Semilocal Convergence of Newton's Method for Finite-Dimensional Variational Inequalities and Nonlinear Complementarity Problems

Zur Erlangung des akademischen Grades eines

DOKTORS DER NATURWISSENSCHAFTEN

von der Fakultät für Mathematik der Universität Karlsruhe genehmigte

DISSERTATION

von

Zhengyu Wang, M. Sc.

aus Nanjing, China

Tag der mündlichen Prüfung:	**21.06.2005**
Referent:	**Prof.Dr. Götz Alefeld**
Korreferent:	**Prof.Dr. Rudolf Lohner**

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To My Mother

Preface

The nonlinear complementarity problem (NCP) is a system of nonlinear inequalities in nonnegative variables, along with a nonlinear equation that expresses the complementarity relationship between the variables and the inequalities. The variational inequality (VI) is a generalization of the nonlinear complementarity problem. Variational inequalities and nonlinear complementarity problems provide a powerful and unifying setting for the study of optimization and equilibrium problems, and serve as the main computational framework for the practical solution.

As one of the most powerful algorithms for solving the VI and the NCP, Newton's method plays an important role in numerical computation, it serves as the prototype of many local, fast methods. However, in the literature one can only find the local convergence results on Newton's method for the VI and the NCP. The local results share the same drawback: before showing the convergence of the method, the existence and some properties of the solution to the original problem have to be assumed, which cannot be verified computationally.

The present research is motivated by the effort to overcome this drawback. By the idea of the Kantorovich theorem, the dissertation meticulously studies the semilocal convergence of Newton's method for variational inequalities and complementarity problems, as well as the various convergence properties including the convergence domain, convergence rate, error estimation etc. These Kantorovich-type theorems established in the dissertation not only provide computationally verifiable conditions to guarantee the convergence of Newton's method, but also provide new existence and uniqueness results for solutions. Moreover, an enclosure method for linear complementarity problems is also proposed in order to estimate the parameters required in the convergence conditions. Numerical results are presented to support the theoretical analysis.

During the period of my study and the preparation of the dissertation, Professor Götz Alefeld of Karlsruhe Universität has been giving me great and circumspect support. It is he who introduced me to interval analysis and automatic differentiation techniques. I have benefitted from the many fruitful and illuminating discussions with him. Here I would express my deep and sincere gratitude to Prof. Dr. Alefeld, for his so kind and so great support to my study, for his careful supervision and for his many illuminating suggestions.

Also, I would appreciate Professor Rudolf Lohner, the second referee of the thesis, for his valuable advice on corrections and improvements of the paper. Specially, I would appreciate Professor Zuhe Shen, who introduced me to nonlinear analysis and recommended me to study in Karlsruhe Universität, for his kindness and great support to my work.

Among the colleagues in Universität Karlsruhe and in Nanjing University, I wish to thank in particular Professor Dongsheng Fu, Dr. Jan Mayer, Dr. Markus Neher, Dr. Uwe Schäfer, Mr. Marco Schnurr, Professor Rong Shao, Mrs. Sonja Sommerfeld, and Professor Xinyuan Wu, for their help with my study and with the preparation of the dissertation. Special thanks to Professor Yaxiang Yuan in Chinese Academy of Sciences, for his friendly support to my study in Karlsruhe.

Zhengyu Wang

Karlsruhe

Contents

Chapter 1

Introduction

1.1 Problems

Definition 1.1. *[14] Let Ω be a nonempty subset of R^n and let f be a mapping from R^n into itself. The variational inequality problem, denoted by $VI(\Omega, f)$, is to find a vector $x^* \in \Omega$ such that*

$$(y - x^*)^T f(x^*) \geq 0, \qquad \forall y \in \Omega.$$

We call $VI(\Omega, f)$ a linear variational inequality if Ω is a polyhedral and f is an affine function, i.e., $f(x) = Mx + q$, where $M \in R^{n\times n}$ and $q \in R^n$. Refer to [11, 12, 31] for linear variational inequalities, for example.

One typically assumes that f is continuously differentiable over an open set $D \subseteq R^n$, and that $\Omega \subset D$ is nonempty, convex and closed. In fact Ω is usually a polyhedral in applications.

In the important special case where Ω is taken to be the nonnegative orthant R^n_+, the variational inequality $VI(\Omega, f)$ is equivalent to the nonlinear complementarity problem [22].

Definition 1.2. *[14] Let f be a mapping from R^n into itself. The nonlinear complementarity problem, denoted by $NCP(f)$, is to find a vector x^* such that*

$$x^* \geq 0, \qquad f(x^*) \geq 0, \qquad x^{*T} f(x^*) = 0.$$

When $f(x) = Mx + q$ for $M \in R^{n\times n}$ and $q \in R^n$, the problem $NCP(f)$ is called linear complementarity problem, which is denoted by $LCP(q, M)$. Refer to Cottle, Pang and Stone [9], or Murty [29] for an extensive treatment of the linear complementarity problem.

Historically, the variational inequality problem was originally introduced as a tool in the study of partial differential equations by Hartman and Stampacchia in [15], and was subsequently expanded by Stampacchia in several papers [24, 25, 42]. The nonlinear complementarity problem first appeared in the Ph.D. dissertation [8] of Cottle.

Let $\Omega \subseteq R^n$ be nonempty. The simplest example of a variational inequality is that of solving a system of equations

$$f(x) = 0$$

in Ω. It is easy to show that if $f(x^*) = 0$, then x^* solves $VI(\Omega, f)$; conversely, if x^* solves $VI(\Omega, f)$ and it is in the interior of Ω, then $f(x^*) = 0$. The various applications of variational inequalities and nonlinear complementarity problems have been well documented in the literature [13, 14], which we will concern in the numerical experiments.

1.2 Newton's Method

For the variational inequality $VI(\Omega, f)$, the most well known algorithm is Newton's method, sometimes it is denoted as basic Newton's method in the literature. The method is to compute a sequence of iterates $\{x^k\}$, such that x^{k+1} solves the k-th linearized problem $VI(\Omega, f^k)$, where

$$f^k(x) = f(x^k) + f'(x^k)(x - x^k), \tag{1.1}$$

and $f'(x)$ denotes the Jacobian matrix of f, i.e., $f'(x) = (\partial f_i(x)/\partial x_j)$. The linearized problem $VI(\Omega, f^k)$ is not a linear variational inequality when Ω fails to be a polyhedral. The actual computation of the solution to each $VI(\Omega, f^k)$ is not of particular concern in the paper. One can state Newton's method for the nonlinear complementarity problem in the similar way, where each linearized problem is a linear complementarity problem. There is a large body of literature on the solution to linear complementarity problems, see [9] and [29] and their references, for example.

It seems from the literature that Robinson proposed Newton's method for variational inequalities and nonlinear complementarity problems originally [36, 37, 38, 39, 40], but did not give a convergence analysis. Subsequently Eaves [10] and Josephy [19] analyzed the method for the variational inequalities with applications to PIES model [5, 6, 17, 18], and independently obtained the convergence results in their technical reports respectively. Josephy presented his results using the notion of a regular solution introduced in Robinson's earlier work [40].

Definition 1.3. *[40] Let x^* be a solution to $VI(\Omega, f)$. Then x^* is called to be regular if there exists a neighborhood N of x^* and a scalar $\delta > 0$ such that for every vector y with $\|y\| < \delta$, there is a unique solution $x(y) \in N$ to the perturbed linearized variational inequality $VI(\Omega, f^y)$, where*

$$f^y(x) = f(x^*) + y + f'(x^*)(x - x^*);$$

moreover, as a function of the perturbed vector y, the solution $x(y)$ is Lipschitz continuous, i.e., there exists a constant $\gamma > 0$ such that whenever $\|y\| < \delta$ and $\|z\| < \delta$, one has

$$\|x(y) - x(z)\| < \gamma \|y - z\|.$$

It is easy to see that if $\Omega = R^n$, the solution x^* is regular if and only if $f'(x^*)$ is nonsingular. Generally, the regularity of the solution x^* to $VI(\Omega, f)$ is hard to be verified except for some special cases.

Proposition 1.4. *[40] Let x^* be a solution to $VI(\Omega, f)$ and let $f'(x^*)$ be positive definite (not necessarily symmetric), then x^* is regular.*

In the case of the nonlinear complementarity problem, we can present a necessary and sufficient condition [40] for x^* to be a regular solution.

Definition 1.5. *[9] Let $A = (a_{ij}) \in R^{n \times n}$. A is said to be*
(a) a Z-matrix if all its off-diagonal elements are nonpositive;
(b) a P-matrix if all its principal minors are positive;
(c) an M-matrix if it is an invertible Z-matrix and has nonnegative inverse;
(d) an H-matrix if there is a vector $d = (d_i)$, $d_i > 0$, such that

$$\sum_{j \neq i} |a_{ij}| d_j < |a_{ii}| d_i, \qquad i = 1, 2, \cdots, n.$$

Remark 1.5.1. *An H-matrix with positive diagonal elements is a P-matrix, an M-matrix is an H-matrix and has positive diagonal elements. The class of H-matrices with positive diagonal elements is an important subclass of P-matrices. See [9].*

Proposition 1.6. *[40] Let x^* be a solution to $NCP(f)$. Define the index sets*

$$I_+ = \{i : x_i^* > 0\}, \qquad I_0 = \{i : x_i^* = f_i(x^*) = 0\}.$$

Then x^* is regular if and only if the following two conditions hold with the index sets I_+ and I_0:
(a) the principal submatrix $(f'(x^*))_{I_+ I_+}$ is nonsingular;
(b) the Schur complement $(f'(x^*))_{I_0 I_0} - (f'(x^*))_{I_0 I_+}[(f'(x^*))_{I_+ I_+}]^{-1}(f'(x^*))_{I_+ I_0}$ is a P-matrix.

It is clear that if $f'(x^*)$ is a P-matrix, then x^* is regular since the class of P-matrices is invariant under principal pivoting [9].

Given the notion of regularity, we can state the convergence result of Newton's method proposed by Josephy [19].

Theorem 1.7. *[14, 19] Let Ω be a nonempty closed and convex subset of R^n. Let $f : R^n \to R^n$ be once continuously differentiable, and x^* be a regular solution to $VI(\Omega, f)$. Then there exists a neighborhood of x^* such that if the starting point x^0 is chosen there, the Newton sequence $\{x^k\}$ is well defined and converges to the solution x^*. Furthermore, if $f'(x)$ is Lipschitz continuous near x^*, then the convergence is quadratic.*

Corollary 1.8. *[19, 33] Let Ω be a nonempty closed and convex subset of R^n. Let $f : R^n \to R^n$ be once continuously differentiable, and let x^* be a solution to $VI(\Omega, f)$ with $f'(x^*)$ being positive definite. Then there exists a neighborhood of x^* such that if the starting point x^0 is chosen there, the Newton sequence $\{x^k\}$ is well defined and converges to the solution x^*. Moreover, if $f'(x)$ is Lipschitz continuous near x^*, then the convergence is quadratic.*

In Eaves's treatment [10], f has the special form:

$$f(y, z) = \begin{pmatrix} c \\ g(z) \end{pmatrix},$$

where $g'(z)$ is assumed to be positive definite in its domain, and the quadratic convergence is established only for z.

Another special case of theorem 1.7 for the nonlinear complementarity problem was established in [33] by using the monotonic norm approach.

Corollary 1.9. *[33] Let $f : R^n \to R^n$ be once continuously differentiable, and x^* be a solution to $NCP(f)$ with $f'(x^*)$ being an H-matrix with positive diagonal elements. Then there exists a neighborhood of x^* such that if the starting point x^0 is chosen there, the Newton sequence $\{x^k\}$ is well defined and converges to the solution x^*.*

One notices that the aforementioned convergence results share the same drawback:
before showing the convergence of the method, the existence and some properties of the solution to the original problem has to be assumed, which cannot be verified computationally.

The present research is motivated by the effort to overcome this drawback. By the idea of the Kantorovich theorem, the dissertation meticulously studies the semilocal convergence of Newton's method for variational inequalities and complementarity problems, as well as the various convergence properties including the convergence domain, convergence rate, error estimation etc. These Kantorovich-type theorems established in the dissertation not only provide computationally verifiable conditions to guarantee the convergence of Newton's method, but also provide new existence and uniqueness results for solutions.

1.3 Structure of Dissertation

The structure of the dissertation is as follows, chapter 2 extends the Kantorovich theorem to variational inequalities, some convergence properties are derived also; chapter 3 establishes the semilocal convergence results specially for nonlinear complementarity problems; chapter 4 proposes an approach of enclosing solutions to linear complementarity problems; implementation details and numerical results are presented in the last chapter.

Chapter 2

Extension of the Kantorovich Theorem

2.1 The Kantorovich Theorem

Let $D \subseteq R^n$ be open and nonempty, and let $f : D \to R^n$ be continuously differentiable. Denote the nonlinear equation $f(x) = 0$ by $NE(f)$. We know that the Newton iterate

$$x^{k+1} = x^k - f'(x^k)^{-1} f(x^k)$$

is just the solution to the linearized problem $NE(f^k)$, i.e., to the system of linear equations

$$f^k(x) = f(x^k) + f'(x^k)(x - x^k) = 0.$$

For the investigation of the method, one of the most powerful convergence analysis tools is the Kantorovich theorem [20], which can provide computationally verifiable conditions of convergence. Since Newton's method for $NE(f)$ and that for $VI(\Omega, f)$ share the same iterative scheme, i.e, their (k+1)-th iterates are all defined as the solutions to their respective k-th linearized problems $NE(f^k)$ and $VI(\Omega, f^k)$ with the same associated affine mapping (1.1), it is promising to extend the Kantorovich theorem to variational inequalities.

Denote the closed ball by $\bar{S}(x, r) := \{y \in R^n : \|y - x\| \leq r\}$, while denote the open ball by $S(x, r) := \{y \in R^n : \|y - x\| < r\}$. The following is the Kantorovich theorem in its classic form for the solution of equations.

Theorem 2.1. *[30] Assume that $f : D \subseteq R^n \to R^n$ is continuously differentiable on a convex set $D_0 \subseteq D$ and that*

$$\|f'(x) - f'(y)\| \leq \gamma \|x - y\|, \qquad \forall x, y \in D_0.$$

Suppose that there exists an $x^0 \in D_0$ such that $\|f'(x^0)^{-1}\| \leq \beta$ and $h = \beta\gamma\eta \leq \frac{1}{2}$, where $\eta \geq \|x^1 - x^0\|$. Set

$$r^* = \frac{1 - \sqrt{1-2h}}{\beta\gamma}, \qquad r^{**} = \frac{1 + \sqrt{1-2h}}{\beta\gamma},$$

and assume that $\bar{S}(x^0, r^*) \subseteq D_0$. Then the Newton sequence $\{x^k\}$ is well defined, remains in $\bar{S}(x^0, r^*)$, and converges to a solution x^* of $f(x) = 0$ which is unique in $S(x^0, r^{**}) \cap D_0$. Moreover, the error estimate

$$\|x^k - x^*\| \leq (\beta\gamma 2^k)^{-1}(2h)^{2^k}, \quad k = 0, 1, 2, \cdots,$$

holds.

Loosely speaking, to prove the theorem, one has to deal with two problems:
(1) to show that the invertibility of $f'(x^1)$ can be concluded from that of $f'(x^0)$ so as to guarantee that x^2 is well defined;
(2) to estimate $\|x^2 - x^1\|$, in order to show that the conditions of theorem 2.1 still hold when x^0 is replaced by x^1.

The first problem can be addressed by the following perturbation lemma [7].

Lemma 2.2. *[7, 30] Let B be an $n \times n$ matrix. B^{-1} exists if and only if there is a matrix A such that A^{-1} exists and*

$$\|A - B\| < \frac{1}{\|A^{-1}\|}.$$

If A^{-1} exists, then

$$\|B^{-1}\| \leq \frac{\|A^{-1}\|}{1 - \|I - A^{-1}B\|} \leq \frac{\|A^{-1}\|}{1 - \|A^{-1}\|\|A - B\|}. \tag{2.1}$$

Here the matrix norm $\|\cdot\|$ is assumed to be subordinate to some vector norm.

The estimation of $\|x^2 - x^1\|$ can be obtained by direct substitution. Thus by the mathematical induction we can prove the well-definedness and the convergence of the Newton sequence to a solution of the nonlinear equation, and other various convergence properties.

The analysis on Newton's method for the variational inequality $VI(\Omega, f)$ differs in some aspects to that on Newton's method for equations. Firstly, the invertibility of $f'(x^0)$ is not sufficient to insure the unique solvability of $VI(\Omega, f^0)$. Secondly, if $VI(\Omega, f^0)$ is uniquely solvable under certain assumption on $f'(x^0)$, we need a powerful extension of lemma 2.2 to show that the assumption imposed on $f'(x^0)$ holds also for $f'(x^1)$, so as to insure that $VI(\Omega, f^1)$ has a unique solution, and then that x^2 is well defined. The last problem is to estimate $\|x^2 - x^1\|$, which is hardly to obtain by direct substitution, if not impossible.

For the first problem, we know if $f'(x^0)$ is positive definite (not necessarily symmetric), then f^0 is strongly monotone, so $VI(\Omega, f^0)$ is uniquely solvable, and x^1 is well-defined. See remark 2.5.1 in the next section. Thus in the extension of the Kantorovich theorem to variational inequalities, $f'(x^0)$ is assumed to be positive definite.

In order to solve the second problem, we need to extend lemma 2.2 to symmetric positive definite matrices. This is given in the next section. We use the definition of the variational inequality and the positive definiteness of the Jacobian matrices of f at the iterates to estimate $\|x^2 - x^1\|$, which is included in the proof of the main result of this chapter.

2.2 Main Result

The following is the extension of lemma 2.2 to symmetric positive definite matrices. The involved matrix norm is subordinate to some vector norm.

Theorem 2.3. *Let B be an $n\times n$ symmetric real matrix. We have*
(a) B is positive definite if and only if there is a symmetric positive definite matrix A such that

$$\|A - B\| < \frac{1}{\|A^{-1}\|};$$

(b) if there is a symmetric positive definite matrix A such that

$$\|A - B\| = \frac{1}{\|A^{-1}\|},$$

then B is either positive semi-definite or positive definite.

Proof. (a) The necessity is straightforward, we prove the sufficiency. Denoting by $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$ the eigenvalues of A, and so A^{-1} has the eigenvalues $\lambda_1^{-1} \ge \lambda_2^{-1} \ge \cdots \ge \lambda_n^{-1}$ since A is symmetric positive definite. It is clear

$$\rho(A - B) \le \|A - B\| < \frac{1}{\|A^{-1}\|} \le \frac{1}{\rho(A^{-1})} = \lambda_1. \tag{2.2}$$

Let $C \in R^{n\times n}$ be symmetric with the eigenvalues $\mu_1 \le \mu_2 \le \cdots \le \mu_n$. From Chapter 2.1 of Ortega and Rheinboldt [30] we know

$$\mu_1 x^T x \le x^T C x \le \mu_n x^T x, \qquad \forall x \in R^n. \tag{2.3}$$

From (2.3), it follows

$$|x^T C x| \le \max\{|\mu_1 x^T x|, |\mu_n x^T x|\} \le \rho(C) x^T x,$$

so by (2.2) we have

$$|x^T(A-B)x| \le \rho(A-B)x^T x < \lambda_1 x^T x, \qquad \forall x \ne 0,$$

which implies $x^T Bx > x^T Ax - \lambda_1 x^T x$ for any $x \ne 0$. And from (2.3) we know $x^T Bx > 0$ for any $x \ne 0$, it means that B is positive definite.
(b) If $\|A-B\| = 1/\|A^{-1}\|$, in the similar way to that in (a), we can prove that $x^T Bx \ge x^T Ax - \lambda_1 x^T x \ge 0$. Letting $A = I$, $B = 0$, we have

$$\|A-B\| = 1 = 1/\|A^{-1}\|,$$

which shows that B is either positive semi-definite or positive definite. □

In the proof of the main result of this chapter we will need the classic existence and uniqueness result, which was established previously in [42]. To state the result, we introduce the following definition.

Definition 2.4. *[30] The mapping $f : R^n \to R^n$ is said to be strongly monotone over $D \subseteq R^n$ if there exists an $\gamma > 0$ such that*

$$(f(x) - f(y))^T (x-y) \ge \gamma \|x-y\|^2, \qquad \forall x, y \in D,$$

where $\|\cdot\|$ denotes any vector norm in R^n.

Theorem 2.5. *[42] Let Ω be a nonempty, closed and convex subset of R^n and let f be a continuous mapping from Ω to R^n. If f is strongly monotone with respect to Ω, then there exists a unique solution to the problem $VI(\Omega, f)$.*

Remark 2.5.1. *For affine mapping $f(x) = Mx + q$, where $M \in R^{n\times n}$ and $q \in R^n$, the strong monotonicity of f is equivalent to the positive definiteness of the matrix M (not necessarily symmetric), see chapter 5.4 of Ortega and Rheinboldt [30]. Thus, if M is positive definite and $\Omega \subseteq R^n$ is nonempty, closed and convex, then $VI(\Omega, f)$ has a unique solution.*

Recall $\tilde{A} = (A + A^T)/2$, where A is a square real matrix. We establish the following Kantorovich-type semilocal convergence of Newton's method for variational inequalities.

Theorem 2.6. *Let $D \subseteq R^n$ be open, let $\Omega \subset D$ be nonempty, convex and closed. Assume that $f : D \to R^n$ is continuously differentiable, and that*

$$\|f'(x) - f'(y)\|_2 \leq \gamma \|x - y\|_2, \qquad \forall x, y \in D_0,$$

where $D_0 \subseteq \Omega$ is convex. Suppose that there is a starting point $x^0 \in D_0$ such that $f'(x^0)$ is positive definite and

$$\|\widetilde{f'(x^0)}^{-1}\|_2 \leq \beta.$$

Denote by x^1 the unique solution to $VI(\Omega, f^0)$ and

$$\|x^1 - x^0\|_2 \leq \eta,$$

where

$$f^0(x) = f(x^0) + f'(x^0)(x - x^0).$$

If

$$h = \beta\gamma\eta \leq \frac{1}{2}, \tag{2.4}$$

and

$$\bar{S}(x^0, r^*) \subseteq D_0, \tag{2.5}$$

where

$$r^* = \frac{1 - \sqrt{1 - 2h}}{\beta\gamma},$$

then the Newton sequence $\{x^k\}$ is well defined, remains in $\bar{S}(x^0, r^*)$, and converges to a solution x^* of the variational inequality $VI(\Omega, f)$, which is contained in $\bar{S}(x^0, r^*)$.

Remark 2.6.1. *If $f'(x^0)$ is positive definite, then $VI(\Omega, f^0)$ has the unique solution x^1. See theorem 2.5 and remark 2.5.1.*

Remark 2.6.2. *Here the open ball $S(x, r)$ and the closed ball $\bar{S}(x, r)$ are all defined by the spectral norm $\|\cdot\|_2$.*

Proof. It is clear that $\beta \neq 0$. If $\gamma = 0$, then we have $f'(x) = f'(x^0)$ for any $x \in D_0$, which by the mean value theorem [30] implies $f(x) = f^0(x)$, and so the Newton iteration terminates at x^1 since it is just the solution to $VI(\Omega, f)$. If $\eta = 0$, then $x^1 = x^0$, since x^1 solves $VI(\Omega, f^0)$ we have

$$(y - x^0)^T f(x^0) = (y - x^1)^T (f(x^0) + f'(x^0)(x^1 - x^0)) \geq 0, \qquad \forall y \in \Omega,$$

which indicates that x^0 is just a solution of $VI(\Omega, f)$, and the Newton iteration terminates at it. So without loss of generality, we assume $\gamma \neq 0$ and

$\eta \neq 0$.
Denote $\eta_0 = \eta$, $\beta_0 = \beta$, $h_0 = h$ and $r_0^* = r^*$. We divide the proof into three parts: (a), (b) and (c).
(a) Firstly we prove that x^2 is well defined. From the inequality

$$1 - 2h_0 \leq 1 - 2h_0 + h_0^2$$

and the assumption (2.4) it follows that

$$\sqrt{1 - 2h_0} \leq 1 - h_0,$$

and so

$$\beta_0 \gamma \eta_0 = h_0 \leq 1 - \sqrt{1 - 2h_0},$$

so we have

$$\eta_0 \leq \frac{1 - \sqrt{1 - 2h_0}}{\beta_0 \gamma} = r_0^*.$$

Since $\|x^1 - x^0\|_2 \leq \eta_0$, we have $x^1 \in \bar{S}(x^0, r_0^*)$, and $x^1 \in D_0$ because $\bar{S}(x_0, r^*) \subseteq D_0$. Considering that

$$\begin{aligned}
\|\widetilde{f'(x^1)} - \widetilde{f'(x^0)}\|_2 &\leq \|f'(x^1) - f'(x^0)\|_2/2 + \|(f'(x^1) - f'(x^0))^T\|_2/2 \\
&= \|f'(x^1) - f'(x^0)\|_2 \leq \gamma \|x^1 - x^0\|_2 \\
&\leq \gamma \eta_0 = h_0/\beta_0 \leq 1/(2\beta_0) < 1/\beta_0,
\end{aligned}$$

one has

$$\|\widetilde{f'(x^1)} - \widetilde{f'(x^0)}\|_2 < 1/\|\widetilde{f'(x^0)}^{-1}\|_2,$$

which, by theorem 2.3, implies that $\widetilde{f'(x^1)}$ is positive definite, and so is $f'(x^1)$. From remark 2.5.1 we know that the problem $VI(\Omega, f^1)$ is uniquely solvable, and x^2 is well defined. Moreover, by the inequality (2.1) one has

$$\|\widetilde{f'(x^1)}^{-1}\|_2 \leq \frac{\beta_0}{1 - \beta_0 \eta_0 \gamma} = \frac{\beta_0}{1 - h_0} = \beta_1.$$

(b) Subsequently we estimate $\|x^2 - x^1\|_2$ and prove that (2.4) and (2.5) still hold when x^0 is replaced by x^1. Considering that $x^1, x^2 \in \Omega$, and that x^1 solves $VI(\Omega, f^0)$ and x^2 solves $VI(\Omega, f^1)$, one has

$$(x^2 - x^1)^T f^0(x^1) = (x^2 - x^1)^T [f(x^0) + f'(x^0)(x^1 - x^0)] \geq 0,$$

$$(x^1 - x^2)^T f^1(x^2) = (x^1 - x^2)^T [f(x^1) + f'(x^1)(x^2 - x^1)] \geq 0.$$

Adding the two inequalities and rearranging the terms, one obtains

$$\begin{aligned}
& (x^1-x^2)^T f'(x^1)(x^1-x^2) \\
\le\ & (x^1-x^2)^T (f(x^1)-f(x^0)-f'(x^0)(x^1-x^0)) \\
\le\ & \|x^1-x^2\|_2 \|f(x^1)-f(x^0)-f'(x^0)(x^1-x^0)\|_2.
\end{aligned} \tag{2.6}$$

Since $x^1 \in \bar{S}(x^0, r_0^*)$, from the assumption (2.5) it follows $x^1 \in D_0$, and so $L[x^0, x^1] = \{\lambda x^0 + (1-\lambda)x^1 | 0 \le \lambda \le 1\} \subseteq D_0$. We have the following inequality [35]

$$\|f(x^1)-f(x^0)-f'(x^0)(x^1-x^0)\|_2 \le \gamma \|x^1-x^0\|_2^2/2. \tag{2.7}$$

Denote the eigenvalues of $\tilde{A}$ by $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$. From (2.3) we know

$$x^T \tilde{A} x \ge \lambda_1 x^T x = \frac{\|x\|_2^2}{\rho(\tilde{A}^{-1})} \ge \frac{\|x\|_2^2}{\|\tilde{A}^{-1}\|_2}.$$

Considering the fact $x^T A x = x^T \tilde{A} x$, one has

$$\begin{aligned}
\|x^1-x^2\|_2^2 / \|\widetilde{f'(x^1)}^{-1}\|_2 &\le (x^1-x^2)^T \widetilde{f'(x^1)} (x^1-x^2) \\
&= (x^1-x^2)^T f'(x^1)(x^1-x^2).
\end{aligned} \tag{2.8}$$

From the inequalities (2.6), (2.7) and (2.8) we have

$$\|x^1-x^2\|_2^2 / \|\widetilde{f'(x^1)}^{-1}\|_2 \le \gamma \|x^1-x^2\|_2 \|x^1-x^0\|_2^2/2.$$

For the same consideration as in the beginning of the proof, we assume that $x^1 \ne x^2$, otherwise the exact solution $x^* = x^1$ has been got, and the iteration can be stopped. Thus

$$\|x^1-x^2\|_2 \le \gamma \|\widetilde{f'(x^1)}^{-1}\|_2 \eta_0^2/2 \le \frac{\beta_0}{1-h_0}\frac{\gamma}{2}\eta_0^2 = \frac{h_0\eta_0}{2(1-h_0)} = \eta_1.$$

Clearly $\eta_1 \le \eta_0/2$. Noting that

$$h_1 = \beta_1 \gamma \eta_1 = \frac{\beta_0}{1-h_0}\gamma \frac{h_0\eta_0}{2(1-h_0)} = \frac{h_0^2}{2(1-h_0)^2} \le \frac{1}{2},$$

condition (2.4) holds when x^0 is replaced by x^1. Let

$$r_1^* = \frac{1-\sqrt{1-2h_1}}{\beta_1 \gamma}.$$

By direct substitution, one has

$$\sqrt{1-2h_1} = (1 - \frac{h_0^2}{(1-h_0)^2})^{1/2} = \frac{\sqrt{1-2h_0}}{1-h_0}, \tag{2.9}$$

and

$$r_1^* = \frac{1-\sqrt{1-2h_0}}{\beta_0\gamma} - \eta_0 = r_0^* - \eta_0,$$

so for any $x \in \bar{S}(x^1, r_1^*)$,

$$\|x - x^0\|_2 \le \|x - x^1\|_2 + \|x^1 - x^0\|_2 \le r_1^* + \eta_0 = r_0^*,$$

i.e., $\bar{S}(x^1, r_1^*) \subseteq \bar{S}(x^0, r_0^*)$, which indicates that the condition (2.5) holds also when x^0 is replaced by x^1.
(c) Here we prove that the Newton sequence is convergent to a solution of $VI(\Omega, f)$, which exists in the ball $\bar{S}(x^0, r^*)$. By mathematical induction it follows that the Newton sequence $\{x^k\}$, starting from x^0, is well defined, remains in $\bar{S}(x^0, r_0^*) = \bar{S}(x^0, r^*)$ and satisfies

$$\|x^{k+1} - x^k\|_2 \le \eta_k = \frac{h_{k-1}\eta_{k-1}}{2(1-h_{k-1})} \le h_{k-1}\eta_{k-1}, \tag{2.10}$$

$$\|\widetilde{f'(x^k)}^{-1}\|_2 \le \beta_k = \frac{\beta_{k-1}}{1-h_{k-1}}, \tag{2.11}$$

and

$$h_k = \beta_k\gamma\eta_k = \frac{h_{k-1}^2}{2(1-h_{k-1})^2} \le 2h_{k-1}^2, \tag{2.12}$$

where $k = 1, 2, \cdots$. From (2.12) we have

$$h_k \le 2h_{k-1}^2 = \frac{1}{2}(2h_{k-1})^2 \le \frac{1}{2}(2h_{k-2})^4 \le \cdots \le \frac{1}{2}(2h_0)^{2^k}. \tag{2.13}$$

From (2.10) and (2.13) we have

$$\begin{aligned} \eta_k &\le h_{k-1}\eta_{k-1} \le h_{k-1}h_{k-2}\eta_{k-2} \le \cdots \le h_{k-1}h_{k-2}\cdots h_0\eta_0 \\ &\le (2h_0)^{2^{k-1}}(2h_0)^{2^{k-2}}\cdots(2h_0)^0\eta_0/2^k = (2h_0)^{2^k-1}\eta_0/2^k. \end{aligned} \tag{2.14}$$

On the other hand, by the mathematical induction, we can see that

$$\{x^{k+1}, x^{k+2}, \cdots\} \subset \bar{S}(x^k, r_k^*), \qquad k = 0, 1, 2, \cdots,$$

which, combined with (2.14) implies that

$$\|x^{k+p} - x^k\|_2 \le r_k^* = \frac{1-\sqrt{1-2h_k}}{\beta_k\gamma} \le 2\eta_k \le (2h_0)^{2^k-1}\eta_0/2^{k-1}, \tag{2.15}$$

i.e., $\{x^k\}$ is a Cauchy sequence which has a limit x^* with $x^* \in \bar{S}(x^k, r_k^*)$ for any $k = 0, 1, \cdots$. Considering

$$(y - x^{k+1})^T (f(x^k) + f'(x^k)(x^{k+1} - x^k)) \geq 0, \qquad \forall y \in \Omega,$$

and the continuity of f and f', we can conclude

$$(y - x^*)^T f(x^*) \geq 0, \qquad \forall y \in \Omega,$$

when $k \to \infty$, i.e., x^* solves $VI(\Omega, f)$. It is clear that $x^* \in \bar{S}(x^0, r^*)$ since $\{x^k\} \subset \bar{S}(x^0, r^*)$. □

2.3 Uniqueness and Convergence Speed

We have shown that $x^* \in \bar{S}(x^0, r^*)$. The following is a further result on the existence domain of the solution x^*.

Theorem 2.7. *If the conditions of theorem 2.6 hold, then*

$$\bar{S}(x^{k+1}, r_{k+1}^*) \subseteq \bar{S}(x^k, r_k^*), \qquad \forall k = 0, 1, \cdots;$$

and

$$\lim_{k \to \infty} \bar{S}(x^k, r_k^*) = \{x^*\},$$

where x^* is the limit of the Newton sequence $\{x^k\}$, and r_k^* is defined as in (2.15).

Proof. It is straightforward in the proof of theorem 2.6 that

$$\bar{S}(x^{k+1}, r_{k+1}^*) \subseteq \bar{S}(x^k, r_k^*).$$

From (2.11) we know $\beta_k \geq \beta_0$ and $\beta_k = 2^k \beta_0$ when $h_0 = \frac{1}{2}$. From (2.13) it follows that

$$0 \leq r_k^* = \frac{1 - \sqrt{1 - 2h_k}}{\beta_k \gamma} \leq \frac{1 - \sqrt{1 - (2h)^{2^k}}}{\beta_0 \gamma} \to 0$$

for $h < \frac{1}{2}$; and

$$r_k^* = \frac{1 - \sqrt{1 - 2h_k}}{\beta_k \gamma} = \frac{1}{2^k \beta_0 \gamma} \to 0$$

for $h = \frac{1}{2}$. Thus the sequence of $\bar{S}(x^k, r_k^*)$ converges to $\{x^*\}$. □

Theorem 2.7 indicates that the limit x^* of $\{x^k\}$ remains in each closed ball $\bar{S}(x^k, r_k^*)$, where the sequence $\{\bar{S}(x^k, r_k^*)\}$ is inclusion monotone. On the uniqueness of the solution we have the following result.

Theorem 2.8. *Let the conditions of theorem 2.6 hold and $S(x^0, r^{**}) \subseteq D_0$, where*

$$r^{**} = \frac{1 + \sqrt{1 - 2h}}{\beta\gamma}.$$

Then the limit x^* of the Newton sequence $\{x^k\}$ is the unique solution of $VI(\Omega, f)$ in the open ball $S(x^0, r^{**})$.

Proof. Denote $r_0^{**} = r^{**}$ and suppose that $x^{**} \in S(x^0, r^{**})$ is a solution of $VI(\Omega, f)$ different to x^* in $S(x^0, r^{**})$. Because $x^1 \in \Omega$ is a solution to $VI(\Omega, f^1)$, by the definition of variational inequalities we have

$$(x^1 - x^{**})^T f(x^{**}) \geq 0,$$

$$(x^{**} - x^1)^T (f(x^0) + f'(x^0)(x^1 - x^0)) \geq 0.$$

Adding the two inequalities and arranging the terms, we have

$$\|x^{**} - x^1\|_2 \leq \frac{1}{2}\gamma\beta_0\|x^{**} - x^0\|_2^2.$$

Assume $\|x^{**} - x^0\|_2 = \theta r_0^{**}$, where $0 \leq \theta < 1$ since x^{**} is assumed to be in the open ball $S(x^0, r_0^{**})$. From (2.9) and (2.11) we know

$$r_1^{**} = \frac{1 + \sqrt{1 - 2h_1}}{\beta_1\gamma} = \frac{\beta_0\gamma}{2}(\frac{1 + \sqrt{1 - 2h_0}}{\beta_0\gamma})^2 = \frac{\beta_0\gamma}{2}(r_0^{**})^2, \tag{2.16}$$

and so $\|x^{**} - x^1\|_2 \leq \theta^2 r_1^{**}$. (2.16) also follows $r_1^{**} = r_0^{**} - \eta_0$, which indicates that $S(x^1, r_1^{**}) \subseteq S(x^0, r_0^{**})$. By induction, we have

$$\|x^{**} - x^k\|_2 \leq \theta^{2^k} r_k^{**} = \theta^{2^k}\frac{1 + \sqrt{1 - 2h_k}}{\beta_k\gamma} \leq \theta^{2^k}\frac{2}{\beta_k\gamma}, \tag{2.17}$$

and by (2.11) we know $\beta_k \geq \beta_0$, and so

$$\|x^{**} - x^k\|_2 \leq \theta^{2^k}\frac{2}{\beta_0\gamma}.$$

Since $0 \leq \theta < 1$, $x^{**} = \lim_{k\to\infty} x^k = x^*$, and the conclusion holds. □

When $h = \frac{1}{2}$, $r^* = r^{**} = 2\eta$, from theorem 2.8 we know x^* is the unique solution to $VI(\Omega, f)$ in the open ball $S(x^0, r^*) = S(x^0, r^{**}) = S(x^0, 2\eta)$. In fact we have the following better result.

Theorem 2.9. *If the conditions of theorem 2.6 hold with $h = \frac{1}{2}$, then the Newton sequence $\{x^k\}$ converges to the solution x^* of the problem $VI(\Omega, f)$ which is unique in the closed ball $\bar{S}(x^0, r^*) = \bar{S}(x^0, r^{**}) = \bar{S}(x^0, 2\eta)$.*

Proof. Obviously $r^* = r^{**} = 2\eta$ when $h = \frac{1}{2}$. The analysis in the proof of theorem 2.8 holds except for the case $\theta = 1$ in (2.17). From (2.17) with $\theta = 1$, we have

$$\|x^{**} - x^k\|_2 \leq \frac{2}{\beta_k \gamma}.$$

When $h = \frac{1}{2}$, from (2.11) and (2.12) it follows that $\beta_k = 2^k \beta$, so

$$\|x^{**} - x^k\|_2 \leq \frac{1}{2^{k-1}} \frac{1}{\beta\gamma},$$

and so $x^{**} = \lim_{k\to\infty} x^k = x^*$, and the conclusion holds. $\square$

The following error estimate can be obtained from the inequality (2.15) immediately.

Theorem 2.10. *If the conditions of theorem 2.6 hold, then we have the error estimate*

$$\|x^k - x^*\|_2 \leq \frac{1}{2^{k-1}} (2h)^{2^k - 1} \eta = (\beta\gamma 2^k)^{-1} (2h)^{2^k}. \tag{2.18}$$

Proof. From (2.15) with $p \to \infty$, the error estimate (2.18) follows. $\square$

The error estimate (2.18) indicates that if $h < \frac{1}{2}$, the Newton sequence converges rapidly, which can be alternately shown by the following quadratic convergence property.

Theorem 2.11. *If the conditions of theorem 2.6 hold with $h < \frac{1}{2}$, then the Newton sequence $\{x^k\}$ is quadratically convergent.*

Proof. Since x^* solves $VI(\Omega, f)$, x^{k+1} solves $VI(\Omega, f^k)$, we have

$$(x^{k+1} - x^*)^T f(x^*) \geq 0,$$

$$(x^* - x^{k+1})^T (f(x^k) + f'(x^k)(x^{k+1} - x^k)) \geq 0.$$

Adding the two inequalities and rearranging the terms, we have

$$\|x^{k+1} - x^*\|_2 \leq \frac{\gamma}{2} \|\widetilde{f'(x^k)}^{-1}\|_2 \|x^k - x^*\|_2^2. \tag{2.19}$$

Noting $x^k \in \bar{S}(x^0, r^*)$, so by the inequality (2.1) we have

$$\|\widetilde{f'(x^k)}^{-1}\|_2 \leq \frac{\beta}{1 - \beta\gamma\|x^k - x^0\|_2} \leq \frac{\beta}{1 - \beta\gamma r^*} = \frac{\beta}{\sqrt{1 - 2h}},$$

and so

$$\|x^{k+1} - x^*\|_2 \leq \frac{\gamma}{2} \frac{\beta}{\sqrt{1 - 2h}} \|x^k - x^*\|_2^2,$$

i.e., the convergence is quadratic. $\square$

The following result shows that the convergence of the Newton sequence is linear when $h = \frac{1}{2}$.

Theorem 2.12. *If the conditions of theorem 2.6 hold with $h = \frac{1}{2}$, then the Newton sequence is linearly convergent.*

Proof. When $h = \frac{1}{2}$, (2.11) and (2.12) imply that $\beta_k = 2^k\beta$ and $h_k = \frac{1}{2}$ respectively. From the error estimate (2.18) we know $\|x^k - x^*\|_2 \leq \frac{1}{2^{k-1}}\eta$. Substituting the relevant terms in (2.19) one has

$$\|x^{k+1} - x^*\|_2 \leq \frac{\gamma}{2} 2^k \beta \frac{1}{2^{k-1}} \eta \|x^k - x^*\|_2 = \frac{1}{2}\|x^k - x^*\|_2,$$

which follows the conclusion. $\square$

Example 2.13. *Consider a simple one-dimensional variational inequality $VI(\Omega, f)$, where $\Omega = [-1, 1]$ and $f(x) = x^2$. Setting $x^0 = \frac{1}{2}$, one can verify that all the assumptions of theorem 2.6 hold with $h = \frac{1}{2}$. The Newton iterates read $x^k = 1/2^{k+1}$, $k \geq 1$. This sequence converges linearly to $x^* = 0$, which is a solution of $VI(\Omega, f)$.*

In the rest of the section we compare theorem 2.6 and corollary 1.8.

Theorem 2.14. *Let $D \subseteq R^n$ be open, let $\Omega \subset D$ be nonempty, closed and convex. Assume that $f : D \to R^n$ is continuously differentiable on a convex set $D_0 \subseteq \Omega$ and that*

$$\|f'(x) - f'(y)\|_2 \leq \gamma\|x - y\|_2, \qquad \forall x, y \in D_0.$$

Let $x^* \in D_0$ be a solution to $VI(\Omega, f)$, where $f'(x^*)$ is positive definite and

$$\|\widetilde{f'(x^*)}^{-1}\|_2 \leq \beta^*.$$

If $\bar{S}(x^*, 1/(\beta^*\gamma)) \subseteq D_0$, then the conditions of theorem 2.6 hold for any starting point $x^0 \in \bar{S}(x^*, \theta/(\beta^*\gamma))$, $0 < \theta \leq \frac{2-\sqrt{2}}{2}$.

Proof. Similar to the part (a) of the proof of theorem 2.6 we can show that $f'(x^0)$ is positive definite, and

$$\|\widetilde{f'(x^0)}^{-1}\|_2 \leq \frac{\beta^*}{1-\theta} = \beta.$$

Thus x^1 is well defined. Since x^* solves $VI(\Omega, f)$, x^1 solves $VI(\Omega, f^0)$, we have

$$(x^1 - x^*)^T f(x^*) \geq 0,$$

$$(x^* - x^1)^T(f(x^0) + f'(x^0)(x^1 - x^0)) \geq 0.$$

Adding the two inequalities and arranging the terms, we have

$$\|x^* - x^1\|_2 \le \frac{\gamma}{2}\|\widetilde{f'(x^0)}^{-1}\|_2\|x^* - x^0\|_2^2 \le \frac{\gamma}{2}\frac{\beta^*}{1-\theta}(\frac{\theta}{\beta^*\gamma})^2,$$

this implies that

$$\|x^1 - x^0\|_2 \le \|x^* - x^0\|_2 + \|x^* - x^1\|_2 \le \frac{\theta}{\beta^*\gamma} + \frac{\gamma}{2}\frac{\beta^*}{1-\theta}(\frac{\theta}{\beta^*\gamma})^2 = \eta.$$

It is easy to verify that if $\theta \le \frac{2-\sqrt{2}}{2}$, then

$$h = \beta\gamma\eta = \frac{\theta^2}{2(1-\theta)^2} + \frac{\theta}{1-\theta} = \frac{2\theta - \theta^2}{2(1-\theta)^2} \le \frac{1}{2}.$$

Let $r = (1 - \sqrt{1-2h})/(\beta\gamma)$. We have

$$r = \frac{1-\sqrt{1-2h}}{\beta\gamma} = \frac{2h}{\beta\gamma(1+\sqrt{1-2h})} \le \frac{2h}{\beta\gamma} = \frac{2\theta-\theta^2}{1-\theta}\frac{1}{\beta^*\gamma}.$$

If $\theta \le \frac{2-\sqrt{2}}{2}$, then

$$r + \frac{\theta}{\beta^*\gamma} = \frac{3\theta - 2\theta^2}{1-\theta}\frac{1}{\beta^*\gamma} \le \frac{1}{\beta^*\gamma}.$$

Hence for any $x \in \bar{S}(x^0, r)$ we have

$$\|x - x^*\|_2 \le \|x - x^0\|_2 + \|x^0 - x^*\|_2 \le r + \frac{\theta}{\beta^*\gamma} \le \frac{1}{\beta^*\gamma},$$

which indicates $S(x^0, r) \subseteq S(x^*, 1/(\beta^*\gamma))$, so $S(x^0, r) \subseteq D_0$, and the conclusion is drawn. $\square$

From theorem 2.14 we can see theorem 2.6 quantitatively interprets corollary 1.8. If $f'(x^*)$ is positive definite, the solution x^* is isolated [43], but not vice versa. So to some extent we can say theorem 2.6 also quantitatively explains the local and quadratic convergence of Newton iteration near the isolated solution to $VI(\Omega, f)$.

By the next result we show that theorem 2.6 is more general than corollary 1.8 in the following sense.

Theorem 2.15. *If the conditions of theorem 2.6 hold, then for any $x \in S(x^0, 1/(\beta\gamma))$, $f'(x)$ is positive definite.*

Proof. Similar to the part (a) of the proof of theorem 2.6, we have

$$\|\widetilde{f'(x)} - \widetilde{f'(x^0)}\|_2 \leq \|f'(x) - f'(x^0)\|_2$$

$$\leq \quad \gamma\|x - x^0\|_2 < 1/\beta \leq 1/\|\widetilde{f'(x^0)}^{-1}\|_2,$$

which, from theorem 2.3, follows that $\widetilde{f'(x)}$ is also positive definite, and so is $f'(x)$. $\square$

When $h < \frac{1}{2}$, since $x^* \in \bar{S}(x^0, r^*) \subseteq S(x^0, 1/(\beta\gamma))$, $f'(x^*)$ is positive definite. When $h = \frac{1}{2}$, since $S(x^0, r^*) = S(x^0, 1/(\beta\gamma))$, x^* might be in the boundary of $S(x^0, 1/(\beta\gamma))$, and from theorem 2.3, it follows that $f'(x^*)$ is either positive definite or positive semi-definite. In example 2.13, we can verify that $f'(x^*)$ is positive semi-definite. In other words, Newton's method is convergent if the starting point x^0 is chosen sufficiently close to a solution x^* with $f'(x^*)$ being positive definite, and could be convergent if x^0 is close to a solution x^* with $f'(x^*)$ being positive semi-definite.

Chapter 3

Special Results for Complementarity Problems

All the convergence results proposed in chapter 2 can be applied to nonlinear complementarity problems, but in many cases the requirement of positive definiteness of $f'(x^0)$ is restrictive. Recall the classic existence result [9]: the linear complementarity problem $LCP(q, M)$ has a unique solution for any column vector q if and only if M is a P-matrix. As a matter of fact, the unique solvability of $LCP(q, M)$ depends on the nature of the matrix M and the column vector q. In some cases, $LCP(q, M)$ could have a unique solution even without the invertibility of M. See [9, 29, 41] for more detailed existence and uniqueness results. This is to say, there is still room for weakening the assumptions on $f'(x^0)$ in theorem 2.6. In this chapter we try to replace the requirement that $f'(x^0)$ is positive definite by an alternate condition: $f'(x^0)$ is an H-matrix with positive diagonal elements. This class of matrices is an important subclass of P-matrices. See [9].

3.1 Preliminaries

Let $A = (a_{ij})$ be an n×n real matrix. Then A is an H-matrix if there is a vector $d = (d_i)$, $d_i > 0$, such that

$$\sum_{j \neq i} |a_{ij}| d_j < |a_{ii}| d_i, \qquad i = 1, 2, \cdots, n. \tag{3.1}$$

Define the comparison matrix $\bar{A} = (\bar{a}_{ij})$ of A, where

$$\bar{a}_{ij} = \begin{cases} |a_{ii}|, & \text{if} \quad i = j, \\ -|a_{ij}|, & \text{if} \quad i \neq j. \end{cases}$$

Using $\bar{A}$, (3.1) can be written as

$$\bar{A}d > 0.$$

Define $\hat{A} = (\hat{a}_{ij})$, where

$$\hat{a}_{ij} = \begin{cases} a_{ii}, & \text{if} \quad i = j, \\ -|a_{ij}|, & \text{if} \quad i \neq j. \end{cases} \tag{3.2}$$

Clearly both $\bar{A}$ and $\hat{A}$ are Z-matrices, and $\bar{A} = \hat{A}$ if A has nonnegative diagonal elements. Remember that A is an M-matrix if and only if A is a Z-matrix and there is a vector $d = (d_i)$, $d_i > 0$ such that $Ad > 0$; A is an H-matrix if and only if $\bar{A}$ is an M-matrix. See [9, 34].

We recall that a vector norm $\|\cdot\|$ is monotonic if for any $x, y \in R^n$,

$$|x| \leq |y| \quad \text{implies} \quad \|x\| \leq \|y\|,$$

where $|x| = (|x_i|)$ and $|y| = (|y_i|)$. It is easy to see that $\|\cdot\|_1$ and $\|\cdot\|_\infty$ are monotonic. Denote $|A| = (|a_{ij}|)$ for an arbitrary matrix $A = (a_{ij})$. We can see that $|A| \leq |B|$ implies $\|A\|_1 \leq \|B\|_1$ and $\|A\|_\infty \leq \|B\|_\infty$. Refer to chapter 2.4 of Ortega and Rheinboldt [30].

The following property of $\hat{A}$ is straightforward.

Proposition 3.1. *Let A and B be $n \times n$ matrices. Then*

$$\|\hat{A} - \hat{B}\| \leq \|A - B\| \tag{3.3}$$

holds for $\|\cdot\|_\infty$ and $\|\cdot\|_1$.

Proof. Noticing that $|a_{ii} - b_{ii}| = |(A - B)_{ii}|$, and that for $i \neq j$

$$|(|a_{ij}| - |b_{ij}|)| \leq |a_{ij} - b_{ij}| = |(A - B)_{ij}|,$$

we have $|\hat{A} - \hat{B}| \leq |A - B|$, and the assertion holds. $\square$

3.2 Convergence Results

From remark 1.5.1 we can see that if $f'(x^0)$ is an H-matrix and has positive diagonal elements, then $f'(x^0)$ is a P-matrix, and $NCP(f^0)$ has the unique solution x^1. Subsequently, we try to show that $f'(x^1)$ is also an H-matrix with positive diagonal elements, which guarantees that x^2 is well defined. For this purpose we need another extension of lemma 2.2 to M-matrices and H-matrices. We estimate the distance between x^1 and x^2 in the proof of the main result of this chapter by using monotonic norm approach.

We establish the following perturbation property of M-matrices.

Theorem 3.2. *Let B be a Z-matrix. Then B is an M-matrix if and only if there is an M-matrix A such that*

$$\|A - B\|_\infty < \frac{1}{\|A^{-1}\|_\infty}.$$

Proof. The necessity is straightforward, we prove the sufficiency. Let $e = (1, 1, \cdots, 1)^T$ and $d = A^{-1}e$. Since A is an M-matrix, $A^{-1} = (\alpha_{ij})_{n\times n} \geq 0$, so $d_i = \sum_{j=1}^n \alpha_{ij} = \sum_{j=1}^n |\alpha_{ij}| \geq 0$. Assume $d_i = 0$, then $\sum_{j=1}^n |\alpha_{ij}| = 0$. This means $\alpha_{ij} = 0$ for all $1 \leq j \leq n$, which is not possible since A^{-1} is invertible. So $d > 0$. Moreover

$$\|d\|_\infty = \max_{1\leq i\leq n}\{|d_i|\} = \max_{1\leq i\leq n}\{\sum_{j=1}^n |\alpha_{ij}|\} = \|A^{-1}\|_\infty.$$

Because

$$\|(A - B)d\|_\infty \leq \|A - B\|_\infty \|d\|_\infty < \|d\|_\infty / \|A^{-1}\|_\infty = 1,$$

we have

$$|(Ad - Bd)_i| = |(e - Bd)_i| = |1 - (Bd)_i| < 1, \qquad i = 1, 2, \cdots, n,$$

so $(Bd)_i > 0$, i.e., $Bd > 0$ for a positive vector $d > 0$, which implies that B is an M-matrix since it has been assumed to be a Z-matrix. □

Corollary 3.3. *Let B be a Z-matrix. Then B is an M-matrix if and only if there is an M-matrix A such that*

$$\|A - B\|_1 < \frac{1}{\|A^{-1}\|_1}.$$

Proof. Since $\|A\|_\infty = \|A^T\|_1$ and A is an M-matrix if and only if its transpose is also an M-matrix, so from theorem 3.2 it follows the conclusion. □

We establish the perturbation property of H-matrices with positive diagonal elements.

Theorem 3.4. *Let B be an $n\times n$ real matrix. Then B is an H-matrix with positive diagonal elements if and only if there is an H-matrix with positive diagonal elements A such that*

$$\|\hat{A} - \hat{B}\|_\infty < \frac{1}{\|\hat{A}^{-1}\|_\infty},$$

where $\hat{A}$ and $\hat{B}$ are defined as in (3.2).

Proof. It is enough to prove the sufficiency. Note that $\hat{B}$ is a Z-matrix, and $\hat{A}$ is an M-matrix since A is assumed to be an H-matrix with positive diagonal elements. We can apply theorem 3.2 and conclude that $\hat{B}$ is an H-matrix with positive diagonal elements. $\square$

The following is an alternate convergence result of Newton's method for nonlinear complementarity problems.

Theorem 3.5. *Let $D \subseteq R^n$ be open and $R^n_+ \subset D$. Assuming that $f : D \to R^n$ is continuously differentiable, $D_0 \subseteq R^n_+$ is convex, and that*

$$\|f'(x) - f'(y)\|_\infty \leq \gamma \|x - y\|_\infty, \qquad \forall x, y \in D_0.$$

Suppose that there exists a starting point $x^0 \in D_0$ such that $f'(x^0)$ is an H-matrix with positive diagonal elements, and

$$\|\overline{f'(x^0)}^{-1}\|_\infty \leq \beta.$$

Denote by x^1 the solution to $NCP(f^0)$, and let

$$\|x^1 - x^0\|_\infty \leq \eta.$$

If

$$h = \beta\gamma\eta \leq \frac{1}{2},$$

and

$$\bar{S}(x^0, r^*) \subseteq D_0,$$

where

$$r^* = \frac{1 - \sqrt{1 - 2h}}{\beta\gamma},$$

then the Newton sequence $\{x^k\}$ is well defined, remains in $\bar{S}(x^0, r^*)$, and converges to a solution x^* of the nonlinear complementarity problem $NCP(f)$, which exists in the closed ball $\bar{S}(x^0, r^*)$.

Remark 3.5.1. *$NCP(f^0)$ is in fact a linear complementarity problem with the matrix $f'(x^0)$, and has a unique solution because $f'(x^0)$ is assumed to be an H-matrix with positive diagonal elements.*

Remark 3.5.2. *Here the open ball $S(x, r)$ and the closed ball $\bar{S}(x, r)$ are all defined by $\| \cdot \|_\infty$.*

Proof. For the same consideration as in theorem 2.6 we assume $\gamma \neq 0$ and $\eta \neq 0$. Denote $\beta_0 = \beta$, $\eta_0 = \eta$, $h_0 = h$, $r_0^* = r^*$. From (3.3) we know

$$\|\widehat{f'(x^1)} - \widehat{f'(x^0)}\|_\infty \leq \|f'(x^1) - f'(x^0)\|_\infty \leq \gamma \|x^1 - x^0\|_\infty < 1/\beta_0,$$

since $\widehat{f'(x^0)} = \overline{f'(x^0)}$ we have

$$\|\widehat{f'(x^1)} - \widehat{f'(x^0)}\|_\infty < \frac{1}{\|\widehat{f'(x^0)}^{-1}\|_\infty} = \frac{1}{\|\overline{f'(x^0)}^{-1}\|_\infty},$$

which, from theorem 3.4 follows that $f'(x^1)$ is also an H-matrix with positive diagonal elements. By the inequality (2.1) we have

$$\|\overline{f'(x^1)}^{-1}\|_\infty \leq \frac{\beta_0}{1 - \beta_0 \eta_0 \gamma} = \frac{\beta_0}{1 - h_0} = \beta_1.$$

Since $f'(x^1)$ is an H-matrix with positive diagonal elements, so by the existence and uniqueness result [9, 41] we know the subproblem $NCP(f^1)$ is uniquely solvable, and x^2 is well-defined. Note

$$x^1 \geq 0, \quad f(x^0) + f'(x^0)(x^1 - x^0) \geq 0, \quad (x^1)^T(f(x^0) + f'(x^0)(x^1 - x^0)) = 0,$$

$$x^2 \geq 0, \quad f(x^1) + f'(x^1)(x^2 - x^1) \geq 0, \quad (x^2)^T(f(x^1) + f'(x^1)(x^2 - x^1)) = 0.$$

(1) Consider the index for which $(x^1)_i = (x^2)_i$. We obtain

$$\begin{aligned}
(\overline{f'(x^1)}|x^2 - x^1|)_i &= -\textstyle\sum_{j\neq i} |f'(x^1)|_{ij} |x^2 - x^1|_j \\
&\leq |f(x^1) - f(x^0) - f'(x^0)(x^1 - x^0)|_i.
\end{aligned}$$

(2) Consider the index for which $(x^2)_i > (x^1)_i$. We have $(x^2)_i > 0$, and so $[f(x^1) + f'(x^1)(x^2 - x^1)]_i = 0$, and

$$[f(x^0) + f'(x^0)(x^1 - x^0) - f(x^1) - f'(x^1)(x^2 - x^1)]_i \geq 0.$$

Since $[\overline{f'(x^1)}]_{ii} = [f'(x^1)]_{ii}$ and $|x^2 - x^1|_i = (x^2 - x^1)_i$, we obtain

$$\begin{aligned}
(\overline{f'(x^1)}|x^2 - x^1|)_i &= (\overline{f'(x^1)})_{ii}(x^2 - x^1)_i - \textstyle\sum_{j\neq i} |f'(x^1)|_{ij} |x^2 - x^1|_j \\
&\leq (f'(x^1)(x^2 - x^1))_i \\
&\leq [f(x^0) + f'(x^0)(x^1 - x^0) - f(x^1)]_i \\
&= |f(x^1) - f(x^0) - f'(x^0)(x^1 - x^0)|_i.
\end{aligned}$$

(3) Consider the index for which $(x^1)_i > (x^2)_i$. We have $(x^1)_i > 0$, and so $[f(x^0) + f'(x^0)(x^1 - x^0)]_i = 0$, and

$$[(f(x^1) + f'(x^1)(x^2 - x^1) - f(x^0) - f'(x^0)(x^1 - x^0)]_i \geq 0.$$

Since $[\overline{f'(x^1)}]_{ii} = [f'(x^1)]_{ii}$ and $|x^2 - x^1|_i = (x^1 - x^2)_i$, we obtain

$$\begin{aligned}
(\overline{f'(x^1)}|x^2 - x^1|)_i &= (\overline{f'(x^1)})_{ii}(x^1 - x^2)_i - \textstyle\sum_{j \neq i} |f'(x^1)|_{ij}|x^2 - x^1|_j \\
&\leq (f'(x^1)(x^1 - x^2))_i \\
&\leq [f(x^1) - f(x^0) - f'(x^0)(x^1 - x^0)]_i \\
&= |f(x^1) - f(x^0) - f'(x^0)(x^1 - x^0)|_i.
\end{aligned}$$

Hence we can deduce that

$$\overline{f'(x^1)}|x^2 - x^1| \leq |f(x^1) - f(x^0) - f'(x^0)(x^1 - x^0)|.$$

Since the inverse of $\overline{f'(x^1)}$ is nonnegative, we obtain

$$|x^2 - x^1| \leq \overline{f'(x^1)}^{-1}|f(x^1) - f(x^0) - f'(x^0)(x^1 - x^0)|.$$

Since the norm $\|\cdot\|_\infty$ is monotonic, it follows that

$$\|x^2 - x^1\|_\infty \leq \|\overline{f'(x^1)}^{-1}\|_\infty\|f(x^1) - f(x^0) - f'(x^0)(x^1 - x^0)\|_\infty.$$

By the similar way as in the proof for theorem 2.6, we can complete the proof. □

We can verify that the following H-matrix, which has positive diagonal elements, is not positive definite:

$$A = \begin{pmatrix} 1 & 2 \\ 0.1 & 1 \end{pmatrix}.$$

Another example illustrates that a positive definite matrix could not be an H-matrix:

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

Thus we can see that theorem 3.5 could be applied to certain nonlinear complementarity problem, to which theorem 2.6 is not applicable, and vice versa.

The following are the convergence properties of Newton's method for nonlinear complementarity problems, the proof for them are similar to those for their counterparts in chapter 2.

Theorem 3.6. *If the conditions of theorem 3.5 hold, then*

$$\bar{S}(x^{k+1}, r^*_{k+1}) \subseteq \bar{S}(x^k, r^*_k), \qquad \forall k = 0, 1, \cdots;$$

and

$$\lim_{k\to\infty} \bar{S}(x^k, r^*_k) = \{x^*\},$$

where x^* is the limit of the Newton sequence.

Theorem 3.7. *Let the conditions of theorem 3.5 hold and $S(x^0, r^{**}) \subseteq D_0$, where*

$$r^{**} = \frac{1+\sqrt{1-2h}}{\beta\gamma}.$$

Then the limit x^* of the Newton sequence $\{x^k\}$ is the unique solution of $NCP(f)$ in the open ball $S(x^0, r^{**})$.

Theorem 3.8. *If the conditions of theorem 3.5 hold with $h = \frac{1}{2}$, then the Newton sequence $\{x^k\}$ converges to the solution x^* of $NCP(f)$, which is unique in the closed ball $\bar{S}(x^0, r^*) = \bar{S}(x^0, r^{**}) = \bar{S}(x^0, 2\eta)$.*

Theorem 3.9. *If the conditions of theorem 3.5 hold, then we have the error estimate*

$$\|x^k - x^*\|_\infty \le \frac{1}{2^{k-1}}(2h)^{2^k-1}\eta = (\beta\gamma 2^k)^{-1}(2h)^{2^k}.$$

Theorem 3.10. *If the conditions of theorem 3.5 hold with $h < \frac{1}{2}$, then the Newton sequence $\{x^k\}$ is quadratically convergent.*

Theorem 3.11. *If the conditions of theorem 3.5 hold with $h = \frac{1}{2}$, then the Newton sequence is linearly convergent.*

We know if $f'(x^*)$ is an H-matrix with positive diagonal elements, then x^* is isolated [14]. The following theorem shows that if a starting point x^0 is close enough to such a solution, the conditions of theorem 3.5 hold. So we can consider theorem 3.5 as a quantitative interpretation of corollary 1.9, and to some extent it is also a quantitative interpretation of the local and quadratic convergence of Newton's method near an isolated solution to the nonlinear complementarity problem.

Theorem 3.12. *Let $D \subseteq R^n$ be open and $R^n_+ \subset D$. Assume that $f : D \to R^n$ is continuously differentiable, $D_0 \subseteq R^n_+$ is convex, and that*

$$\|f'(x) - f'(y)\|_\infty \le \gamma\|x - y\|_\infty, \qquad \forall x, y \in D_0.$$

Let $x^* \in D_0$ be a solution to $NCP(f)$, where $f'(x^*)$ is an H-matrix with positive diagonal elements, and

$$\|\overline{f'(x^*)}^{-1}\|_\infty \le \beta^*.$$

If $\bar{S}(x^*, 1/(\beta^*\gamma)) \subseteq D_0$, then the conditions of theorem 3.5 hold for any starting point $x^0 \in \bar{S}(x^*, \theta/(\beta^*\gamma))$, $0 < \theta \leq \frac{2-\sqrt{2}}{2}$.

By the next result we show that theorem 3.5 is more general than corollary 1.9 in the following sense.

Theorem 3.13. *If the conditions of theorem 3.5 hold, then for any $x \in S(x^0, 1/(\beta\gamma))$, $f'(x)$ is an H-matrix with positive diagonal elements.*

Theorem 3.13 indicates that if $h < \frac{1}{2}$, $f'(x^*)$ is an H-matrix with positive diagonal elements; if $h = \frac{1}{2}$, $f'(x^*)$ could not be such matrix. This means that Newton's method could be convergent if the starting point x^0 is chosen sufficiently close to a solution x^*, for which $f'(x^*)$ is not an H-matrix or has nonpositive diagonal elements.

All the convergence results of this chapter hold also for the norm $\|\cdot\|_1$.

Chapter 4

Enclosing Solutions of Linear Complementarity Problems

Theorem 2.6 and 3.5 provide the computational conditions to guarantee the convergence of Newton's method for complementarity problems. In order to apply the theorems, one has to find the upper bound η of the distance between the starting point x^0 and the first Newton iterate x^1. For this purpose an apparent approach is to compute x^1 by algorithms for solving linear complementarity problems, for example by the various principal pivoting methods and iterative methods [9, 29]. However, this approach is not economic and unnecessary in many cases. Instead of computing x^1 exactly, if we can compute an interval $[x]$ such that x^1 is guaranteed to be contained in it, then we can estimate $\|x^1 - x^0\|$ by

$$\|x^1 - x^0\| \leq \sup_{x \in [x]} \{\|x - x^0\|\}. \tag{4.1}$$

In the literature there are very few enclosing methods for the linear complementarity problem $LCP(q, M)$, except for [2, 3], in which the authors develop the Moore test [28] and Miranda's theorem [26] for the well known Pang's formula [32],

$$\min\{x, Mx + q\} = 0, \tag{4.2}$$

where min is taken componentwise. Both of the two papers provide sufficient conditions for insuring the existence of the solution to the linear complementarity problem in a given interval. However, they do not point out how to compute such an interval enclosing solutions. The present chapter establishes an approach to construct an interval in which the unique solution to the linear complementarity problem, associated with an H-matrix with positive diagonal elements, is contained. A variable dimension bounding procedure is also given to compute the exact solution.

We will use interval analysis in this chapter, see [1, 27] for an extensive treatment. Here we just refer to some necessary notations. Denote the one-dimensional real closed interval by $[x] = [\underline{x}, \overline{x}]$, where $\underline{x} \leq \overline{x}$ are real numbers. Denote the n-dimensional real closed interval by $[x] = ([x])_i$, where each component $([x])_i$ is a one-dimensional interval. Also we can write an n-dimensional interval as $[x] = [\underline{x}, \overline{x}]$, where $\underline{x}, \overline{x} \in R^n$ and $\underline{x} \leq \overline{x}$ holds componentwise. Define the midpoint of an interval by $m([x]) = (\underline{x} + \overline{x})/2$ and the width by $w([x]) = (\overline{x} - \underline{x})/2$, and define $|[x]| = \max\{|\underline{x}|, |\overline{x}|\}$, where the max operator denotes the componentwise maximum of two vectors.

If an enclosure $[x] = [\underline{x}, \overline{x}]$ of x^1 has been obtained, apparently one can componentwise estimate

$$|x^1 - x^0| \leq |[x] - x^0|,$$

which can be computed easily. Hence for a monotonic vector norm $\|\cdot\|$, (4.1) can be expressed as

$$\begin{aligned} \|x^1 - x^0\| &\leq \sup\{\|x - x^0\| : x \in [x]\} \\ &= \||[x] - x^0|\| \\ &= \|\max\{|\overline{x} - x^0|, |\underline{x} - x^0|\}\|. \end{aligned} \tag{4.3}$$

4.1 Existence Test

We begin with giving an existence test for the solution to the nonlinear complementarity problem $NCP(f)$ by using a more general equivalent formulation [9]. Let Δ be a diagonal matrix with positive diagonal elements. Also we call Δ a positive diagonal matrix. Let

$$p(x) := \max\{0, x - \Delta f(x)\}. \tag{4.4}$$

It is known that x solves $NCP(f)$ if and only if x is a fixed point of the mapping $p(x)$, i.e., if $x = p(x)$, which can also be written equivalently

$$\min\{x, \Delta f(x)\} = 0.$$

(4.2) is a special case of this equation. See [9].

Introduce an interval operator

$$\max\{0, [x]\} := [\max\{0, \underline{x}\}, \max\{0, \overline{x}\}],$$

where $[x]$ is an n-dimensional interval. Notice that this interval operator is inclusion monotonic, i.e., $[x] \subseteq [y]$ implies $\max\{0, [x]\} \subseteq \max\{0, [y]\}$.

The following is an existence test for the solution to the nonlinear complementarity problem $NCP(f)$.

Theorem 4.1. *Let $[x]$ be an n-dimensional interval, and let $f'([x])$ be an interval extension of f' over $[x]$. If for some fixed point $x \in [x]$ and a positive diagonal matrix Δ,*

$$\Gamma(x, [x], \Delta) := \max\{0, x - \Delta f(x) + (I - \Delta f'([x]))([x] - x)\} \subseteq [x], \quad (4.5)$$

then there is a solution of $NCP(f)$ in $\Gamma(x, [x], \Delta)$. If there is a solution x^* of $NCP(f)$ in $[x]$, then $x^* \in \Gamma(x, [x], \Delta) \cap [x]$.

Proof. For any $y \in [x]$ we have

$$y - \Delta f(y) \in x - \Delta f(x) + (I - \Delta f'([x]))([x] - x),$$

see [28]. By the property of inclusion monotonicity of $\max\{0, [x]\}$, we have

$$\begin{aligned} p(y) &= \max\{0, y - \Delta f(y)\} \\ &\in \max\{0, x - \Delta f(x) + (I - \Delta f'([x]))([x] - x)\}, \end{aligned}$$

i.e., $\Gamma(x, [x], \Delta)$ is an interval extension of the mapping $p(\cdot)$ over $[x]$. Thus the condition (4.5) implies that $p(\cdot)$ maps $[x]$ into itself, from which, combining with the continuity of $p(\cdot)$, it follows that $p(\cdot)$ has a fixed point $x^* \in [x]$. Let $x^* \in [x]$ be a solution of $NCP(f)$. Clearly

$$x^* = p(x^*) \in \max\{0, x - \Delta f(x) + (I - \Delta f'([x]))([x] - x)\},$$

which indicates that $x^* \in \Gamma(x, [x], \Delta) \cap [x]$. □

Theorem 4.1 indicates that if we can find an interval $[x]$, for which the condition (4.5) holds, then an inclusion monotonic sequence $\{[x^k]\}$ can be computed, where

$$[x^{k+1}] := \Gamma(x^k, [x^k], \Delta^k) \cap [x^k], \qquad k = 0, 1, \cdots, \quad (4.6)$$

$[x]^0 = [x]$, $x^k \in [x^k]$, Δ^k is a positive diagonal matrix. And we can guarantee that a solution x^* to $NCP(f)$ is contained in each interval $[x^k]$. An approximation of x^* can also be automatically given by some $x^k \in [x^k]$ with the componentwise error less than $|[x^k] - x^k|$, although the exact solution x^* has not been computed yet. A common choice of x^k is $x^k = m([x^k])$, for which the error is componentwise less than the width $w([x^k])$.

The following corollary is a non-existence result.

Corollary 4.2. *If*

$$\Gamma(x, [x], \Delta) \cap [x] = \emptyset, \quad (4.7)$$

then there is no solution to $NCP(f)$ in $[x]$.

If neither the inclusion (4.5) nor the condition (4.7) holds for the interval $[x]$, then we can conclude nothing, but we can still compute the sequence $\{[x^k]\}$ iteratively. If for some iterate $[x^k]$ the inclusion (4.5) holds, then the existence of the solution to $NCP(f)$ in $[x^k]$ can be guaranteed, and we can improve the enclosure by continuing the iteration (4.6) since the next enclosure $[x^{k+1}]$ is not wider than its predecessor $[x^k]$. If $[x^k] = \emptyset$, we terminate the iteration and can conclude that there is no solution in the interval $[x^0] = [x]$.

4.2 Enclosing Solutions

In the rest of this chapter we study the linear complementarity problem $LCP(q, M)$, where M is an H-matrix with positive diagonal elements. It is known that the problem has a unique solution for any column vector q [41]. In this section, we will construct an interval $[x]$ for which the inclusion (4.5) holds, and so the unique solution of $LCP(q, M)$ can be enclosed by the interval.

The interval operator defined in theorem 4.1 has the following simple form for the general linear complementarity problem $LCP(q, M)$:

$$\Gamma(x, [x], \Delta) = \max\{0, x - \Delta(Mx + q) + (I - \Delta M)([x] - x)\}. \tag{4.8}$$

In order to find an interval $[x]$ satisfying (4.5), one has to meticulously choose the positive diagonal matrix Δ, the interval $[x]$ and the point x. Because each diagonal entry of M is assumed to be positive, we define $\Delta = diag(m_{ii}^{-1})$ in the rest of this chapter.

We know an H-matrix with positive diagonal elements must be nonsingular [9], so $Mx + q = 0$ has a unique solution. We have the following enclosure of the solution of $LCP(q, M)$, where M is an H-matrix with positive diagonal elements. In general, the enclosure method is not applicable to the problem $LCP(q, M)$ when M is positive definite.

Theorem 4.3. *Assume that M is an H-matrix with positive diagonal elements, and $\Delta = diag(m_{ii}^{-1})$. Let $\bar{x}$ satisfy $M\bar{x} + q = 0$ and let $d = (d_i) \in R^n$, $d_i \geq 0$ such that $\bar{M}d \geq 0$ and $d_i > 0$ for any index i with $\bar{x}_i < 0$. Let*

$$s := \begin{cases} 0, & \textit{if} \quad \bar{x} \geq 0, \\ \max\{-\bar{x}_i/d_i : \bar{x}_i < 0\}, & \textit{otherwise}, \end{cases}$$

and $[x] = [\bar{x} - sd, \bar{x} + sd]$. Then the unique solution of $LCP(q, M)$ is contained in $\Gamma(\bar{x}, [x], \Delta)$.

Proof. It is clear that $(I - \Delta\bar{M})d \geq 0$ and

$$(I - \Delta M)[-d, d] = [-(I - \Delta\bar{M})d, (I - \Delta\bar{M})d].$$

Therefore, for the interval $[x] = [\bar{x} - sd, \bar{x} + sd]$ we can write (4.8) as

$$\Gamma(\bar{x}, [x], \Delta) = \max\{0, [\bar{x} - s(I - \Delta\bar{M})d, \bar{x} + s(I - \Delta\bar{M})d]\}.$$

Notice $(I - \Delta\bar{M})d \leq d$. For the case $\bar{x}_i \geq 0$, we can see

$$\underline{(\Gamma(\bar{x}, [x], \Delta)_i} = \max\{0, \bar{x}_i - s((I - \Delta\bar{M})d)_i\} \geq \bar{x}_i - s((I - \Delta\bar{M})d)_i \geq \bar{x}_i - sd_i$$

and

$$\overline{(\Gamma(\bar{x}, [x], \Delta)_i} = \bar{x}_i + s((I - \Delta\bar{M})d)_i \leq \bar{x}_i + sd_i,$$

so we have

$$(\Gamma(\bar{x}, [x], \Delta)_i \subseteq [\bar{x}_i - sd_i, \bar{x}_i + sd_i].$$

For the case $\bar{x}_i < 0$, we can see

$$\underline{(\Gamma(\bar{x}, [x], \Delta)_i} = 0 \geq \bar{x}_i - sd_i,$$

and

$$\overline{(\Gamma(\bar{x}, [x], \Delta)_i} = \max\{0, \bar{x}_i + s((I - \Delta\bar{M})d)_i\} \leq \bar{x}_i + sd_i$$

since $\bar{x}_i + sd_i \geq 0$, so we have

$$(\Gamma(\bar{x}, [x], \Delta)_i \subseteq [\bar{x}_i - sd_i, \bar{x}_i + sd_i],$$

which follows the conclusion. $\square$

4.3 Variable Dimension Iteration

Applying theorem 4.3 to the starting linearized problem $NCP(f^0)$, we can enclose x^1 by the interval $[x]$ constructed in the theorem, and can get an estimate of $\|x^1 - x^0\|$ given in (4.3). Furthermore we can compute an inclusion monotonic sequence of intervals by (4.6) to improve the estimate if necessary. The following theorem indicates that it is enough to compute the next iterate in (4.6) for a problem with smaller dimension, instead of the original problem.

Theorem 4.4. *Suppose that the conditions of theorem 4.3 hold. Denote*

$$s = \max_{\bar{x}_i < 0}\{-\frac{\bar{x}_i}{d_i}\} = -\frac{\bar{x}_k}{d_k},$$

where $\bar{x}_k < 0$, and denote by x^* the unique solution to $LCP(q, M)$. Then $x_k^* = 0$.

Proof. It is clear that $\bar{x}_k + sd_k = 0$. Thus $x_k^* = 0$ is concluded from the fact: $x_k^* \in [\bar{x}_k - sd_k, \bar{x}_k + sd_k] \cap R_+^n = [0, 0]$. □

Let $\bar{x}$ satisfy $M\bar{x} + q = 0$. If $\bar{x} \geq 0$, then $\bar{x}$ is just the solution to $LCP(q, M)$; if it has negative components, from theorem 4.4 it follows that at least one vanishing component of the exact solution x^* can be determined. Let $[x]$ be given as in theorem 4.3. Denote

$$\alpha = \{i : (\Gamma(\bar{x}, [x], \Delta))_i = [0, 0]\},$$

and denote by $\bar{\alpha}$ the complement set of α. As shown above, if $\bar{x} \ngeq 0$, then $\alpha \neq \emptyset$, so if $\alpha = \emptyset$, we have got a solution $x^* = \bar{x}$ to $LCP(q, M)$. If $\alpha \neq \emptyset$, we can guarantee the components of the solution x^* of $LCP(q, M)$ indexed by α to be 0, although x^* has not been computed yet. Block the vectors x^*, q and the matrix M

$$x^* = \begin{pmatrix} x_\alpha^* \\ x_{\bar{\alpha}}^* \end{pmatrix}, \qquad q = \begin{pmatrix} q_\alpha \\ q_{\bar{\alpha}} \end{pmatrix}, \qquad M = \begin{pmatrix} M_{\alpha\alpha} & M_{\alpha\bar{\alpha}} \\ M_{\bar{\alpha}\alpha} & M_{\bar{\alpha}\bar{\alpha}} \end{pmatrix}.$$

Since $x_\alpha^* = 0$, from the complementarity condition one can see that $x_{\bar{\alpha}}^*$ solves $LCP(q_{\bar{\alpha}}, M_{\bar{\alpha}\bar{\alpha}})$. Because any principal submatrix of an H-matrix is still an H-matrix, theorem 4.3 is applicable to $LCP(q_{\bar{\alpha}}, M_{\bar{\alpha}\bar{\alpha}})$, which has smaller dimension.

The application of theorem 4.3 depends on the computation of the vector d. Choosing $u > 0$, for example $u = (1, 1, \cdots, 1)^T$, we know $\bar{M}d = u$ has the unique solution $d = \bar{M}^{-1}u \geq 0$, and

$$m_{ii}d_i = u_i + \sum_{j \neq i} |m_{ij}| d_j \geq u_i > 0,$$

i.e., $d_i > 0$. Block d and u as $d = (d_\alpha^T, d_{\bar{\alpha}}^T)^T$ and $u = (u_\alpha^T, u_{\bar{\alpha}}^T)^T$, respectively. Since $\bar{M}_{\bar{\alpha}\alpha} \leq 0$ and $d_\alpha > 0$, we have

$$\bar{M}_{\bar{\alpha}\bar{\alpha}} d_{\bar{\alpha}} = u_{\bar{\alpha}} - \bar{M}_{\bar{\alpha}\alpha} d_\alpha \geq 0,$$

which indicates that we can use d_α when applying 4.3 to $LCP(q_{\bar{\alpha}}, M_{\bar{\alpha}\bar{\alpha}})$.

Since in application of theorem 4.3, we either get the exact solution x^* or compute at least one vanishing component of it, it is enough to apply theorem 4.3 to at most n reduced problems with the form $LCP(q_{\bar{\alpha}}, M_{\bar{\alpha}\bar{\alpha}})$, in order to obtain the exact solution x^*. We call such method a variable dimension iteration, which is described as follows.

Algorithm 4.5. ***(Variable Dimension Iteration)***
Input $q \in R^n$ and $M \in R^{n \times n}$ which is an H-matrix and has positive diagonal

elements. Denote by $[x]$ the output enclosure.
Step 1(Initialization) *Compute $d > 0$ such that $\bar{M}d = u = (1, 1, \cdots, 1)^T$, set $I := \{1, 2, \cdots, n\}$, $\alpha := I$, $\beta := \emptyset$, and choose $\epsilon \geq 0$.*
Step 2(Computing enclosure) *Compute $\bar{x} = (\bar{x}_i)$ such that $M\bar{x} + q = 0$, compute*

$$s = \max_{x_i < 0, i \in \alpha} \{-\frac{\bar{x}_i}{d_i}\}$$

and

$$[x]_i = [\max\{0, \bar{x}_i - sd_i + s/m_{ii}\}, \max\{0, \bar{x}_i + sd_i - s/m_{ii}\}],$$

where $i \in \alpha$.
Step 3(Stopping criteria) *Compute*

$$p = \max_{i \in \alpha} |\overline{x}_i - \underline{x}_i|.$$

If $p \leq \epsilon$, then output the enclosure $[x]$ and terminate the algorithm; otherwise, set

$$\beta := \beta \cup \{i \in \alpha : [x]_i = [0, 0]\}$$

and $\alpha := I - \beta$, go to step 2.

Algorithm 4.5 will compute an enclosure of the exact solution x^* in at most n loops, where a loop means the procedure from step 2 to step 3. The width of the enclosure is componentwise less than $\epsilon/2$. It is clear that the exact solution will be obtained if choosing $\epsilon = 0$.

Chapter 5

Numerical Experiments

Theorem 2.6 and 3.5 provide the computational conditions to guarantee the convergence of Newton's method for variational inequalities and complementarity problems. The purpose of this chapter is to test the applicability of the theorems. Since there are very few real variational inequalities in the literature, we restrict our experiments to nonlinear complementarity problems.

5.1 Implementation Details

In numerical experiments we apply the following variant of theorem 3.5, in which we choose $D_0 = \bar{S}(x^0, 2\eta_0)$. It is easy to see that $\bar{S}(x^0, r^*)$ is contained in D_0 if $h = \beta\eta\gamma \leq \frac{1}{2}$.

Theorem 5.1. *Let $D \subseteq R^n$ be open, $R^n_+ \subset D$, and let $f : D \to R^n$ be continuously differentiable. Let $x^0 \in R^n_+$, and let $f'(x^0)$ be an H-matrix and have positive diagonal elements with*

$$\|\overline{f'(x^0)}^{-1}\|_\infty \leq \beta.$$

Let x^1 denote the unique solution to $NCP(f^0)$ and

$$\|x^1 - x^0\|_\infty \leq \eta.$$

Assume that $\bar{S}(x^0, 2\eta) \subset D$, and that

$$\|f'(x) - f'(y)\|_\infty \leq \gamma\|x - y\|_\infty, \qquad \forall x, y \in \bar{S}(x^0, 2\eta).$$

If

$$h = \beta\gamma\eta \leq \frac{1}{2},$$

then the Newton sequence $\{x^k\}$ is well defined, remains in $\bar{S}(x^0, 2\eta)$, and converges to a solution x^* of $NCP(f)$, which is contained in $\bar{S}(x^0, 2\eta)$.

We test the applicability of theorem 5.1 for five examples via Matlab 6.5 on a PC. For each example we set

$$x^0 := (1, \cdots, 1)^T,$$

and apply theorem 5.1 in the following way.

Let x^k be known. We have to invert the matrix $\overline{f'(x^k)}$ in order to verify whether or not $f'(x^k)$ is an H-matrix. If $f'(x^k)$ is an H-matrix and has positive diagonal elements, we compute

$$\beta_k = \|\overline{f'(x^k)}^{-1}\|_\infty.$$

When $f'(x^k)$ is an H-matrix with positive diagonal elements, $NCP(f^k)$ has a unique solution, where

$$f^k(x) = f(x^k) + f'(x^k)(x - x^k).$$

$NCP(f^k)$ is in fact the linear complementarity problem

$$LCP(f(x^k) - f'(x^k)x^k, f'(x^k)). \tag{5.1}$$

We apply algorithm 4.5 to (5.1) with the choice $\epsilon = 1e-15$, so as to compute the enclosure $[x^{k+1}]$ of the unique solution of it. By (4.3) we compute

$$\eta_k = \||[x^{k+1}] - x^k|\|_\infty,$$

and set

$$x^{k+1} := m([x^{k+1}]).$$

Note that x^{k+1} is an approximation of the unique solution of (5.1) with the error less than $\epsilon/2$ componentwise.

In general, we could evaluate f' and estimate the Lipschitz constant γ_k of f' over the closed ball $\bar{S}(x^k, 2\eta_k)$ via the interval computation and automatic differentiation techniques, see [35]. Because the numerical examples in this chapter are not too complex, in coding we use manual computation to give the formulae of evaluating f' and of estimating its Lipschitz constant.

We report

$$h_k = \beta_k \eta_k \gamma_k, \qquad k = 0, 1, \cdots, k^*,$$

for which $h_{k^*} \le \frac{1}{2}$ and $h_k > \frac{1}{2}$ holds for $0 \le k \le k^* - 1$.

If $\eta_k \le \epsilon = 1e - 15$, we terminate the computation, and report

$$\tilde{x} := x^{k+1}$$

as an approximation of the exact solution x^*. Considering that x is a solution of $NCP(f)$ if and only if $\min\{x, f(x)\} = 0$, see [32], we report the value

$$\|\min\{\tilde{x}, f(\tilde{x})\}\|_\infty$$

as a measurement of the preciseness of the approximate solution $\tilde{x}$. The inclusion $\tilde{x} \in \bar{S}(x^{k^*}, 2\eta_{k^*})$ is also verified.

5.2 Numerical Results

Example 1. Let

$$f(x) = \begin{pmatrix} 3x_1^2 + 2x_1x_2 + 2x_2^2 \\ 2x_1^2 + x_1 + 5x_2^2 - 5 \end{pmatrix}.$$

We get

Table 1

k	h_k
0	4.480000000000000e+000
1	1.796666666666667e+000
2	1.983606557377060e-001

with $k^* = 2$,

$$x^{k^*} = \begin{pmatrix} 0 \\ 1.016666666666667e + 000 \end{pmatrix},$$

$\eta_{k^*} = 1.653005464480883e - 002$, and get

$$\tilde{x} = x^6 = (0, 1)^T$$

with

$$\| \min\{\tilde{x}, f(\tilde{x})\}\|_\infty = 0.$$

We have

$$\begin{aligned} \|\tilde{x} - x^{k^*}\|_\infty &= 1.666666666666661e - 002 \\ &\leq 3.306010928961767e - 002 = 2\eta_{k^*}, \end{aligned}$$

which indicates that $\tilde{x} \in \bar{S}(x^{k^*}, 2\eta_{k^*})$.

Example 2. Let

$$f(x) = \begin{pmatrix} 9x_1^2 + 2x_1x_2 + 2x_2^2 + x_3 - 2x_4 - 6 \\ 2x_1^2 + 6x_2^2 + 3x_2 + 3x_3 + 2x_4 - 2 \\ 3x_1^2 + x_1x_2 + 2x_2^2 + 12x_3 + 3x_4 - 1 \\ x_1^2 + 2x_2^2 + 2x_3 + 2x_4^2 + 12x_4 \end{pmatrix}.$$

We get

Table 2

k	h_k
0	7.139453398738613e+000
1	1.864409122527345e+000
2	5.711166356596502e-001
3	3.241410280772485e-002

with $k^* = 3$,

$$x^{k^*} = \begin{pmatrix} 7.918856434193208e-001 \\ 1.844193264594170e-001 \\ 0 \\ 0 \end{pmatrix},$$

$\eta_{k^*} = 2.261871037195052e-003$, and get

$$\tilde{x} = x^7 = \begin{pmatrix} 7.919820808120031e-001 \\ 1.821513560751179e-001 \\ 0 \\ 0 \end{pmatrix}$$

with

$$\|\min\{\tilde{x}, f(\tilde{x})\}\|_\infty = 4.440892098500626e-016.$$

We have

$$\begin{aligned} \|\tilde{x} - x^{k^*}\|_\infty &= 2.267970384299101e-003 \\ &\leq 4.523742074390103e-003 = 2\eta_{k^*}, \end{aligned}$$

which indicates that $\tilde{x} \in \bar{S}(x^{k^*}, 2\eta_{k^*})$.

Example 3. Consider $NCP(f)$, where $f(x) = \nabla g(x)$,

$$g(x) = \sum_{j=1}^{5} e_j x_j + \sum_{i=1}^{5}\sum_{j=1}^{5} c_{ij} x_i x_j + \sum_{j=1}^{5} d_j x_j^3,$$

the e_j, c_{ij} and d_j are given in table 3, see [16].

Table 3

j	1	2	3	4	5
e_j	-15	-27	-36	-18	-12
c_{1j}	30	-20	-10	32	-10
c_{2j}	-20	39	-6	-31	32
c_{3j}	-10	-6	10	-6	-10
c_{4j}	32	-31	-6	39	-20
c_{5j}	-10	32	-10	-20	30
d_j	4	8	10	6	2

We get

Table 4

k	h_k
0	8.983718736411477e-001
1	1.268063520890801e-001

with $k^* = 1$,

$$x^{k^*} = \begin{pmatrix} 5.771443120443256e-001 \\ 8.691545919474093e-001 \\ 1.317488519671896e+000 \\ 7.508180538040421e-001 \\ 4.208261791923880e-001 \end{pmatrix},$$

$\eta_{k^*} = 8.327449205204705e-002$, and get

$$\tilde{x} = x^6 = \begin{pmatrix} 5.242668812739169e-001 \\ 8.826745559564113e-001 \\ 1.258478528366829e+000 \\ 7.411507267992281e-001 \\ 3.355687869800365e-001 \end{pmatrix}$$

with

$$\|\min\{\tilde{x}, f(\tilde{x})\}\|_\infty = 6.994405055138486e-015.$$

We have

$$\begin{aligned} \|\tilde{x} - x^{k^*}\|_\infty &= 8.525739221235151e-002 \\ &\leq 1.665489841040941e-001 = 2\eta_{k^*}, \end{aligned}$$

which indicates that $\tilde{x} \in \bar{S}(x^{k^*}, 2\eta_{k^*})$.

Example 4. Let $\phi(x) = (\phi_i(x_i))$ with $\phi_i(x_i) = e^{x_i}$, let

$$M = \frac{1}{h^2} \begin{pmatrix} H & -I & & \\ -I & H & \ddots & \\ & \ddots & \ddots & -I \\ & & -I & H \end{pmatrix} \in R^{n\times n},$$

where $h = 1/(n+1)$,

$$H = \begin{pmatrix} 4 & -1 & & \\ -1 & 4 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{pmatrix} \in R^{\sqrt{n}\times\sqrt{n}}.$$

Set $x^* = (0, 1, 0, 1, \cdots, 1)^T \in R^n$ and let $q = (q_i)^T \in R^n$ as in [4]:

$$q_i = -\begin{cases} (Mx^*)_i + e^{x_i^*}, & \text{if } x_i^* > 0, \\ (Mx^*)_i + e^{x_i^*} - \xi_i, & \text{otherwise,} \end{cases}$$

where ξ_i is a random nonnegative number. Let $f(x) = \phi(x) + Mx + q$. The problem $NCP(f)$ has a unique solution x^*, and is the result of the application of centered five points difference method to an equilibrium problem given in [23]. The nonnegative random numbers are generated in $[0, 1]$. We perform the numerical experiments for the case $n = 9$ and get

Table 5

k	h_k
0	2.199881344962741e-001

with $k^* = 0$, $\eta_{k^*} = 9.994809069174520e - 001$. We have

$$\|x^* - x^0\|_\infty = 1 \leq 1.998961813834904e + 000 = 2\eta_{k^*},$$

which indicates that $\tilde{x} \in \bar{S}(x^{k^*}, 2\eta_{k^*})$.

Example 5. Let $\phi(x) = (\phi_i(x_i))$ with $\phi_i(x_i) = (x_i + 1)^3 - i$, and let

$$M = \begin{pmatrix} 1 & 2 & 2 & \cdots & 2 \\ 0 & 1 & 2 & \cdots & 2 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 2 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix} \in R^{n \times n}.$$

Furthermore, let $x^* = (x_i^*)$ with

$$x_i^* = \begin{cases} 0, & \text{if} \quad i \bmod 7 = 0, \\ i, & \text{otherwise.} \end{cases}$$

$q = (q_i)$ is chosen such that

$$q_i = \begin{cases} i - (Mx^*)_i - s_i(x_i^*), & \text{if} \quad i \bmod 7 = 0, \\ -(Mx^*)_i - s_i(x_i^*), & \text{otherwise.} \end{cases}$$

Let $f(x) = \phi(x) + Mx + q$. The problem $NCP(f)$ has a unique solution x^* and can be found in [4]. We perform the numerical experiments for the case $n = 10$, and get

Table 6

k	h_k
0	4.978082710810089e+004
1	3.228462762280312e+005
2	8.098622412333274e+004
3	2.154793637151195e+004
4	5.699905960651396e+003
5	1.458547108142570e+003
6	3.257926206342722e+002
7	3.893138642914219e+001
8	3.588485395622169e+000
9	3.900827115527714e-002

with $k^* = 9$, $\eta_{k^*} = 1.736591041838764e - 003$. We have

$$\begin{aligned} \|x^* - x^{k^*}\|_\infty &= 1.732093619922992e - 003 \\ &\leq 3.473182083677529e - 003 = 2\eta_{k^*}, \end{aligned}$$

which indicates that $\tilde{x} \in \bar{S}(x^{k^*}, 2\eta_{k^*})$.

Final Remark. Numerical results support the theoretical analysis given before, and indicate that the conditions in theorem 5.1 can serve as a numerical validation of both the convergence of Newton's method and the existence of solutions. Moreover, the computational enclosure $\bar{S}(x^{k^*}, 2\eta_{k^*})$ of the exact solution is also available as soon as the conditions of theorem 5.1 are fulfilled. For numerical validation of solutions of nonlinear complementarity problems, see [4].

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