{k+1}(t) + g(t) + Mv \geq 0, v \geq 0\}. \end{aligned} \quad (4.4)$$

Now we show $x_k(t) \in \mathcal{B}(x_0, \gamma)$ for $t \in [0, T_0]$ and $k = 1, 2, \dots$. Note that

$$\|x_1(t) - x_0(t)\| = \left\| \int_0^t (Ax_0(s) + By(x_0(s)) + f(s)) ds \right\| \leq c_0 T_0 \leq \gamma.$$

Suppose $\|x_k(t) - x_0(t)\| \leq \gamma$. From Theorem 2.2, we have

$$\begin{aligned} \|x_{k+1}(t) - x_0(t)\| &\leq (\|A\| + \mathcal{L}\|B\|\|N\|)T_0\gamma + c_0 T_0 \\ &\leq T_0(\gamma\kappa + c_0) \\ &\leq \gamma. \end{aligned}$$

Thus $x_k(t) \in \mathcal{B}(x_0, \gamma)$ for $t \in [0, T_0]$ and $k = 0, 1, \dots$. Moreover, we have

$$\begin{aligned} \|x_{k+1} - x_k\| &\leq (\|A\| + \mathcal{L}\|B\|\|N\|)T_0\|x_k - x_{k-1}\| \\ &\leq (\kappa T_0)^k c_0 T_0 \\ &= c_0 T_0 \left(\frac{\kappa\gamma}{c_0 + \kappa\gamma} \right)^k. \end{aligned}$$

Then $\{x_k\}$ is a Cauchy sequence in $C[0, T_0]$ and thus there is $x^* \in C[0, T_0]$ such that $\lim_{k \rightarrow \infty} x_k = x^*$ and

$$x^*(t) = x_0(t) + \int_0^t (Ax^*(s) + By(x^*(s)) + f(s))ds$$

for $t \in [0, T_0]$. This implies that x^* is a solution of the least-element LCS (1.7). Moreover, from the Lipschitz continuity of y and f , $\dot{x} = Ax + By + f$ is continuous on $[0, T_0]$, that is, $x^* \in C^1[0, T_0]$.

Now we show that the solution x^* is unique. Suppose there are two solutions u and v . Then by the Lipschitz continuity of the least-element solution y , we have

$$\|u - v\| \leq (\|A\| + \mathcal{L}\|B\|\|N\|)T_0\|u - v\| = \kappa T_0\|u - v\|.$$

Since $\kappa T_0 < 1$, we must have $u = v$.

(iii) This result is directly from Theorem 3.2.

(iv) Since the right-hand-side function $Ax(t) + y(x(t)) + f(t)$ is Lipschitz continuous on $[0, T_0]$, the implicit least-element time-stepping scheme (1.8) has at least linear convergence rate. \blacksquare

Now we use the following example to illustrate the least-element LCS (1.7) and the implicit least-element time-stepping scheme (1.8) for the differential Z-matrix LCS.

Example 4.1 We consider the following differential Z-matrix LCS

$$\begin{aligned} \frac{d}{dt} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} &= \begin{bmatrix} -\alpha_1 & 0 \\ 0 & -\alpha_2 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{bmatrix} \alpha_3 & 0 & 0 & -\alpha_3 \\ 0 & \alpha_4 & \alpha_4 & 0 \end{bmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} + f(t) \\ 0 &\leq \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} \perp \begin{bmatrix} -1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} + g(t) \geq 0. \end{aligned} \quad (4.5)$$

The given matrices and functions in this example are

$$\begin{aligned} A &= \begin{bmatrix} -\alpha_1 & 0 \\ 0 & -\alpha_2 \end{bmatrix}, \quad B = \begin{bmatrix} -\alpha_3 & 0 & 0 & \alpha_3 \\ 0 & \alpha_4 & \alpha_4 & 0 \end{bmatrix}, \quad N = \begin{bmatrix} -1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \end{bmatrix}, \\ M &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad f(t) = \begin{pmatrix} \alpha_5 \sin(\omega t) \\ 0 \end{pmatrix}, \quad g(t) \equiv 0. \end{aligned}$$

We can compute the Lipschitz constant \mathcal{L} of the least-element solution $y(\cdot)$ and find

$$\mathcal{L} = 1 \quad \text{and} \quad \kappa = \|A\| + \mathcal{L}\|B\|\|N\| = \max\{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}.$$

The solution set of the LCP in (4.1) can be explicitly given as
 $\text{SOL}(Nx(t), M)$

$$= \left\{ \left\{ \begin{pmatrix} x_1(t) \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} x_1(t) \\ x_2(t) \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} x_1(t) \\ 0 \\ x_2(t) \\ 0 \end{pmatrix}, \begin{pmatrix} x_1(t) \\ x_2(t) \\ x_2(t) \\ 0 \end{pmatrix} \right\}, \quad x_1(t) \geq 0, x_2(t) \geq 0 \right. \\ \left. \left\{ \begin{pmatrix} 0 \\ 0 \\ 0 \\ -x_1(t) \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ x_2(t) \\ -x_1(t) \end{pmatrix}, \begin{pmatrix} 0 \\ x_2(t) \\ 0 \\ -x_1(t) \end{pmatrix}, \begin{pmatrix} 0 \\ x_2(t) \\ x_2(t) \\ -x_1(t) \end{pmatrix} \right\}, \quad x_1(t) < 0, x_2(t) \geq 0, \right.$$

and the least-element solution is

$$y(Nx(t)) = \begin{cases} \begin{pmatrix} x_1(t) \\ 0 \\ 0 \\ 0 \end{pmatrix}, & x_1(t) \geq 0, x_2(t) \geq 0 \\ \begin{pmatrix} 0 \\ 0 \\ 0 \\ -x_1(t) \end{pmatrix}, & x_1(t) < 0, x_2(t) \geq 0. \end{cases}$$

The corresponding least-element solution system is

$$\begin{cases} \dot{x}_1(t) = -(\alpha_1 + \alpha_3)x_1(t) + \alpha_5 \sin(\omega t), \\ \dot{x}_2(t) = -\alpha_2 x_2(t), \end{cases} \quad x_2(t) \geq 0.$$

A continuously differentiable solution of DLCS (4.1) corresponding to the least-element solutions exists and can be given by

$$x(t) = \begin{pmatrix} \frac{\alpha_5(\alpha_1 + \alpha_3) \sin(\omega t) - \omega \alpha_5 \cos(\omega t)}{(\alpha_1 + \alpha_3)^2 + \omega^2} + c_1 e^{-(\alpha_1 + \alpha_3)t} \\ c_2 e^{-\alpha_2 t} \end{pmatrix}, \quad x(0) = (x_1(0), x_2(0))^T$$

for any initial value $x(0)$ with $x_2(0) \geq 0$. If we choose the initial value $x(0) = (0, 1)^T$ and parameters

$$\alpha_1 = 1, \quad \alpha_2 = 2, \quad \alpha_3 = 3, \quad \alpha_4 = 1.3, \quad \alpha_5 = 1.2, \quad \omega = 10,$$

the exact solution corresponding to the least-element solutions is

$$x(t) = \begin{pmatrix} \frac{4.8 \sin(10t) - 12 \cos(10t)}{116} + \frac{3}{29} e^{-4t} \\ e^{-2t} \end{pmatrix}, \quad x(0) = (0, 1)^T.$$

Now, we consider the implementation of the generalized Newton method. For $x_1(t) > 0$, the least element solution $y(Nx(t))$ has one positive entry $y_1(Nx(t)) > 0$. By Theorem 2.2, let $D = \text{diag}(1, 0, 0, 0)$, we obtain

$$Y = (I - D + DM)^{-1}D = D \in \partial y(Nx(t)).$$

Choose the time step size $h = 0.1 < 1/3\kappa = 1/9$. By Theorem 3.2,

$$I - h(A - BYN) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - h \begin{pmatrix} -\alpha_1 - \alpha_3 & 0 \\ 0 & -\alpha_2 \end{pmatrix} \in \partial F(x(t)).$$

It is nonsingular and bounded. We can use it in the generalized Newton method (3.3). Similarly, we can give the generalized Jacobian for the case $x_1(t) = 0$ and $x_1(t) \leq 0$.

It is worth noting that choosing a non-least element solution from $\text{SOL}(Nx(t), M)$, we cannot have a Lipschitz continuous solution, and use the generalized Newton method (3.3).

A matrix $M \in R^{n \times n}$ is called a *hidden Z-matrix* [8], if there exist Z-matrices X and Y in $R^{n \times n}$ and nonnegative vectors r and s in R^n such that X is nonsingular and

$$MX = Y, \quad r^T X + s^T Y > 0. \quad (4.6)$$

The class of hidden Z-matrices contains the class of Z-matrices. An H-matrix with positive diagonals is a hidden Z-matrix. All results concerning the class of Z-matrices in this paper can be extended to the class of hidden Z-matrices, by using Theorems 3.11.17 – 3.11.19 and their proof in [8]. In particular, the least-element solution z^* of the LCP(q, M) with respect to the partial ordering $\preceq_{\mathcal{C}}$ can be obtained by solving the following linear programming problem

$$\begin{aligned} & \text{minimize} && e^T X^{-1} z \\ & \text{subject to} && z \geq 0, \quad q + Mz \geq 0, \end{aligned}$$

where $\mathcal{C} = \text{pos}X$ is the pointed convex cone and X is the Z-matrix in (4.6).

Final Remark

In this paper, we propose a superlinearly convergent generalized Newton method (3.3) with a specific matrix in the generalized Jacobian to solve the system of nonlinear equations with linear complementarity constraints (1.4) in the implicit or semi-implicit time-stepping scheme (1.3). We show the generalized Newton method is well-defined and converges superlinearly for M being a nondegenerate matrix or a Z-matrix. It is worth noting that the solution set of the nondegenerate matrix or Z-matrix linear complementarity constraints can be unbounded. The right-hand side of the ordinary differential equation in the nondegenerate matrix or Z-matrix linear complementarity system is multifunction. We show that the least-element solution of the Z-matrix linear complementarity constraints is Lipschitz continuous with a computable Lipschitz constant \mathcal{L} . Example 4.1 shows that it is necessary to choose the least-element solution at each time t to get a solution $x(t) \in C^1[0, T]$.

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