TRANSFORMATIONS OF VARIABLES AND TRANSFORMATIONS OF EQUATIONS VIA THE PERTURBED NEWTON METHOD FRAMEWORK*

Alexey F. Izmailov^{1,2} and Mikhail V. Solodov³

February 7, 2025

ABSTRACT

We show that the Newton method applied to a system of nonlinear equations after transformation of its variables and the Newton method applied to a transformation of the equations themselves (nonlinear preconditioning) can be interpreted within the general perturbed Newtonian framework. This gives an insight into the nature of those methods from a unified perspective, as well as some new convergence results in the case when solutions are singular.

Key words: nonlinear equation; Newton-type method; perturbed Newton method; transformation of variables; transformation of equations; nonsingular solution; singular solution; 2-regularity; super-linear convergence; linear convergence.

AMS subject classifications. 65J15, 49M15.

¹ VMK Faculty, OR Department, Lomonosov Moscow State University (MSU), Uchebniy Korpus 2, Leninskiye Gory, 119991 Moscow, Russia.

Email: solodov@impa.br

^{*} This research was supported by the Russian Science Foundation Grant 23-11-20020 (https://rscf.ru/en/project/23-11-20020/), by CNPq Grant 306775/2023-9, by FAPERJ Grant E-26/200.347/2023, and by PRONEX-Optimization.

Email: izmaf@cs.msu.ru

² Derzhavin Tambov State University (TSU), Internationalnaya 33, 392000 Tambov, Russia.

³ IMPA – Instituto de Matemática Pura e Aplicada, Estrada Dona Castorina 110, Jardim Botânico, Rio de Janeiro, RJ 22460-320, Brazil.

1 Introduction

Consider the system of nonlinear equations

$$\Phi(x) = 0,\tag{1.1}$$

where $\Phi : \mathbb{R}^n \to \mathbb{R}^n$ is a given mapping. For a given iterate $x \in \mathbb{R}^n$ such that Φ is differentiable at x, the basic *Newton method* (NM) for solving (1.1) generates the next iterate as $x + \xi$, where ξ satisfies the linear iteration system

$$\Phi(x) + \Phi'(x)\xi = 0.$$
 (1.2)

Assuming that \bar{x} is a nonsingular solution of (1.1), that is, $\Phi'(\bar{x})$ is nonsingular, local convergence and rate of convergence properties of this basic algorithm belong to classics of numerical analysis. Specifically, if Φ is differentiable near \bar{x} , with its derivative being continuous at \bar{x} , any starting point $x^0 \in \mathbb{R}^n$ close enough to such \bar{x} uniquely defines an iterative sequence of the NM, this sequence converges to \bar{x} , and the rate of convergence is superlinear; see, e.g., [20, Theorem 2.2]. The case of singular solutions will be discussed in Section 2.

The perturbed Newtonian framework is given by

$$\Phi(x) + \Phi'(x)\xi = \omega(x), \tag{1.3}$$

with some mapping $\omega : \mathbb{R}^n \to \mathbb{R}^n$ characterizing perturbations/differences with respect to the basic NM. We refer to the iteration $x + \xi$ with ξ defined by (1.3) as the *perturbed Newton method* (pNM). We emphasize that (1.3) is not necessarily related to some inexactness in solving the NM subproblem (1.2) as, for instance, in [7]. Indeed, the nature of ω in (1.3) can be rather different, as would be the case, in particular, for our developments concerning transformation of variables and transformation of equations.

For the case of nonsingular solutions, conditions on ω ensuring that local convergence properties of the NM are preserved for the pNM were studied in [20, Section 2.1]. Singular solutions will be addressed in Section 2, where in particular a new result, specifically relevant for transformation of variables, will be obtained (Theorem 2.1(c)). For related pNM frameworks, including more general settings, see the recent survey [22] and references therein, and in particular [11, 12, 17, 21].

Consider now a given solution \bar{x} of (1.1), and a transformation of variables $\varphi : U \to \mathbb{R}^n$, where U is a neighborhood of some $\bar{z} \in \mathbb{R}^n$, $\varphi(\bar{z}) = \bar{x}$. Consider the basic NM for the transformed equation

$$\Psi(z) = 0, \tag{1.4}$$

where $\Psi: U \to \mathbb{R}^n$ is defined by

$$\Psi(z) = \Phi(\varphi(z)). \tag{1.5}$$

For a motivation of such constructions, see, e.g., [3]. Under the appropriate assumptions on φ , we shall show that the NM applied to the transformed equation (1.4) can be interpreted as the pNM (1.3) for the original equation (1.1). Specifically, convergence properties of the NM applied to (1.4) can be recovered from the known properties of the pNM (1.3). Apart

from giving an insight from the unified principles, this line of analysis also leads to some new results in the case of singular solutions.

Next, consider the case when transformation is applied not to the variables but rather to the equations. Let V be a neighborhood of 0 in \mathbb{R}^n and a mapping $\psi : V \to \mathbb{R}^n$ be such that $\psi(0) = 0, \ \psi(V)$ a neighborhood in \mathbb{R}^n of a solution \bar{x} of (1.1). Let $\Psi : \Phi^{-1}(V) \to \mathbb{R}^n$ be defined by

$$\Psi(x) = \psi(\Phi(x)), \tag{1.6}$$

and consider the problem

$$\Psi(x) = 0. \tag{1.7}$$

This kind of transformations are discussed as a possible form of a nonlinear preconditioner in [5, p. 184]; for related constructions in the context of discretized partial differential equations, see, e.g., [6, 9]. Again, under the appropriate assumptions on ψ , we shall show that the NM applied to (1.7) can be interpreted as the pNM (1.3) for the original equation (1.1). In particular, convergence properties of the former follow from convergence results for the latter.

In Section 2, we provide the needed preliminaries regarding the pNM in cases of nonsingular and singular solutions, with a new result established in Theorem 2.1(c). In Section 3, these results are applied to transformations of variables. In Section 4, we consider transformations of equations.

Some words about our notation and terminology are in order. The null space and the range space of a linear operator A will be denoted by ker A and im A, respectively. For any $\bar{x}, \bar{\xi} \in \mathbb{R}^n$, and any given scalars $\varepsilon > 0$ and $\delta > 0$, we define the set

$$K_{\varepsilon,\delta}(\bar{x}; \bar{\xi}) = \{ x \in \mathbb{R}^n \mid ||x - \bar{x}|| \le \varepsilon, ||||\bar{\xi}||(x - \bar{x}) - ||x - \bar{x}||\bar{\xi}|| \le \delta ||x - \bar{x}|| ||\bar{\xi}|| \}.$$

A set $S \subset \mathbb{R}^n$ is said to be starlike with respect to $\bar{x} \in \mathbb{R}^n$ if $tx + (1-t)\bar{x} \in S$ holds for all $x \in S$ and $t \in (0, 1]$. A vector $\xi \in \mathbb{R}^n$, with $\|\xi\| = 1$, is called an excluded direction for a set S starlike with respect to \bar{x} if $\bar{x} + tv \notin S$ for all t > 0. A set S starlike with respect to \bar{x} is called asymptotically dense at \bar{x} if the corresponding set of excluded directions is thin, i.e., the complement of the latter is open and dense in the unit sphere in \mathbb{R}^n (with topology induced from \mathbb{R}^n).

If $\Phi : \mathbb{R}^n \to \mathbb{R}^n$ is twice differentiable at $\bar{x} \in \mathbb{R}^n$, it is 2-regular at \bar{x} in the direction $\bar{\xi} \in \mathbb{R}^n$ if

$$\operatorname{im} \Phi'(\bar{x}) + \Phi''(\bar{x})[\bar{\xi}, \ker \Phi'(\bar{x})] = \mathbb{R}^n.$$
(1.8)

For some background and usage of the notion of 2-regularity see, e.g., [1] and references therein. Some more recent applications (possibly with reduced smoothness assumptions on Φ) can be found in [2, 11, 12, 13, 14, 17, 18, 19, 22, 23, 24].

Recall that for a given integer r, a mapping $\varphi : U \to V$ is a C^r -diffeomorphism of an open set $U \subset \mathbb{R}^n$ onto an open set $V \subset \mathbb{R}^n$ if φ is a bijection, r times continuously differentiable on U, and φ^{-1} is r times continuously differentiable on V. Recall also that the derivative $\varphi'(x)$ of a C^1 -diffeomorphism is necessarily nonsingular for all $x \in U$.

Finally, for a mapping $v : \mathbb{R}^n \to \mathbb{R}^n$, the notation $v(x) = O(||x - \bar{x}||)$ as $x \to \bar{x}$ means that there exists c > 0 such that $||v(x)|| \le c||x - \bar{x}||$ for all $x \in \mathbb{R}^n$ close enough to \bar{x} . Accordingly, $v(x) = o(||x - \bar{x}||)$ as $x \to \bar{x}$, means that $v(x)/||x - \bar{x}|| \to 0$ as $x \in \mathbb{R}^n \setminus \{\bar{x}\}$ tends to \bar{x} .

2 Preliminaries

If \bar{x} is a singular solution of (1.1), that is, $\Phi'(\bar{x})$ is singular, there may exist points $x \in \mathbb{R}^n$ arbitrarily close to \bar{x} , such that $\Phi'(x)$ is singular, and the NM iteration from x is not welldefined. Nevertheless, even in this case, if Φ is twice differentiable at \bar{x} , and there exists $\bar{\xi} \in \ker \Phi'(\bar{x})$ such that Φ is 2-regular at \bar{x} in the direction $\bar{\xi}$ (recall (1.8)), it follows from [15, Theorem 6.1] that there exists a large (asymptotically dense at \bar{x}) starlike set of starting points $x^0 \in \mathbb{R}^n$ uniquely defining an iterative sequence of the NM, this sequence converges to \bar{x} , and the rate of convergence is linear with the asymptotic common ratio equal to 1/2. Observe that nonsingularity of $\Phi'(\bar{x})$ implies (1.8) with any $\bar{\xi} \in \mathbb{R}^n$, including $\bar{\xi} = 0$. However, (1.8) may certainly hold (with nonzero $\bar{\xi}$) even at singular solutions.

For the pNM (1.3), conditions on ω ensuring local convergence are given in [20, Section 2.1] for the case of nonsingular solutions, and in [17] for the case when the weaker 2-regularity condition above is satisfied; see also the recent survey of related material for the 2-regular case in [22]. We summarize the corresponding results relevant for our developments in Theorem 2.1 below, also providing one addition useful specifically for dealing with transformation of variables.

We shall make use of the unique decomposition of every $x \in \mathbb{R}^n$ into the sum $x = x_1 + x_2$ with $x_1 \in (\ker \Phi'(\bar{x}))^{\perp}$, $x_2 \in \ker \Phi'(\bar{x})$. Let Π be the orthogonal projector onto $(\operatorname{im} \Phi'(\bar{x}))^{\perp}$ in \mathbb{R}^n . Observe that with this definition, the 2-regularity condition (1.8) is equivalent to saying that the linear operator $x \mapsto \Phi'(\bar{x}) + \Pi \Phi''(\bar{x})[\bar{\xi}, x] : \mathbb{R}^n \to \mathbb{R}^n$ is nonsingular, and also to saying that the linear operator

$$B(\bar{\xi}) : \ker \Phi'(\bar{x}) \to (\operatorname{im} \Phi'(\bar{x}))^{\perp}, \quad B(\bar{\xi})x = \Pi \Phi''(\bar{x})[\bar{\xi}, x],$$

is nonsingular. The latter interpretation, in particular, makes it clear that 2-regularity is indeed a directional property, i.e., it holds in a direction $\bar{\xi}$ if and only if it holds in a direction $t\bar{\xi}$, for any $t \neq 0$.

Theorem 2.1 (a) Let Φ be differentiable near a solution \bar{x} of (1.1), with its derivative being continuous at \bar{x} . If $\Phi'(\bar{x})$ is nonsingular, and

$$\omega(x) = o(\|x - \bar{x}\|) \tag{2.1}$$

as $x \to \bar{x}$, then any starting point $x^0 \in \mathbb{R}^n$ close enough to \bar{x} uniquely defines an iterative sequence of the pNM (1.3), this sequence converges to \bar{x} , and the rate of convergence is superlinear. Moreover, the rate of convergence is quadratic provided

$$\omega(x) = O(\|x - \bar{x}\|^2)$$
(2.2)

as $x \to \bar{x}$, and the derivative of Φ is Lipschitz-continuous with respect to \bar{x} , that is,

$$\Phi'(x) - \Phi'(\bar{x}) = O(||x - \bar{x}||)$$
(2.3)

as $x \to \bar{x}$.

(b) Let Φ be twice differentiable near \bar{x} , with its second derivative being Lipschitz-continuous with respect to \bar{x} , that is,

$$\Phi''(x) - \Phi''(\bar{x}) = O(\|x - \bar{x}\|) \tag{2.4}$$

as $x \to \bar{x}$. If Φ is 2-regular at \bar{x} in a direction $\bar{\xi} \in \ker \Phi'(\bar{x})$, that is, (1.8) holds, and (2.2) holds as well, complemented by

$$\Pi\omega(x) = O(\|x - \bar{x}\| \|x_1 - \bar{x}_1\|) + O(\|x - \bar{x}\|^3)$$
(2.5)

as $x \to \bar{x}$, then there exist $\varepsilon > 0$ and $\delta > 0$ such that any starting point $x^0 \in K_{\varepsilon,\delta}(\bar{x}, \bar{\xi})$ uniquely defines an iterative sequence of the pNM (1.3), this sequence converges to \bar{x} , and the rate of convergence is linear with the asymptotic common ratio equal to 1/2.

(c) If in item (b) it additionally holds that

$$\Pi\omega(x) = o(\|x - \bar{x}\|^2)$$
(2.6)

as $x \to \bar{x}$, then there exists a set $S \subset \mathbb{R}^n$ starlike with respect to \bar{x} and asymptotically dense at \bar{x} , and such that any starting point $x^0 \in S$ uniquely defines an iterative sequence of the pNM (1.3), this sequence converges to \bar{x} , and the rate of convergence is linear with the asymptotic common ratio equal to 1/2.

Before talking about the proofs of the items in Theorem 2.1 (or citing the proofs), some general comments are in order. Of course, the local convergence and rate of convergence results for the basic NM are recovered from Theorem 2.1 by taking $\omega \equiv 0$. The convergence domain in item (b) of Theorem 2.1 is $K_{\varepsilon,\delta}(\bar{x}, \bar{\xi})$, and it need not be asymptotically dense at \bar{x} , even if one would consider the union of such domains coming with all appropriate directions $\bar{\xi} \in \ker \Phi'(\bar{x})$ (i.e., those in which Φ is 2-regular at \bar{x}). For the basic NM (without perturbations), the argument in the proof of item (i) of [15, Theorem 6.1] allows to further extend the convergence domain and obtain an asymptotically dense set. As commented at the end of Section 2 of [17], this kind of an extension for pNM would require further assumptions on the perturbation terms, and (2.6) in item (c) of Theorem 2.1 is precisely an example of such an assumption on ω . The result in item (c) of Theorem 2.1 is new. This assumption may seem to be somewhat restrictive in general, but as we shall see, it holds in the situation of transformation of variables in Section 3. It does not hold for transformation of equations in Section 4.

Proof. [of Theorem 2.1]

Item (a) follows from [20, Theorem 2.12], while item (b) is by [17, Theorem 1] (see also [22, Theorem 1]). Therefore, we only need to prove item (c).

Consider any $\xi^0 \in \mathbb{R}^n$, with $\|\xi^0\| = 1$, such that Φ is 2-regular at \bar{x} in the direction ξ^0 . Then by [22, Lemma 1], which a sharper version of [17, Lemma 1], there exists $\tau > 0$ such that for $x = \bar{x} + t\xi^0$ with any $t \in (0, \tau]$, the pNM iteration (1.3) has the unique solution $\xi(x)$, and

$$x + \xi(x) - \bar{x} = \frac{1}{2}\pi(x - \bar{x}) + O(\|\omega(x)\|) + O(\|\|x - \bar{x}\|^{-1}\|\Pi\omega(x)\|) + O(\|x - \bar{x}\|^{2})$$

as $t \to 0$, where π is a positively homogeneous mapping from the cone of directions $\xi \in \mathbb{R}^n$ of 2-regularity of Φ at \bar{x} to \mathbb{R}^n , defined by

$$\pi(\xi) = \frac{1}{2} (\xi_2 + (B(\xi))^{-1} \Pi \Phi''(\bar{x})[\xi, \xi_1]).$$
(2.7)

Taking into account (2.2) and (2.6), this implies that

$$x + \xi(x) - \bar{x} = \frac{1}{2}t\pi(\xi^0) + o(t)$$
(2.8)

as $t \to 0$.

Assume now that Φ is 2-regular at \bar{x} in the direction $\pi(\xi^0)$. If $\pi(\xi^0) = 0$, then this implies that $\Phi'(\bar{x})$ is nonsingular, in which case the needed (and much stronger) assertion follows from item (a) of the theorem. Therefore, in what follows, we suppose that $\pi(\xi^0) \neq 0$.

Fix $\varepsilon > 0$ and $\delta > 0$ according to item (b) of the theorem for $\overline{\xi} = \pi(\xi^0)$. From (2.8) we have that if $\tau = \tau(\xi^0) > 0$ is taken small enough, it holds that $||x + \xi(x) - \overline{x}|| \le \varepsilon$, and assuming that $\pi(\xi^0) \neq 0$, we also have that

$$\begin{aligned} \|\|\pi(\xi^{0})\|(x+\xi(x)-\bar{x})-\|x+\xi(x)-\bar{x}\|\pi(\xi^{0})\| &= \frac{1}{2}\|\|\pi(\xi^{0})\|(t\pi(\xi^{0})+o(t))\\ &-\|t\pi(\xi^{0})+o(t)\|\pi(\xi^{0})\|\\ &= o(t)\\ &\leq \delta\|x+\xi-\bar{x}\|\|\pi(\xi^{0})\|. \end{aligned}$$

Therefore, $x + \xi \in K_{\varepsilon,\delta}(\bar{x}; \pi(\xi^0))$, and by item (b) of the theorem applied with the starting point $x^0 = x + \xi$, we conclude that the pNM uniquely defines the sequence with the needed convergence and rate of convergence properties.

Next, define S as the union of the sets $\{\bar{x} + t\xi^0 \mid t \in (0, \tau(\xi^0)]\}$ over all $\xi^0 \in \mathbb{R}^n$ such that Φ is 2-regular at \bar{x} in the two directions ξ^0 and $\pi(\xi^0)$. This set S is evidently starlike with respect to \bar{x} , and the excluded directions for this set are those $\xi \in \mathbb{R}^n$, with $\|\xi\| = 1$, satisfying either det $B(\xi) = 0$, or det $B(\xi) \neq 0$ but det $B(\det B(\xi)\pi(\xi)) = 0$. Indeed, according to the interpretation of 2-regularity given before the statement of the theorem, the former exactly means violation of 2-regularity of Φ at \bar{x} in the direction ξ , while the latter characterizes the case when 2-regularity holds in the direction ξ but is violated in the direction det $B(\xi)\pi(\xi)$, which is equivalent to saying that 2-regularity is violated in the direction $\pi(\xi)$. Since $B(\cdot)$ depends linearly on its argument, det $B(\xi)$ is a homogeneous polynomial in ξ . Moreover, from (2.7) and from the formula for the inverse of a matrix through its adjugate matrix, it follows that det $B(\det B(\xi)\pi(\xi))$ is also a homogeneous polynomial in ξ . Therefore, all excluded directions belong to the null sets of the specified two homogeneous polynomials, which are both nontrivial: the assumption that Φ is 2-regular at \bar{x} in a direction $\bar{\xi} \in \ker \Phi'(\bar{u})$ implies that det $B(\bar{\xi}) \neq 0$ and

$$\det B(\det B(\bar{\xi})\pi(\bar{\xi})) = \det B\left(\frac{1}{2}\det B(\bar{\xi})\bar{\xi}\right) \neq 0.$$

This implies that the set of excluded directions is thin, and hence, S is asymptotically dense at \bar{x} .

3 Transformations of variables

In this section we discuss a version of the NM applied to the equation with transformed variables. For a given solution \bar{x} of (1.1), let an open neighborhood U of some $\bar{z} \in \mathbb{R}^n$ and a mapping $\varphi : U \to \mathbb{R}^n$ be such that $\varphi(\bar{z}) = \bar{x}, \varphi(U)$ is an open neighborhood of \bar{x} in \mathbb{R}^n , and φ is a C^1 -diffeomorphism of U onto $\varphi(U)$. Therefore, φ can be regarded as a smooth nonsingular local transformation of variables in \mathbb{R}^n , with the new variable $z \in U$ related to the original one $x \in \varphi(U)$ by the equality $x = \varphi(z)$.

We consider the basic NM for the transformed equation given by (1.4) and (1.5). Assuming that Φ is differentiable on $\varphi(U)$, by the chain rule we have that Ψ is differentiable on U and

$$\Psi'(z) = \Phi'(\varphi(z))\varphi'(z) \quad \forall z \in U.$$
(3.1)

In particular, continuity of Φ' at $x = \varphi(z)$ implies continuity of Ψ' at z, and the Jacobians $\Psi'(z)$ and $\Phi'(x)$ are nonsingular and singular simultaneously. Therefore, for a given iterate $z \in U$, the next iterate is $z + \zeta$, where ζ satisfies

$$\Psi(z) + \Psi'(z)\zeta = 0. \tag{3.2}$$

The issue to investigate are precise relations between the iterates produced this way and the NM for the original equation (1.1), which naturally leads to the pNM scheme (1.3). To that end, it makes sense to consider the following procedure that we call the *Newton method with transformed variables* (NMTV). We start with an iterate $x \in \varphi(U)$ serving as an approximation of the solution \bar{x} of the original equation (1.1), transform it into $z = \varphi^{-1}(x)$, compute ζ satisfying (3.2), ensuring somehow that $z + \zeta \in U$, and then restore $\varphi(z + \zeta)$ as the new iterate for the original equation. The question is how does the displacement $\xi = \varphi(z + \zeta) - x$ fit (1.2), or more precisely, what are the properties of the corresponding perturbation term ω in (1.3). This question is natural, as one is primarily interested in the performance of the algorithm in the original (rather than transformed) variables. In addition, our interpretation provides a new insight for this technique of variable transfromation, from a unified perspective (which includes many other Newtonian techniques), and gives new results in the case of singular solutions.

Consider, for a start, the case of an affine transformation $\varphi(z) = Az + b$, where A is a nonsingular $n \times n$ matrix, and $b \in \mathbb{R}^n$. Then, by (3.1), it holds that

$$\Psi'(z) = \Phi'(Az+b)A \quad \forall z \in U.$$

Further, ζ solves (3.2) with Ψ defined in (1.5) if and only if

$$0 = \Phi(Az+b) + \Phi'(Az+b)A\zeta = \Phi(x) + \Phi'(x)\xi$$

holds with $x = \varphi(z) = Az + b$ and $\xi = A\zeta = A(z + \zeta) + b - x = \varphi(z + \zeta) - x$, i.e., this ξ exactly solves (1.2). These observations recover the folklore fact that the NM is "invariant" with respect to nonsingular affine transformations of variables [8]. It is certainly natural to ask if any similar properties can be established for transformations that are not necessarily affine.

For instance, if Φ is continuously differentiable near \bar{x} , and $\Phi'(\bar{x})$ is nonsingular, then from the classical Implicit Function Theorem (e.g., [10, Theorem 1B.1]) it easily follows that for any $\bar{z} \in \mathbb{R}^n$, one can choose U and φ in such a way that in addition to the properties specified above, it will hold that $(\varphi'(\bar{z})$ is the identity and)

$$\Phi(\varphi(z)) = \Phi'(\bar{x})(z - \bar{z}) \quad \forall z \in U.$$

Then according to (1.5), the transformed equation (1.4) is linear, with a nonsingular matrix, and the unique solution of the iteration system (3.2) is $\zeta = \bar{z} - z$. Thus, the NM for the equation (1.4) hits its unique solution \bar{z} in a single step. Therefore, a single iteration of the NMTV produces $\bar{x} = \varphi(\bar{z})$ provided the current iterate x is in U. Considering this from the viewpoint of the pNM, we have that for x close enough to \bar{x} , the displacement $\xi = \varphi(z + \zeta) - x = \bar{x} - x$ fits (1.3) with

$$\omega(x) = \Phi(x) - \Phi'(x)(x - \bar{x}), \qquad (3.3)$$

and by the Mean-Value Theorem [20, Theorem A.10], it holds that

$$\|\omega(x)\| = \|\Phi(x) - \Phi(\bar{x}) - \Phi'(x)(x - \bar{x})\| \le \sup_{t \in [0, 1]} \|\Phi'(tx + (1 - t)\bar{x}) - \Phi'(x)\| \|x - \bar{x}\|.$$

Hence, the NMTV used with the specified transformation of variables fits the pNM with the perturbation term satisfying (2.1), as $x \to \bar{x}$, or even (2.2) provided Φ' is Lipschitz-continuous with respect to \bar{x} , that is, (2.3) holds as $x \to \bar{x}$.

Generally, suppose that the displacement ζ is uniquely defined by (3.2), $\zeta = O(||z - \bar{z}||)$ as $z \to \bar{z}$, and $z + \zeta \in U$. Observe that these properties are guaranteed for $z = \varphi^{-1}(x)$, for any x close enough to \bar{x} , if \bar{x} is a nonsingular solution of (1.1). Indeed, in this case, \bar{z} is a nonsingular solution of (1.4), and the needed properties follow by the standard local properties of the step of the NM (see, e.g., [20, Theorem 2.2]) applied to the equation (1.4), and by the fact that $z \to \bar{z}$ as $x \to \bar{x}$.

From (1.5)–(3.2) we then have that

$$0 = \Phi(\varphi(z)) + \Phi'(\varphi(z))\varphi'(z)\zeta = \Phi(x) + \Phi'(x)\xi - \Phi'(x)(\xi - \varphi'(z)\zeta)$$
(3.4)

with $\xi = \varphi(z + \zeta) - x$. Therefore, the NMTV fits (1.3) with

$$\omega(x) = \Phi'(x)(\varphi(z+\zeta) - \varphi(z) - \varphi'(z)\zeta), \qquad (3.5)$$

where both z and ζ are uniquely defined through x, and therefore, ω can indeed be regarded as a function of x only. Employing again the Mean-Value Theorem [20, Theorem A.10], we derive the estimate

$$\begin{aligned} \|\varphi(z+\zeta) - \varphi(z) - \varphi'(z)\zeta\| &\leq \sup_{t\in[0,1]} \|\varphi'(t(z+\zeta) + (1-t)z) - \varphi'(z)\| \|\zeta\| \\ &= o(\|\zeta\|) \\ &= o(\|\zeta\|) \\ &= o(\|\zeta-\bar{z}\|) \\ &= o(\|\varphi^{-1}(x) - \varphi^{-1}(\bar{x})\|) \\ &= o(\|\varphi^{-1}(x) - \varphi^{-1}(\bar{x})\|) \\ &= o(\|(\varphi^{-1})'(\bar{x})(x-\bar{x}) + o(\|x-\bar{x}\|)\|) \\ &= o(\|x-\bar{x}\|) \end{aligned}$$
(3.6)

as $x \to \bar{x}$, where the assumption that φ is a C^1 -diffeomorphism was also used. Moreover, assuming that φ is a C^2 -diffeomorphism, this argument leads to the estimate

$$\|\varphi(z+\zeta) - \varphi(z) - \varphi'(z)\zeta\| = O(\|x-\bar{x}\|^2).$$
(3.7)

Combining (3.5) with (3.6) and (3.7), we respectively obtain (2.1) and (2.2). Assuming that \bar{x} is a nonsingular solution of (1.1), this allows to apply item (a) of Theorem 2.1 to derive the following result.

Proposition 3.1 Let Φ be differentiable near a solution \bar{x} of (1.1), with its derivative being continuous at \bar{x} , and assume that $\Phi'(\bar{x})$ is nonsingular. Let an open neighborhood U of some $\bar{z} \in \mathbb{R}^n$ and a mapping $\varphi : U \to \mathbb{R}^n$ be such that $\varphi(\bar{z}) = \bar{x}$, $\varphi(U)$ is an open neighborhood of \bar{x} in \mathbb{R}^n , and φ is a C^1 -diffeomorphism of U onto $\varphi(U)$.

Then any starting point $x^0 \in \mathbb{R}^n$ close enough to \bar{x} uniquely defines an iterative sequence of the NMTV, this sequence converges to \bar{x} , and the rate of convergence is superlinear. Moreover, the rate of convergence is quadratic provided the derivative of Φ is Lipschitz-continuous with respect to \bar{x} , that is, (2.3) holds as $x \to \bar{x}$, and φ is a C^2 -diffeomorphism.

Taking into account the first equality in (3.4), observe that in the case of a linearizing diffeomorphism, (3.5) is the same as (3.3).

We now turn our attention to the case when \bar{x} is a singular solution of (1.1). From (3.1) it follows that

$$\operatorname{im} \Psi'(\bar{z}) = \operatorname{im} \Phi'(\bar{x}), \quad \operatorname{ker} \Psi'(\bar{z}) = (\varphi'(\bar{z}))^{-1} \operatorname{ker} \Phi'(\bar{x}).$$
 (3.8)

Assume that Φ is twice differentiable near \bar{x} , with its second derivative Lipschitz-continuous with respect to \bar{x} , and let Φ be 2-regular at \bar{u} in some nonzero direction $\bar{\xi} \in \ker \Phi'(\bar{x})$. Set $\bar{\zeta} = (\varphi'(\bar{z}))^{-1} \bar{\xi} \in \ker \Psi'(\bar{z})$. From (3.1) it then follows that

$$\Psi''(\bar{z})[\bar{\zeta},\,\zeta] = \Phi''(\bar{x})[\varphi'(\bar{z})\bar{\zeta},\,\varphi'(\bar{z})\zeta] + \Phi'(\bar{x})\varphi''(\bar{z})[\bar{\zeta},\,\zeta],$$

and hence, according to (3.8),

$$\Pi \Psi''(\bar{z})[\bar{\zeta},\,\zeta] = \Pi \Phi''(\bar{x})[\bar{\xi},\,\varphi'(\bar{z})\zeta]$$

for $\zeta \in \mathbb{R}^n$, implying that 2-regularity of Φ at \bar{x} in the direction $\bar{\xi}$ is equivalent to 2-regularity of Ψ at \bar{z} in the direction $\bar{\zeta}$.

Furthermore, for any $\tilde{\varepsilon} > 0$ and $\tilde{\delta} > 0$, there exist $\varepsilon > 0$ and $\delta > 0$ such that the inclusion $x \in K_{\varepsilon,\delta}(\bar{x}, \bar{\xi})$ implies the inclusion $z = \varphi^{-1}(x) \in K_{\tilde{\varepsilon},\tilde{\delta}}(\bar{z}, \bar{\zeta})$. Indeed, observe first that since φ is a C^1 -diffeomorphism, similarly to the intermediate relations in (3.6) one derives the estimates

$$x - \bar{x} = O(\|z - \bar{z}\|), \quad z - \bar{z} = O(\|x - \bar{x}\|)$$
(3.9)

as $z \to \overline{z}$ and $x \to \overline{x}$, respectively. And in particular, for any $\tilde{\varepsilon} > 0$, if $||x - \overline{x}|| \le \varepsilon$ with $\varepsilon > 0$ small enough, then $||z - \overline{z}|| \le \tilde{\varepsilon}$. By the standard formula for the derivative of the inverse mapping [10, Theorem 1A.1], we have that

$$\varphi^{-1}(x) = \varphi^{-1}(\bar{x}) + (\varphi^{-1})'(\bar{x})(x - \bar{x}) + o(||x - \bar{x}||)$$

= $\bar{z} + (\varphi'(\bar{z}))^{-1}(x - \bar{x}) + o(||x - \bar{x}||),$ (3.10)

and

$$\begin{aligned} & \left\| \|(\varphi'(\bar{z}))^{-1}\bar{\xi}\| \|x - \bar{x}\| - \|(\varphi'(\bar{z}))^{-1}(x - \bar{x})\| \|\bar{\xi}\| \right\| \\ & \leq \| \|x - \bar{x}\|(\varphi'(\bar{z}))^{-1}\bar{\xi} - \|\bar{\xi}\|(\varphi'(\bar{z}))^{-1}(x - \bar{x})\| \\ & \leq \|(\varphi'(\bar{z}))^{-1}\| \| \|x - \bar{x}\|\bar{\xi} - \|\bar{\xi}\|(x - \bar{x})\| . \end{aligned}$$

$$(3.11)$$

Employing (3.10)–(3.11), we derive the following chain of estimates

$$\begin{split} \left\| \|\bar{\zeta}\|(z-\bar{z}) - \|z-\bar{z}\|\bar{\zeta}\| &= \left\| \|(\varphi'(\bar{z}))^{-1}\bar{\xi}\|(\varphi^{-1}(x)-\bar{z}) - \|\varphi^{-1}(x)-\bar{z}\|(\varphi'(\bar{z}))^{-1}\bar{\xi}\| \right\| \\ &= \left\| \|(\varphi'(\bar{z}))^{-1}\bar{\xi}\|(\varphi'(\bar{z}))^{-1}(x-\bar{x}) - \|(\varphi'(\bar{z}))^{-1}\bar{\xi}\| + o(\|x-\bar{x}\|) \right) \\ &= \left\| (\varphi'(\bar{z}))^{-1}\| \left\| \|(\varphi'(\bar{z}))^{-1}\bar{\xi}\| (x-\bar{x}) - \|(\varphi'(\bar{z}))^{-1}(x-\bar{x})\| \bar{\xi}\| \right\| \\ &+ o(\|x-\bar{x}\|) \\ &= \left\| (\varphi'(\bar{z}))^{-1}\| \left\| \frac{\|(\varphi'(\bar{z}))^{-1}\bar{\xi}\|}{\|\bar{\xi}\|} \right\| \|\bar{\xi}\| (x-\bar{x}) \\ &- \frac{\|(\varphi'(\bar{z}))^{-1}(x-\bar{x})\|}{\|(\varphi'(\bar{z}))^{-1}\bar{\xi}\|} \|\bar{\xi}\| + o(\|x-\bar{x}\|) \\ &\leq \left\| (\varphi'(\bar{z}))^{-1}\|^2 \right\| \|\bar{\xi}\| (x-\bar{x}) - \|x-\bar{x}\|\bar{\xi}\| \\ &+ \|(\varphi'(\bar{z}))^{-1}\|^2 \left\| \|\bar{x}-\bar{x}\| - \frac{\|(\varphi'(\bar{z}))^{-1}(x-\bar{x})\|}{\|(\varphi'(\bar{z}))^{-1}\bar{\xi}\|} \|\bar{\xi}\| \right\| \|\bar{\xi}\| \\ &+ o(\|x-\bar{x}\|) \\ &= O\left(\left\| \|\bar{\xi}\| (x-\bar{x}) - \|x-\bar{x}\|\bar{\xi}\| \right) \\ &+ o(\|x-\bar{x}\|) \\ &= O\left(\left\| \|\bar{\xi}\| (x-\bar{x}) - \|x-\bar{x}\|\bar{\xi}\| \right) + o(\|x-\bar{x}\|) \|\bar{\xi}\| \right\|) \\ &+ o(\|x-\bar{x}\|) \\ &= O\left(\left\| \|\bar{\xi}\| (x-\bar{x}) - \|x-\bar{x}\|\bar{\xi}\| \right) + o(\|x-\bar{x}\|) \\ &= O\left(\left\| \|\bar{\xi}\| (x-\bar{x}) - \|x-\bar{x}\|\bar{\xi}\| \right) + o(\|x-\bar{x}\|) \end{split}$$

as $x \to \bar{x}$. Taking also into account the first relation in (3.9), this implies that for any $\tilde{\delta} > 0$ there exist $\varepsilon > 0$ and $\delta > 0$ such that the inclusion $x \in K_{\varepsilon,\delta}(\bar{x}, \bar{\xi})$ implies that

$$\left\| \|\bar{\zeta}\|(z-\bar{z}) - \|z-\bar{z}\|\bar{\zeta}\right\| \le \widetilde{\delta}\|\bar{\zeta}\|\|z-\bar{z}\|,$$

completing the proof of the fact that $z \in K_{\tilde{\varepsilon}, \tilde{\delta}}(\bar{z}, \bar{\zeta})$.

Therefore, assuming that $x \in K_{\varepsilon,\delta}(\bar{x}, \bar{\xi})$ with sufficiently small $\varepsilon > 0$ and $\delta > 0$, we can use the characterization of the NM step near a singular solution of a nonlinear equation, given in [15, Lemma 4.1] (see also [13, Lemma 1]), applying it to the equation (1.4). This yields that ζ is uniquely defined by (3.2), $\zeta = O(||z - \bar{z}||)$ as $z \to \bar{z}$, and $z + \zeta \in U$. Then from (3.7) (that holds assuming that φ is a C^2 -diffeomorphism) we have that ω defined in (3.5) satisfies (2.2) and

$$\Pi\omega(x) = \Pi(\Phi'(x) - \Phi'(\bar{x}))(\varphi(z+\zeta) - \varphi(z) - \varphi'(z)\zeta) = O(||x-\bar{x}||^3)$$

as $x \to \bar{x}$, implying both (2.5) and (2.6). These estimates on the perturbation term allow to apply item (c) of Theorem 2.1, which yields the following result.

Proposition 3.2 Let Φ be twice differentiable near \bar{x} , with its second derivative being Lipschitz-continuous with respect to \bar{x} , that is, (2.4) holds as $x \to \bar{x}$, and let Φ be 2-regular at \bar{x} in a direction $\bar{\xi} \in \ker \Phi'(\bar{x})$, that is, (1.8) holds. Let an open neighborhood U of some $\bar{z} \in \mathbb{R}^n$ and a mapping $\varphi: U \to \mathbb{R}^n$ be such that $\varphi(\bar{z}) = \bar{x}$, $\varphi(U)$ is an open neighborhood of \bar{x} in \mathbb{R}^n , and φ is a C^2 -diffeomorphism of U onto $\varphi(U)$.

Then there exists a set $S \subset \mathbb{R}^n$ starlike with respect to \bar{x} and asymptotically dense at \bar{x} , and such that any starting point $x^0 \in S$ uniquely defines an iterative sequence of the NMTV, this sequence converges to \bar{x} , and the rate of convergence is linear with the asymptotic common ratio equal to 1/2.

4 Transformations of equations

We next discuss the case when transformation is applied not to the variables but rather to the equations. Let an open neighborhood V of 0 in \mathbb{R}^n and a mapping $\psi : V \to \mathbb{R}^n$ be such that $\psi(0) = 0$, $\psi(V)$ is an open neighborhood in \mathbb{R}^n of a solution \bar{x} of (1.1), and ψ is a C^1 -diffeomorphism of V onto $\psi(V)$. Let $\Psi : \Phi^{-1}(V) \to \mathbb{R}^n$ be given by (1.6).

Assuming that Φ is differentiable on some neighborhood $O \subset \Phi^{-1}(V)$ of \bar{x} , by the chain rule we have that Ψ is differentiable on O and

$$\Psi'(x) = \psi'(\Phi(x))\Phi'(x) \quad \forall x \in O,$$
(4.1)

and in particular, continuity of Φ' at $x \in O$ implies continuity of Ψ' at x, and the Jacobians $\Psi'(x)$ and $\Phi'(x)$ are nonsingular and singular simultaneously.

For a given current iterate $x \in O$, the basic NM for the transformed equation (1.7), with Ψ defined in (1.6), generates the next iterate as $x + \xi$, where ξ satisfies

$$\Psi(x) + \Psi'(x)\xi = 0,$$

and we shall refer to this iteration process as the Newton method with transformed equations (NMTE).

Employing (1.6) and (4.1), the iteration equation of the NMTE takes the form

$$\psi(\Phi(x)) + \psi'(\Phi(x))\Phi'(x)\xi = 0,$$

and hence, according to (1.3),

$$\omega(x) = \Phi(x) + \Phi'(x)\xi = \Phi(x) - (\psi'(\Phi(x)))^{-1}\psi(\Phi(x)).$$
(4.2)

Again with the use of the Mean-Value Theorem [20, Theorem A.10], we obtain that

$$\begin{aligned} \|\psi(\Phi(x)) - \psi'(\Phi(x))\Phi(x)\| &= \|\psi(\Phi(x)) - \psi(0) - \psi'(\Phi(x))\Phi(x)\| \\ &\leq \sup_{t \in [0, 1]} \|\psi'(t\Phi(x)) - \psi'(\Phi(x))\| \|\Phi(x)\| \end{aligned}$$
(4.3)

and hence,

$$\psi(\Phi(x)) = \psi'(\Phi(x))\Phi(x) + o(\|\Phi(x)\|)$$
(4.4)

as $x \to \bar{x}$. Combining this with (4.2), we obtain that

$$\omega(x) = o(\|\Phi(x)\|) = o(\|\Phi'(\bar{x})(x-\bar{x}) + o(\|x-\bar{x}\|)\|) = o(\|x-\bar{x}\|)$$
(4.5)

as $x \to \bar{x}$.

Moreover, assuming that ψ is a C²-diffeomorphism, from (4.3) we have that

$$\|\psi(\Phi(x)) - \psi'(\Phi(x))\Phi(x)\| \le \sup_{t \in [0,1]} \sup_{\theta \in [0,1]} \|\psi''(\theta t \Phi(x) + (1-\theta)\Phi(x))\|(t-1)\|\Phi(x)\|^2,$$

and (4.4) takes the stronger form

$$\psi(\Phi(x)) = \psi'(\Phi(x))\Phi(x) + O(\|\Phi(x)\|^2).$$

If Φ' is Lipschitz-continuous with respect to \bar{x} , again making use of the Mean-Value Theorem [20, Theorem A.10], from (4.2) we then obtain that

$$\begin{aligned}
\omega(x) &= O(\|\Phi(x)\|^2) \\
&= O(\|\Phi(\bar{x}) + \Phi'(\bar{x})(x - \bar{x}) + O(\|x - \bar{x}\|^2\|^2)) \\
&= O((\|\Phi'(\bar{x})(x_1 - \bar{x}_1) + O(\|x - \bar{x}\|^2\|^2)) \\
&= O(\|x_1 - \bar{x}_1\|^2) + O(\|x - \bar{x}\|^3)
\end{aligned}$$
(4.6)

as $x \to \bar{x}$.

The obtained (under the corresponding assumptions) estimates (4.5) and (4.6) allow to apply items (a) and (b) of Theorem 2.1, giving the following two propositions, respectively.

Proposition 4.1 Let Φ be differentiable near a solution \bar{x} of (1.1), with its derivative being continuous at \bar{x} , and assume that $\Phi'(\bar{x})$ is nonsingular. Let an open neighborhood V of 0 in \mathbb{R}^n and a mapping $\psi: V \to \mathbb{R}^n$ be such that $\psi(0) = 0$, $\psi(V)$ is an open neighborhood in \mathbb{R}^n of \bar{x} , and ψ is a C^1 -diffeomorphism of V onto $\psi(V)$.

Then any starting point $x^0 \in \mathbb{R}^n$ close enough to \bar{x} uniquely defines an iterative sequence of the NMTE, this sequence converges to \bar{x} , and the rate of convergence is superlinear. Moreover, the rate of convergence is quadratic provided the derivative of Φ is Lipschitz-continuous with respect to \bar{x} , that is, (2.3) holds as $x \to \bar{x}$, and ψ is a C^2 -diffeomorphism.

Proposition 4.2 Let Φ be twice differentiable near \bar{x} , with its second derivative being Lipschitz-continuous with respect to \bar{x} , that is, (2.4) holds as $x \to \bar{x}$, and let Φ be 2-regular at \bar{x} in a direction $\bar{\xi} \in \ker \Phi'(\bar{x})$, that is, (1.8) holds. Let an open neighborhood V of 0 in \mathbb{R}^n and a mapping $\psi : V \to \mathbb{R}^n$ be such that $\psi(0) = 0$, $\psi(V)$ is an open neighborhood in \mathbb{R}^n of \bar{x} , and ψ is a C^2 -diffeomorphism of V onto $\psi(V)$.

Then there exist $\varepsilon > 0$ and $\delta > 0$ such that any starting point $x^0 \in K_{\varepsilon,\delta}(\bar{x}, \bar{\xi})$ uniquely defines an iterative sequence of the NMTE, this sequence converges to \bar{x} , and the rate of convergence is linear with the asymptotic common ratio equal to 1/2.

Observe that one cannot apply in this case item (c) of Theorem 2.1 to obtain an asymptotically dense convergence domain, because the estimate (2.6) cannot be guaranteed: since

 ψ appears as an outer mapping in the composition defined in (1.6), application of Π to the corresponding ω does not allow to improve the estimate (4.6).

Preconditioners actually used in [5, 6, 9] are different, and much more involved by structure than what is discussed above, i.e., they are not just compositions of Φ with some transformation ψ . However, in the case of a nonsingular solution (and this is certainly the case in the cited references), the following general observations are applicable.

Suppose that one has at hand some iterative process generating, for a current iterate $x \in \mathbb{R}^n$, a displacement $\xi \in \mathbb{R}^n$ such that

$$x + \xi - \bar{x} = o(||x - \bar{x}||) \quad (\text{ or } O(||x - \bar{x}||^2)) \tag{4.7}$$

as $x \to \bar{x}$. Observe that these properties are guaranteed if the process in question is the NM for the equation (1.7) with $\Psi : \mathbb{R}^n \to \mathbb{R}^n$ satisfying the appropriate smoothness requirements, and being such that \bar{x} is a nonsingular solution of (1.7). Moreover, one can use, say, the Gauss-Newton method and $\Psi : \mathbb{R}^n \to \mathbb{R}^m$ with $m \ge n$, assuming that ker $\Psi'(\bar{x}) = \{0\}$.

According to (1.3), employing again the Mean-Value Theorem [20, Theorem A.10], from (4.7) we obtain that under the appropriate smoothness requirements on Φ ,

$$\begin{aligned} \|\omega(x)\| &= \|\Phi(x) + \Phi'(x)\xi\| \\ &\leq \|\Phi(x) - \Phi(\bar{x}) - \Phi'(x)(x - \bar{x}) + \Phi'(x)(x + \xi - \bar{x})\| \\ &\leq \sup_{t \in [0, 1]} \|\Phi'(tx + (1 - t)\bar{x}) - \Phi'(x)\| \|x - \bar{x}\| + \|\Phi'(x)(x + \xi - \bar{x})\| \\ &= o(\|x - \bar{x}\|) \quad (\text{ or } O(\|x - \bar{x}\|^2)) \end{aligned}$$
(4.8)

as $x \to \bar{x}$. Assuming that \bar{x} is a nonsingular solution of (1.1), these estimates allow to interpret the iterative process in question as the pNM. However, this is of course merely a matter of interpretation: one can apply item (a) of Theorem 2.1, with the resulting conclusions about superlinear (or quadratic) local convergence of the process in question, but this is given directly by (4.7), or by local convergence theories of the specific methods applied to (1.7), yielding (4.7).

The case of a singular solution \bar{x} of (1.1) is a whole different story, even if it becomes nonsingular for (1.7) in the sense that ker $\Psi'(\bar{x}) = \{0\}$ (assuming that $m \ge n$). In the latter case, (1.7) is called a defining system for the solution \bar{x} of (1.1) (and the approach itself is sometimes called bordering, or unfolding-cut), and there exists quite a rich literature on this approach to numerical treatment of nonlinear equations with singular solutions; see, e.g., [16, Section 5], as well as more recent considerations in [4, 25], and references therein. However, (4.8) does not imply the estimates on the perturbation term needed for the pNM in this case, and this is only natural since the behavior of the iterative process in question (superlinear convergence, following from (4.7)) and of the basic Newton method for (1.1) (linear convergence with the asymptotic common ratio equal to 1/2) is totally different.

Declarations

Conflicts of Interest. The author declare that they have no conflict of interest of any kind related to the manuscript.

Data Availability Statement. Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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