Newton's method and secant methods:

A long-standing

relationship from vectors to matrices

M. MONSALVE y M. RAYDAN

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Newton's method and secant methods: A long-standing relationship from vectors to matrices

Marlliny Monsalve [*]   Marcos Raydan [†]

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Abstract

Nonlinear matrix equations arise in different scientific topics, such as applied statistics, control theory, and financial mathematics, among others. As in many other scientific areas, Newton's method has played an important role when solving these matrix problems. Under standard assumptions, the specialized Newton's methods that have been developed for specific problems exhibit local and q-quadratic convergence and require a suitable initial guess. They also require, as usual, a significant amount of computational work per iteration, that in this case involve several matrix factorizations per iterations. As expected, whenever a Newton's method can be developed, a secant method can also be developed. Indeed, more recently, secant methods for solving specific nonlinear matrix problems have been developed opening a new line of research. As in previous scenarios, these specialized secant methods exhibit local and q-superlinear convergence, also require a suitable initial guess, and avoid the use of derivatives in the formulation of the schemes.

In this review we start by recalling the presence of Newton's method and the secant methods, and also their classical relationship, in different and sometimes unexpected scenarios for vector problems. Then we present and describe the state of the art in the use of Newton's method and also the secant method in the space of matrices. A second objective is to present a unified approach for describing the features of these classical schemes, that in the space of matrices represent an interesting research area with special features to be explored.

Keywords: Newton's method, secant method, nonlinear matrix problems.

1 Introduction

Newton's method has played a fundamental role in the development of numerical algorithms for solving scientific computing problems in general. It is simple to describe, and so it is appealing, because it appears naturally from considering a Taylor approximation to a certain function associated with the problem at hand. It has been rediscovered several times through history for solving specialized problems. Moreover, historically, whenever a Newton's method has been proposed to solve specific problems, secant methods have also

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[*]Departamento de Computación, Facultad de Ciencias, Universidad Central de Venezuela, Ap. 47002, Caracas 1041-A, Venezuela (marlliny.monsalve@ciens.ucv.ve).

[†]Departamento de Cómputo Científico y Estadística, Universidad Simón Bolívar, Ap. 89000, Caracas 1080-A, Venezuela (mraydan@usb.ve). Partially supported by the Scientific Computing Center at UCV.

been developed for the same problem. The main reason is that secant methods avoid the explicit knowledge of derivatives at the cost of reducing the asymptotic convergence from q-quadratic to q-superlinear, which in practice can be seldom appreciated.

One of the objectives of this review is to unify the Newton-secant connection for several scenarios and for important applications. Special attention is paid to the historical process in the space of vectors, describing some of the equivalent well-known methods. The other main objective is to present some of the recent developments for solving matrix problems using Newton's method as well as secant methods. In that case the movement from vectors to matrices is an intriguing and attractive topic that has produces several impressive specialized Newton's method, and quite recently some secant methods that retain the fundamental principles: No explicit knowledge of derivatives and q-superlinear convergence.

In a general setting, let us consider the following nonlinear problem:

$$\text{given } F : H \to H \text{ find } X_* \in H \text{ such that } F(X_*) = 0, \tag{1}$$

where H is a normed space, and F is a Fréchet differentiable map. We denote by F' the Fréchet derivative of F, and by $\|X\|$ the norm of X. If H is an inner product space, then $\|X\|^2 = \langle X, X \rangle$ will be the norm induced by the inner product. During the presentation of our review we will consider the finite dimensional space $H = \mathbb{R}^n$ for vector problems, and depending on the application, we will consider $H = \mathbb{C}^{n \times n}$ or $H = \mathbb{R}^{n \times n}$ for matrix problems.

The well-known Newton's method for solving equation (1) can be written, in a general framework, as:

Algorithm 1 Newton's method

1: Given $X_0 \in H$
2: **for** $k = 0, 1, \cdots$ **do**
3: $\quad$ Solve $F'(X_k)S_k = -F(X_k)$
4: $\quad$ $X_{k+1} = X_k + S_k$
5: **end for**

Note that we need F' to find S_k at each iteration of Algorithm 1 and in order to obtain F' we can use the Taylor series for F about X,

$$F(X + S) = F(X) + F'(X)S + R(S), \tag{2}$$

where $R(S)$ is such that

$$\lim_{\|S\| \to 0} \frac{\|R(S)\|}{\|S\|} = 0.$$

The Taylor expansion (2) allows us to identify the application of $F'(X)$ on S which is required to solve the linear problem of step 3 in Algorithm 1.

As a general principle, whenever a Newton's method is applicable, a suitable secant method can be obtained, that hopefully has interesting features to exploit. For example,

in the well-known scalar case, the secant method does not require the derivative, and only uses function evaluations. In that case $f : \mathbb{C} \to \mathbb{C}$, and the secant method can be written as follow:

$$x_{k+1} = x_k - \frac{f(x_k)}{a_k},$$

where a_k satisfies that $f(x_k) = f(x_{k-1}) + a_k(x_k - x_{k-1})$ for $k \geq 0$, and $x_{-1}, x_0 \in \mathbb{C}$ are given. Notice that $a_k = f'(x_k)$ for all k yields the scalar Newton iteration. In a recent work [137], a full investigation is included on the historical development of the secant method for one variable.

For different scenarios, from vector problems to matrix problems, we will discuss in this review specialized Newton's methods and the suitable secant methods that have been developed to solve problem (1).

2 Vector problems

Let $F : \mathbb{R}^n \to \mathbb{R}^n$. Consider the linear model $M_k(x) = F(x_k) + J(x_k)(x - x_k)$ that approximates F at x_k, where $J(x_k)$ represents the Jacobian matrix at x_k. Notice that $M_k(x_k) = F(x_k)$. The next iterate, x_{k+1}, in Newton's method is obtained by solving $M_k(x_{k+1}) = 0$. Therefore, $x_{k+1} = x_k + s_k$, where s_k satisfies the linear system of equations $J(x_k)s_k = -F(x_k)$. Solving this linear system for every k represents the computational effort of Newton's method. The next result shows, under standard assumptions, the local and q-quadratic convergence of Newton's method for solving (1). For a proof see [54].

Theorem 2.1 *Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a continuously differentiable function in an open and convex set $D \subset \mathbb{R}^n$. Let us assume that there exists $x_* \in \mathbb{R}^n$ and $r, \beta > 0$, such that $N(x_*, r) \subset D$, $F(x_*) = 0$, $J(x_*)^{-1}$ exists with $\|J(x_*)^{-1}\| \leq \beta$, and $J \in Lip_\gamma(N(x_*, r))$. Then there exists $\epsilon > 0$ such that for all $x_0 \in N(x_*, \epsilon)$, the sequence $\{x_k\}_{k \geq 0}$ generated by the iteration $x_{k+1} = x_k - J(x_k)^{-1}F(x_k)$, is well-defined, converges to x_*, and satisfies*

$$\|x_{k+1} - x_*\| \leq \beta\gamma\|x_k - x_*\|^2, \quad \forall k \geq 0. \tag{3}$$

In here, we introduce the notation $J \in Lip_\gamma(N(x_*, r))$ which means that there exists $\gamma > 0$ such that for every $x, y \in N(x_*, r)$ it follows that $\|J(x) - J(y)\| \leq \gamma\|x - y\|$, where $N(x_*, r)$ denotes the open ball with center x_* and radius r. From (3) we conclude that Newton's method has local and q-quadratic convergence when the matrix $J(x_*)$ is non-singular, which is clearly a great advantage. On the negative side, Newton's method only has local convergence, so it requires globalization strategies to be practically effective and needs to solve a linear system of equations per iteration. Concerning globalization strategies, there are two main possibilities that can be associated with Newton-type methods and also with secant-type methods: Line search strategies and trust region schemes. In this work we do not concentrate on the issue of globalization techniques. For a complete treatment of this topic we recommend the book by Bertsekas [15], the book by Conn et al. [40], the book by Fletcher [68], and the book by Nocedal and Wright [133]. In the general setting of Banach spaces, Newton's method, as presented in Algorithm 1, has been

extensively studied. The most important theoretical tool in that case to prove the convergence of Newton's method is the well-known Newton-Kantorovich Theorem that has been extended and applied to several different problems. For a complete survey of Newton's method in Banach spaces and the Newton-Kantorovich Theorem, see the recent book by Argyros [4]. A historical review about the convergence analysis of Newton's method can be found in [134].

For solving problem (1) when $F : \mathbb{R}^n \to \mathbb{R}^n$ there also exist the so-called secant-type methods, also known as quasi-Newton methods [24]. The main feature of the secant methods is that they do not require the explicit knowledge of the Jacobian map, $J(x)$. As in the development of Newton's method, at every iteration k, the following linear model is solved to obtain x_{k+1}

$$\widehat{M_k}(x) = F(x_k) + A_k(x - x_k). \tag{4}$$

In the vector case, A_k is an $n \times n$ matrix that is expected to approximate $J(x_k)$. Clearly if $A_k = J(x_k)$, for all k, then Newton's method is recovered. However, the idea is to avoid the use of $J(x_k)$, and so the matrix A_k is obtained among those that satisfy $F(x_{k-1}) = \widehat{M_+}(x_{k-1})$. When this condition is imposed, we obtain the so-called secant equation,

$$A_k s_{k-1} = y_{k-1}, \tag{5}$$

where $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = F(x_k) - F(x_{k-1})$. As in the scalar case, equation (4) satisfies $\widehat{M_k}(x_k) = F(x_k)$ and the next iterate, x_{k+1}, is the one that satisfies $\widehat{M_k}(x_{k+1}) = 0$. Any method generated by this procedure is known as a secant-type method or a quasi-Newton method, and can be written as

$$x_{k+1} = x_k - A_k^{-1} F(x_k),$$

where the vector x_0 and the matrix A_0 must be given.

Notice that equation (5) represents a linear system of n equations and n^2 unknowns (the n^2 elements of A_k) which implies that there are infinitely many ways of building the matrix A_k at every iteration. A very successful way of building A_k at every k was proposed by Broyden [26], and later analyzed by Dennis [50]. The so-called Broyden's method is given by the following formula for A_{k+1}

$$A_{k+1} = A_k + \frac{(y_k - A_k s_k)s_k^t}{s_k^t s_k}. \tag{6}$$

The formula (6) for building A_{k+1} is obtained as the closest matrix to A_k that satisfies the secant equation (5), see [54, 68]. Broyden's method has been extended in several ways and has produced a significant body of research for many different problems. For a complete description of Broyden's method, its extensions and applications see, e.g., [27, 54, 123, 133, 175].

Broyden's algorithm can be written as

Algorithm 2 Broyden's method

1: Given $x_0 \in \mathbb{R}^n$, $A_0 \in \mathbb{R}^{n \times n}$
2: **for** $k = 0, 1, \cdots$ **do**
3:     Solve $A_k s_k = -F(x_k)$ $\triangleright$ For s_k
4:     $x_{k+1} = x_k + s_k$
5:     $y_{k+1} = F(x_{k+1}) + F(x_k)$
6:     $A_{k+1} = A_k + \dfrac{(y_k - A_k s_k)s_k^t}{s_k^t s_k}$
7: **end for**

The next result establishes, under standard assumptions, the local and q-superlinear convergence of Broyden's method for solving (1). For details and a full proof see [54].

Theorem 2.2 *Under the same hypothesis of Theorem 2.1, there exist positive constants ϵ and δ such that if $\|x_0 - x_*\|_2 \leq \epsilon$ and $\|A_0 - J(x_*)\|_2 \leq \delta$, then the sequence $\{x_k\}$ generated by Algorithm 2 is well defined and converges q-superlinearly to x_*.*

One of the most popular variants of Broyden's method is the so-called inverse Broyden's method in which the inverse of the Jacobian matrix, $J(x_k)^{-1}$, is directly approximated at every iteration [54]. The computational cost of the inverse version is similar to the standard Broyden's method except that the calculation of the vector s_k, in Step 3 of Algorithm 2, requires a matrix-vector product instead of the solution of a linear system. For the inverse version we have that

$$A_{k+1}^{-1} = A_k^{-1} + \frac{(s_k - A_k^{-1}y_k)y_k^t}{y_k^t y_k}, \tag{7}$$

and A_0^{-1} must be given. As in the standard Broyden's method the matrix A_{k+1}^{-1} given according to (7) solves an optimization problem, that in this case is stated as

$$\min_{B \in Q(y_k, s_k)} \|B^{-1} - A_k^{-1}\|_2,$$

where $Q(y_k, s_k) = \{B \in \mathbb{C}^{n \times n} : Bs_k = y_k\}$. In other words, A_{k+1} satisfies the secant equation and A_{k+1}^{-1} is the closest nonsingular matrix to A_k^{-1}. Once again, under standard assumptions the inverse Broyden's method is locally and q-superlinearly convergent [52, 53, 54]. The inverse Broyden's method will play an important role in Section 3, where we describe the secant-type extensions recently developed for matrix problems.

Under some special assumptions on F, for solving (1), or for some special problems, a faster rate of convergence than q-quadratic can be observed for Newton's method (q-order p, where $p > 2$). Moreover, some special methods have been developed at some additional cost per iteration to accomplish that kind of very fast convergence (see, e.g., [64, 78, 110, 163, 168, 172]). For some of those special cases, under the same circumstances for which Newton's method shows a q-order p convergence, for $p > 2$, the secant-type methods also

show a speed of convergence faster than q-superlinear, see for example [65, 85]. In the scalar case, the relationship between the speed of Newton's method and the speed of the secant method has been characterized [146].

As well as Newton's method, the secant-type methods have also been extended and analyzed for solving nonlinear problems in Hilbert spaces, see e.g., [75, 150]. Newton's method has been extended for solving nonsmooth systems of nonlinear equations [36, 124, 149], and has been combined with interior point methods [76]. Similarly, the secant-type methods have also been extended for nonsmooth problems [35, 116, 125, 139], and have been combined with inexact schemes and nonstandard globalization strategies [18, 71].

2.1 Unconstrained optimization problems

The relationship between Newton's method and secant methods has been suitably exploited in the development of numerical optimization algorithms, and hence it represents one of the most important topics to illustrate the historical connection between them.

For solving smooth unconstrained optimization problems, the traditional approach is to solve a nonlinear system with the gradient vector of the objective function, $f : \mathbb{R}^n \to \mathbb{R}$, i.e., find $x \in \mathbb{R}^n$ such that $\nabla f(x) = 0$. Hence, for unconstrained optimization, we recover problem (1) with $F(x) = \nabla f(x)$. Let us consider, without loss of generality, the minimization problem.

The methods we consider belong to a large family of iterative methods that can be written in a generic fashion as follows

$$x_{k+1} = x_k + \alpha_k d_k, \tag{8}$$

where d_k is a search direction, usually chosen as a descent direction i.e., $d_k^t \nabla f(x_k) < 0$, and $\alpha_k > 0$ is the step length in the direction d_k. Both d_k and α_k can be chosen to guarantee convergence to local minimizers, according to some standard globalization strategies. A very important family can be obtained by choosing the search direction as follows

$$d_k = -H_k^{-1} \nabla f(x_k),$$

where H_k is a nonsingular and symmetric matrix that pretends to approximate the Hessian matrix of f at x_k. Different ways of choosing d_k and different ways of choosing α_k produce different methods. Two well-known methods are obtained when $H_k = I$, for all k, which is known as the steepest descent method, the Cauchy method [30], or simply the gradient method; and $H_k = \nabla^2 f(x_k)$ (the Hessian at x_k) for all k, that produces Newton's method. Notice that any possible scheme that approximates the inverse of the Hessian matrix to obtain d_k can be viewed as an inverse preconditioning strategy for the Cauchy method [118]. See [34] for a preconditioning strategy of that kind, based on solving a suitable differential equation by means of a marching scheme that improves the quality of the approximation when k increases.

In practice, the direction d_k in Newton's method is obtained by solving the following linear system of equations

$$\nabla^2 f(x_k) d_k = -\nabla f(x_k),$$

that can be solved inexactly, i.e., by using an iterative linear scheme and stopping prematurely the internal solver, by monitoring the value of $\|F(x_k)\|$. The idea of stopping prematurely the internal iterative solver goes back to Pereyra [138], who developed such a combined scheme for solving two point boundary value problems, and was later generalized and formalized by Dembo et al. [56]. The inexact Newton's method has been associated with globalization strategies [57], nonsmooth problems [124], and Krylov subspace methods [10, 25].

For the Newton iteration to be well-defined, we must assume that f is twice continuously differentiable in the domain of interest. Moreover, in order to guarantee that the Newton's direction is a descent direction, it is enough to assume that the Hessian matrix is symmetric and positive definite (PD) for all k. In that case, the inverse of the Hessian is also PD and so

$$\nabla f(x_k)^t d_k = -\nabla f(x_k)^t \nabla^2 f(x_k)^{-1} \nabla f(x_k) < 0.$$

There exists several well-known techniques to modify the search direction to guarantee that the descent condition is satisfied, including modified factorization techniques [54, 133], and solving optimization subproblems as in the trust region approach [40]. Not all descent directions are of the same quality. The quality of a descent direction d_k can be measured with the cosine that it forms with the negative gradient direction

$$\cos \theta_k = \frac{-g_k^t d_k}{\|g_k\| \, \|d_k\|}.$$

Concerning the secant-type methods, in order to reduce the computational effort required by Newton's method, Davidon introduced [45] a very clever idea for optimization, that provides a way of approximating the derivative (Hessian matrix) using only the gradient information evaluated at each iterate. Davidon's method was the first secant method for vector problems, and its computational advantages were immediately appreciated in [69]. These very successful methods, called also quasi-Newton methods, are the natural secant extension of Newton's method for problems in vector spaces. For a complete discussion of quasi-Newton methods, see [53, 54]. The most successful ones are the DFP, the BFGS, and the SR1 methods. All these methods belong to the family described in (8), where now the matrix H_k is built according to some recipe to satisfy the secant equation (5). Hence, H_k will depend not only on x_k, but also on H_{k-1} and x_{k-1}, see, e.g., [54, 133]. As in the Newton's method, it is always possible to guarantee that d_k is a descent direction, and as before, the direction can be obtained inexactly [70]. The secant methods for unconstrained optimization have also been extended for nonsmooth problems [35, 116, 125].

2.2   Constrained optimization problems

Let us now discuss the extensions of Newton's method and secant methods for solving the constrained optimization problem, also known as the nonlinear programming problem,

$$\text{minimize} \, f(x) \quad \text{subject to} \quad h(x) = 0 \text{ and } \quad g(x) \leq 0, \tag{9}$$

where $f : \mathbb{R}^n \to \mathbb{R}$, $h : \mathbb{R}^n \to \mathbb{R}^m$, and $g : \mathbb{R}^n \to \mathbb{R}^p$. In the form (9) the problem is quite general; it includes the unconstrained case when $m = p = 0$, and it also includes as special cases linear and quadratic programs in which the constraint maps, h and g, are affine and f is linear or quadratic, respectively. A function that plays a key role in constrained optimization is the Lagrangian function defined by

$$L(x, \lambda, \mu) = f(x) + \lambda^T h(x) + \mu^T g(x),$$

where $\lambda \in \mathbb{R}^m$ and $\mu \in \mathbb{R}^p$ are the Lagrange multiplier vectors.

We start our discussion with the following general observation: For unconstrained optimization problems using either Newton's method or quasi-Newton methods, we need to solve a sequence of symmetric linear systems of equations. On the other hand, for solving (9), extending both the Newton's method and the secant formulations, the standard and proper approach is to solve a sequence of quadratic programming problems in which, at every iteration, the Hessian of the quadratic objective function is the Hessian of the Lagrangian function or a secant approximation to the Hessian. This approach is called the Successive Quadratic Programming (SQP) approach for solving (9). Several important observations are in order. The success of the SQP methods depends on the existence of rapid and robust schemes for solving quadratic programs. Fortunately, there are good algorithms to solve them, and an excellent review on this topic can be found in [20]. There are good implementations in both cases that guarantee local and fast convergence, i.e., q-quadratic for Newton's extension and q-superlinear for secant extensions (see [15, 68, 133] for details).

As it usually happens, the earliest reference of an SQP algorithm was concerned with the extension of Newton's method [173], and later SQP-type methods were developed to extend the secant method. The first secant-SQP method was introduced by Garcia-Palomares and Mangasarian [73]. Further extensions and convergence analysis (local and global) for SQP-Newton's method can be found for example in [41, 59, 142], and for SQP-secant methods in [22, 29, 55, 70, 84, 141, 167]. Besides the SQP approach, there are some other options to extend Newton's method and secant methods for solving (9). For instance, the study of Newton's method applied directly to the first order necessary conditions for (9) can be found in [77, 161, 165], and a diagonalized multiplier version of the SQP-secant method was discussed in [166]. See also Tapia [167] for optional extensions of the secant method for solving (9), El-Bakry et al. [59] for the application of a Newton interior-point methods for nonlinear programming problems, and Boggs et al. [21] for a special treatment of the large-scale case. A quasi-Newton interior-point method for nonlinear programming has also been analyzed in [122], and the connection of the trust-region globalization strategy with SQP-type methods has received special attention, see e.g., [31, 51, 58].

2.3 Additional vector problems

Besides the numerical optimization area, and the closely related topic of nonlinear systems of algebraic equations, there are many other general vector-space scientific computing prob-

lems and some specific applications in which the relationship between Newton's method and the secant methods appears.

In the numerical solution of nonlinear differential equations the traditional approach is to discretize the region of interest and also the differential operators, and then solve the associated nonlinear system of equation via numerical methods. As in some previously described scenarios, the first attempts involved Newton's method. For example, in the special case of Two Point Boundary Value Problems (TPBVP) the use of Newton's method is analyzed in [2], and an inexact Newton's version is introduced in [138]. Later on, as it usually happens, quasi-Newton methods were introduced for solving TPBVP, see e.g., [83]. For a general discussion on the numerical solution of TPBVP see [5]. Some other classical differential equation problems have also been attacked by Newton-type methods which are not related to discretization schemes, see e.g., [164].

Another more recent case, in which the relationship between Newton's method and the secant method can be observed, is the so called parareal method that exploits parallelism in time discretization for solving general nonlinear differential equations. It was introduced for solving Partial Differential Equations (PDE) by Lions, Maday and Turinici [115], and after been extended in several ways, it was recently analyzed by Gander and Vandewalle [72]. In [72], the authors observed the connection of the parareal method with multiple shooting, as analyzed by Chartier and Phillipe [32], for which quadratic convergence can be established since the multiple shooting method can be viewed as Newton's method. In [72], they also analyze a variant first proposed by Baffico et al. [6] that clearly resembles the secant method, and indeed, they establish superlinear convergence for that variant. Nevertheless, as far as we know, the connection between the superlinearly convergent variants of the parareal method and the classical secant method has not been pointed out in the literature.

The numerical solution of optimal control problems is another interesting area in which Newton's method, and some of its variations, has played a very important role. In particular, Newton's method has been combined with suitable globalization strategies specially adapted to optimal control problems in [84, 104, 170]. Moreover, SQP-type extensions have been proposed where the control variables receive a special treatment [55, 111].

Finally, we close this subsection describing some additional standard and well-known scientific computing vector problems for which Newton's method (or a closely related q-quadratically or even faster convergent scheme) was proposed without being aware of the connection, when the related numerical techniques were originally introduced. In most cases, these methods are still known and referred in the literature by their original names, although the connection with Newton's method has been established. For these problems, no secant counterpart has ever been developed.

The well-known *iterative refinement* scheme for solving linear systems of the form $Ax = b$ is a very good example of how Newton's method is rediscovered for a special application. Indeed, if an approximate solution, $\bar{x}$, has been already obtained by any method, and from that initial vector we apply Newton's method on the (linear) map $F(x) = Ax - b$ we obtain an improved solution $\bar{x}_+$ as follows:

$$\bar{x}_+ = \bar{x} - F'(\bar{x})^{-1}F(\bar{x}) = \bar{x} + A^{-1}r(\bar{x}),$$

where the residual vector is defined for any x as $r(x) = b - Ax$. In practice, to take advantage of any possible already obtained factorization of A, it is better to proceed as follows: Compute $r(\bar{x}) = b - A\bar{x}$, solve $As = r(\bar{x})$, update the solution $\bar{x}_+ = \bar{x} + s$, and repeat if necessary. This last procedure is what is known in the literature as iterative refinement, and the clear connection with Newton's method is seldom described. For the iterative refinement process it has been established local and fast convergence as well as stability when combined with LU factorizations [90, 158].

A topic in which Newton's method appears in a perhaps surprising way is the use of inverse power shifted iteration algorithms for computing an eigenvalue - eigenvector pair (eigenpair) of a given real $n \times n$ matrix A. In the symmetric case, Peters and Wilkinson [140] observed the connection between Newton's method and the iterative calculation of an eigenpair $(\hat{x}, \hat{\lambda})$ by considering the $(n + 1) \times (n + 1)$ nonlinear system:

$$(A - \lambda I)x = 0, \quad \frac{1}{2}(1 - x^T x) = 0,$$

where the normalization $\|x\|_2 = 1$ is included. Then, Newton's method or the so-called projected Newton's method from an initial x_0, such that $\|x_0\|_2 = 1$, are obtained by solving iteratively the linear system

$$\begin{pmatrix} A - \lambda I & -x \\ -x^T & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta \lambda \end{pmatrix} = - \begin{pmatrix} (A - \lambda I)x \\ \frac{1}{2}(1 - x^T x) \end{pmatrix} \tag{10}$$

and then setting $x_+ = (x + \Delta x)/\|x + \Delta x\|_2$, and $\lambda_+ = \lambda + \Delta \lambda$. If the normalization is not included when computing x_+ then this would be Newton's method applied to the $(n + 1) \times (n + 1)$ nonlinear system. If the normalization is considered, then it is the projected Newton's method. If the normalization is not included, then local q-quadratic convergence is immediately obtained. Surprisingly, it is established in Tapia and Whitley [168] that if the normalization is forced at every iteration, then the intriguing local q-order of convergence is $1 + \sqrt{2}$, which represents a superquadratic order of convergence. To observe the connection with inverse power shifted iterations, it suffices to note that the first equation in (10) implies that (see [168] for details)

$$(A - \lambda I)x_+ = (\Delta \lambda)x,$$

i.e., the new eigenvector estimate is a scalar multiple of the one given by inverse power shifted iterations. In the projected Newton's method it can be established that the new eigenvalue estimate is given by

$$\lambda_+ = \frac{x^T A x_+}{x^t x_+}.$$

It is well-know that the so-called Rayleigh quotient iteration uses systematically the closely related estimate

$$\lambda_+ = \frac{x_+^T A x_+}{x_+^t x_+},$$

for which the faster q-cubic convergence is observed.

For nonsymmetric matrices, when convergence is observed, the rate of the previously mentioned inverse iterations is in general slower than in the symmetric case. For example, when convergence is observed, the Rayleigh quotient iteration converges q-quadratically instead of q-cubically. Unfortunately there are examples that show that the inverse iterations can fail in the nonsymmetric case [9]. See [163] for a discussion on how to combine different inverse power iterations to improve the chance of convergence. Variants of Newton's method have also been applied for approximating several matrix eigenpairs simultaneously [1, 119].

Another interesting and attractive topic for which Newton's method appeared, without knowing it explicitly, is the problem of finding the best function approximation in the uniform norm, also known as the infinity norm. The classical Chebyshev alternating theorem suggests ways for numerically computing the best uniform approximation $p*$ to $f \in C[a, b]$ by functions p from a Haar system $\phi := \{\phi_1, \cdots, \phi_n\}$. The first effective algorithm, based on the alternating theorem, was proposed by Remez in 1934 [147]. This algorithm iteratively repeats two distinct steps that involve nonlinear systems of n algebraic equations, and finding the n roots of some related polynomials. It was soon identified that Remez algorithm had quadratic convergence to $p*$. Later on, it was established under mild assumptions (mainly that f is C^1) that Remez method could be viewed as Newton's method for a certain convenient nonlinear map [38, 132]; see also [169]. For additional details on this topic see [37], and also [143].

3 Matrix problems

In the space of square matrices, problem (1) can be written as

$$\text{Given } F : \mathbb{C}^{n \times n} \to \mathbb{C}^{n \times n} \quad \text{find } X_* \in \mathbb{C}^{n \times n} \text{ such that } F(X_*) = 0. \tag{11}$$

Newton's method (Algorithm 1) has also played an important role in the historical process of the algorithm development for solving specific nonlinear matrix problems. Moreover, as we will discuss in this section, in the space of matrices the algorithm structure is heavily problem dependent, and as discussed before for vector problems, Newton's method has been reinvented several times.

Let us list some of the most important nonlinear matrix problems frequently considered in the literature for special applications, and the associated map F.

- *Matrix inverse.* One of the oldest and most common nonlinear matrix problem is to compute the inverse of a nonsingular A, that appears associated with the solution of linear systems, and more recently associated with the art of building suitable preconditioning strategies for iterative methods [33, 34]. For this problem, $F(X) = X^{-1} - A$.

- *Matrix p-th root.* For this problem, $F(X) = X^p - A$ where $p \in \mathbb{N}$ and $p \geq 2$. The case $p = 2$ has been extensively studied for several decades, see e.g. [19, 87, 91, 99, 126], whereas the general case, $p > 2$, has been recently considered, see e.g.

[16, 47, 48, 100, 159]. Computing the square root ($p = 2$) of a given matrix is useful for solving some boundary value problems [152] and also appears in the modelling of flow problems [121]; and the general case ($p > 2$) appears associated with Markov processes [79] among other applications. For a complete discussion on matrix p-th roots see [92].

- *Matrix sign function.* The sign of a matrix extends naturally the concept of the sign of a complex number [108]. Given a matrix A with no pure imaginary eigenvalues, the sign of A is given by

$$S = sign(A) = A(A^2)^{-1/2},$$

where $A^{1/2}$ is the principal square root of A, that will be fully described later. See [92] for several equivalent definitions of the matrix sign function and its properties. The sign function is useful for solving Riccati equations, that will be discussed later. It is also useful for solving some specialized eigenvalue problems [97]. Among the many equivalent definitions, a practical one states that the sign of a matrix A is the square root of the identity that commutes with A [106]. This last equivalent definition motivates to use $F(X) = X^2 - I$, and then apply suitable iterative methods starting from $X_0 = A$.

- *Riccati equations.* The nonlinear map associated with Riccati equations is $F(X) = XA + A^T X - XBB^T X + C^T C$ where A, B and C are given matrices with some special properties, and the solution X is square and usually required to have some special properties [112]. Riccati equations arise naturally in control problems [3, 11, 14, 43, 113, 148].

- *Quadratic equations.* Given the matrices A, B, and C, the quadratic matrix equation $AX^2 + BX + C = 0$ arises in control theory [43, 46, 94]. In this case, the nonlinear map is $F(X) = AX^2 + BX + C$.

- *Matrix rational equations.* The nonlinear map associated with matrix rational equations is

$$F(X) = X \pm A^* X^{-p} A - Q,$$

where A is a given matrix, Q is a Hermitian positive definite matrix, and p is a positive integer. The cases $p = 1$ or $p = 2$ have received special attention in the last few years. Matrix rational equations appear in a wide variety of applications [60, 61, 62, 81, 102, 130, 145, 174].

- *Matrix logarithm and matrix exponential.* For computing the logarithm of a given matrix A [39, 105], we consider the map $F(X) = e^X - A$ where

$$e^X = I + X + \frac{X^2}{2!} + \cdots + \frac{X^k}{k!} + \cdots$$

Similarly, for computing the exponential of a given matrix A [93, 127], we consider the map $F(X) = \ln X - A$.

A key aspect that plays a crucial role in the space of matrices is the numerical stability of the proposed methods. In general, Newton's method is numerically stable, but in many cases simplified versions of it, that are mathematically equivalent and computationally appealing, are not numerically stable (i.e. a small perturbation Δ_k in X_k may lead to divergence of the sequence obtained by replacing X_k by $X_k + \Delta_k$).

It is worth mentioning that, although nonlinear problems are the natural ones associated with problem (11), there exist important applications for which the map F in (11) is a linear map that, despite being linear, represent difficult problems to solve, and so they deserve special attention. Moreover, quite frequently the iterative methods associated with nonlinear problems, solve a linear matrix problem per iteration. The best known of these linear matrix problems is the so-called Sylvester equation [162], that appears, e.g., in the solution of control theory problems [43]:

$$AX - XB = C, \tag{12}$$

where $X, C \in \mathbb{C}^{n \times p}$ and A and B are square matrices of order n and p respectively. Note that $B = -A^T$ yields the well-known Lyapunov equation [120]. The necessary and sufficient condition for (12) to have a unique solution is that the set of eigenvalues of A and B have an empty intersection. This key theoretical result was originally established by Sylvester [162]. For a full description of the theoretical properties of Sylvester equations see [43, 95]. For solving (12) a wide variety of numerical schemes have been proposed, ranging from direct methods that are based on the Kronecker product to iterative methods of different types, see e.g. [8, 44, 74, 98, 103, 128] and references therein.

As we mentioned before, whenever a Newton's method is proposed, it is possible to define a secant scheme. Recently some authors have developed secant methods for nonlinear matrix problems that inherited, as much as possible, the features of the classical secant methods in previous scenarios (e.g., scalar equations, nonlinear algebraic systems of equations). A general secant method for solving (11) should be given by the following iteration

$$X_{k+1} = X_k - A_k^{-1} F(X_k),$$

where $X_{-1} \in \mathbb{C}^{n \times n}$ and $X_0 \in \mathbb{C}^{n \times n}$ are given, and A_{k+1} is a suitable linear operator that satisfies

$$A_{k+1} S_k = Y_k, \tag{13}$$

where $S_k = X_{k+1} - X_k$ and $Y_k = F(X_{k+1}) - F(X_k)$. Equation (13) is known as the *matrix secant equation*.

Notice that one $n \times n$ matrix is enough to satisfy the matrix secant equation (13), i.e., the operator A_{k+1} can be obtained as a matrix of the same dimension of the step S_k and the map-difference Y_k. In that sense, there is a resemblance with the scalar case, in which one equation is required to find one unknown. Hence, once X_{k+1} has been obtained, the matrix A_{k+1} can be computed at each iteration by solving a linear system of n^2 equations. The proposed algorithm, and an important inverse variant, can be summarized as follows [129, 131]:

Algorithm 3 General secant method for matrix problems
- 1: Given $X_{-1} \in \mathbb{C}^{n \times n}$, $X_0 \in \mathbb{C}^{n \times n}$
- 2: **Set** $S_{-1} = X_0 - X_{-1}$
- 3: **Set** $Y_{-1} = F(X_0) - F(X_{-1})$
- 4: **Solve** $A_0 S_{-1} = Y_{-1}$ $\qquad\qquad\qquad$ ▷ for A_0
- 5: **for** $k = 0, 1, \cdots$ until convergence **do**
- 6: $\quad$ **Solve** $A_k S_k = -F(X_k)$ $\qquad\qquad$ ▷ for S_k
- 7: $\quad$ **Set** $X_{k+1} = X_k + S_k$
- 8: $\quad$ **Set** $Y_k = F(X_{k+1}) - F(X_k)$
- 9: $\quad$ **Solve** $A_{k+1} S_k = Y_k$ $\qquad\qquad$ ▷ for A_{k+1}
- 10: **end for**

We can generate the sequence $B_k = A_k^{-1}$, instead of A_k, and obtain an inverse version that solves only one linear system of equations per iteration:

Algorithm 4 Inverse secant method
- 1: Given $X_{-1} \in \mathbb{C}^{n \times n}$, $X_0 \in \mathbb{C}^{n \times n}$
- 2: **Set** $S_{-1} = X_0 - X_{-1}$
- 3: **Set** $Y_{-1} = F(X_0) - F(X_{-1})$
- 4: **Solve** $B_0 Y_{-1} = S_{-1}$ $\qquad\qquad\qquad$ ▷ for B_0
- 5: **for** $k = 0, 1, \cdots$ until convergence **do**
- 6: $\quad$ **Set** $S_k = -B_k F(X_k)$
- 7: $\quad$ **Set** $X_{k+1} = X_k + S_k$
- 8: $\quad$ **Set** $Y_k = F(X_{k+1}) - F(X_k)$
- 9: $\quad$ **Solve** $B_{k+1} Y_k = S_k$ $\qquad\qquad$ ▷ for B_{k+1}
- 10: **end for**

Solving a secant method that deals with $n \times n$ matrices is the most attractive feature of Algorithms 3 and 4, in sharp contrast with the standard extension of quasi-Newton methods for general Hilbert spaces, (see e.g. [75, 150]), that in this context would involve $n^2 \times n^2$ linear operators to approximate the derivative of F. Clearly, dealing with $n \times n$ matrices for solving the related linear systems significantly reduces the computational cost associated with the linear algebra of the algorithm.

In order to discuss some theoretical issues of the proposed general secant methods, let us consider the standard assumptions of Theorem 2.1 but using $\mathbb{C}^{n \times n}$ instead of $\mathbb{R}^n$. We begin by noticing that the operator A_k does not approximate $F'(X_k)$ as in previous scenarios due to dimensional discrepancies. Indeed, $F'(X_k) \in \mathbb{C}^{n^2 \times n^2}$ and $A_k \in \mathbb{C}^{n \times n}$. However, fortunately, $F'(X_k)S_k$ and $A_k S_k$ both live in $\mathbb{C}^{n \times n}$, which turns out to be the suitable approximation since, using the secant equation (13), we have that

$$A_{k+1} S_k = Y_k = F(X_{k+1}) - F(X_k) = F'(X_k)S_k + R(S_k). \tag{14}$$

Subtracting $F'(X_*)S_k$ in both sides of (14), and taking norms we obtain

$$\|A_{k+1}S_k - F'(X_*)S_k\| \leq \|F'(X_k) - F'(X_*)\|\|S_k\| + \|R(S_k)\|,$$

for any subordinate norm $\| \, . \, \|$. Using now that $F'(X) \in Lip_\gamma(N(X_*, r))$, and dividing by $\|S_k\|$ we have

$$\frac{\|A_{k+1}S_k - F'(X_*)S_k\|}{\|S_k\|} \leq \gamma\|E_k\| + \frac{\|R(S_k)\|}{\|S_k\|}, \tag{15}$$

where $E_k = X_k - X_*$ represents the error matrix.

Form this inequality we observe that, if convergence is attained, the left hand side tends to zero when k goes to infinity, and so the sequence $\{A_k\}$, generated by Algorithm 2, tends to the Fréchet derivative, $F'(X_*)$, when they are both applied to the direction of the step S_k.

In the next subsections we will discuss the specialized versions of Newton's method when applied to some of the nonlinear matrix problems listed above. We will also present the recent development of secant methods for solving some of them.

3.1 Inverse of a matrix

Let us start by describing the application of Newton's method for computing the inverse of a given matrix A. As we mentioned before, for this problem the associated map F is defined as follow

$$F(X) = X^{-1} - A. \tag{16}$$

Applying the suitable Taylor's expansion, discussed in (2), to (16) we obtain that

$$F(X + H) = (X + H)^{-1} - A = X^{-1} - X^{-1}HX^{-1} - A + O(H^2),$$

and so $F'(X)H = -X^{-1}HX^{-1}$. In here, we are using the fact that if B is a nonsingular matrix and C is any other matrix then

$$(B + C)^{-1} = B^{-1} - B^{-1}CB^{-1} + O(\|B^2\|).$$

Consequently, forcing the step 3 in Algorithm 1 yields

$$\begin{aligned} -X_k^{-1}H_kX_k^{-1} &= -(X_k^{-1} - A) \\ H_k &= X_k - X_kAX_k, \end{aligned}$$

which implies that the Newton iteration, from an initial guess X_0, to find the inverse of A is given by

$$X_{k+1} = X_k + H_k = 2X_k - X_kAX_k. \tag{17}$$

Notice that, the Fréchet derivative F' cannot be obtained explicitly, and instead it is obtained implicitly in the product $F'(X)H$, which is enough to identify the step H. The implicit representation of F' is a frequent event, as we will see in the following subsections, when applying Newton's method to solve nonlinear matrix problems.

The iterative method (17) has been historically known as Schulz method [153] who first introduced it in the early 30's. It has been established that if $X_0 = \frac{A^*}{\|A\|_2 \|A^*\|_2}$, then Schulz method possesses global convergence [86], it is a numerical stable scheme [160], and it clearly has local q-quadratic convergence. Moreover, if A does not have an inverse, it converges to the pseudoinverse of A, denoted by $A^\dagger$ (also known as the generalized inverse) [86, 92, 135, 160].

A secant method has also been defined to find the root of (16) [131]. For that, let us consider the general secant method applied to (16)

$$
\begin{aligned}
X_{k+1} &= X_k - S_{k-1}(F(X_k) - F(X_{k-1}))^{-1}F(X_k) \\
&= X_k - (X_k - X_{k-1})(X_k^{-1} - X_{k-1}^{-1})^{-1}(X_k^{-1} - A),
\end{aligned}
\tag{18}
$$

that after several algebraic manipulations can be reduced as

$$
X_{k+1} = X_{k-1} + X_k - X_{k-1}AX_k,
\tag{19}
$$

which avoids the inverse matrix calculations per iteration associated with iteration (18). Notice the resemblance between (19) and Schulz method for solving the same problem. The method described in (19), denoted as the secant-Schulz method, converges locally and q-superlinearly to the inverse of A. Moreover, when A has no inverse, it converges locally and q-superlinearly to $A\dagger$. It has also been established that the secant-Schulz method generates a stable iteration [131]. It is important to note that the q-superlinear convergence implies the well-known Dennis-Moré condition [52, 54]

$$
\lim_{k \to \infty} \frac{\|A_k S_k - F'(X_*)S_k\|}{\|S_k\|} = 0,
$$

that establishes the most important property of the sequence $\{A_k\}$ generated by the secant-Schulz method.

We now present an experiment to illustrate the typical behavior of the secant-Schulz iterative method when compared to the Schulz method for computing the inverse of a given matrix. For this experiment we consider the symmetric and positive definite matrix `poisson` from the Matlab gallery with $n = 400$. In this case, choosing $X_{-1} = 0.5 * I$ and $X_0 = A^T/\|A\|_2^2$ for the secant-Schulz and the same X_0 for the Newton-Schulz guarantees global convergence for both methods [131] . We report the results in Table 1, and the semilog of the relative error in Figure 1.

Table 1: Performance of secant-Schulz and Newton-Schulz for finding the inverse of $A =$ `gallery('poisson',20)` when $n = 400$, $X_{-1} = 0.5 * I$, and $X_0 = A^T/\|A\|_2^2$.

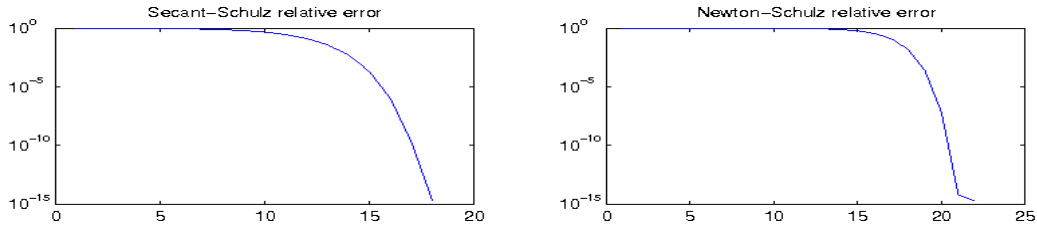| Method	Iter	$\|X_k - X_*\|/\|X_*\|$
Secant-Schulz	18	1.95e-15
Newton-Schulz	22	1.87e-15

Figure 1: Semilog of the relative error associated with Table 1.

3.2 Square root

Let us now consider $F(X) = X^2 - A$ with $A \in \mathbb{C}^{n \times n}$ for computing square roots of A. In this case, $F(X) = 0$ might have no solutions, finitely many solutions or infinitely many solutions. For a theoretical discussion on the existence of square roots for a given matrix, see [89, 95]. Nevertheless, when A has no eigenvalue in the set $\mathbb{R}^- = \{x \in \mathbb{R} : x \leq 0\}$, then there exists a unique square root X_* such that the real part of all its eigenvalues is positive. This special solution is known as the *principal square root* of A, and it is denoted by $X_* = A^{1/2}$. The principal square root can be characterized when A is *diagonalizable*, i.e., if there exists $W \in \mathbb{C}^{n \times n}$ such that

$$W^{-1}AW = \Lambda = diag(\lambda_1, \lambda_2, \cdots \lambda_n),$$

where $\lambda_1, \lambda_2, \cdots \lambda_n$ are the eigenvalues of A. Note that in that case

$$A = W\Lambda W^{-1} = (W\Lambda^{1/2}W^{-1})(W\Lambda^{1/2}W^{-1}),$$

where $\Lambda^{1/2} = diag(\sqrt{\lambda_1}, \sqrt{\lambda_2}, \cdots, \sqrt{\lambda_2})$ and so $A^{1/2} = W\Lambda^{1/2}W^{-1}$. For details see [92]. The special interest in $A^{1/2}$ is based on the role it plays for several applications, e.g., Markov processes [79, 101, 171], modelling of flow problems [121], and applications related to the logarithm of a matrix [39, 105].

Newton's method and specialized versions of it, for computing the principal square root of a matrix, has received significant attention for many years [79, 87, 91, 99, 126, 154]. For Newton's method, once again, we need to identify the Fréchet derivative $F'(X)$ using the Taylor expansion (2)

$$F(X + S) = (X + S)^2 - A = X^2 - A + XS + SX + S^2.$$

Hence, we obtain the following algorithm

Algorithm 5 Newton's method for $F(X) = X^2 - A$

1: Given $X_0 \in \mathbb{C}^{n \times n}$
2: **for** $k = 0, 1, \cdots$ **do**
3:    Solve $X_k S_k + S_k X_k = -F(X_k)$ ▷ For S_k
4:    $X_{k+1} = X_k + S_k$
5: **end for**

17

Notice that the linear problem in Step 3, that needs to be solved to obtain the step S_k, is a Sylvester equation. As we mentioned before, solving a Sylvester equation is not an easy problem, that requires a significant amount of computational effort. Algorithm 5 is a stable scheme that has q-quadratic convergence to $A^{1/2}$ when $X_0 = A$ or $X_0 = mI$ for $m > 0$ [87].

In order to avoid the solution of a Sylvester equation per iteration, several variants of Newton's method have emerged. In [87, 91, 92] several of these variants are described and analyzed. Many of them assume that X_0 is chosen such that $X_0 A = A X_0$, which imply that $A X_k = X_k A$ and $X_k S_k = S_k X_k$ for all $k \geq 0$ [87]. As a consequence, S_k can be explicitly obtained, from Step 3 of Algorithm 5, as $S_k = \frac{1}{2}[X_k^{-1} A - X_k]$ or $S_k = \frac{1}{2}[A X_k^{-1} - X_k]$, and two simplified variants of Newton's method are obtained:

$$(I): \quad Y_{k+1} = \frac{1}{2} \left[Y_k + Y_k^{-1} A \right] \tag{20}$$

$$(II): \quad Z_{k+1} = \frac{1}{p} \left[Z_k + A Z_k^{-1} \right] . \tag{21}$$

In Higham [87] it is established that if A is diagonalizable and no real eigenvalue of A belongs to $\mathbb{R}^-$, then the sequence of matrices generated by (20), or (21), converges q-quadratically to $A^{1/2}$ when $Y_0 = Z_0 = mI$ for $m > 0$. On the negative side, these iterations are numerically unstable unless the following restrictive condition holds

$$\frac{1}{2} \left| 1 - (\lambda_j / \lambda_i)^{1/2} \right| \leq 1 \quad \text{for } 1 \leq i, j, \leq n, \tag{22}$$

where the λ_i's are the eigenvalues of A. If A is Symmetric and Positive Definite (SPD) the condition (22) is equivalent to $\kappa_2(A) \leq 9$ [87]. Due to this unacceptable condition the schemes given by (20) and (21) are of no practical use.

In contrast, several additional stable variants have been proposed and analyzed for the matrix square root problem, that are also based on Newton's method. A complete description of some of these variants can be found in [91]. We now present some of the most relevant Newton-type stable options:

- Denman and Beavers [49] propose a specialized iteration for Riccati equations, that reduced to the square root problem produces the following coupled scheme:

$$\begin{aligned} Y_{k+1} &= \frac{1}{2} \left[Y_k + Z_k^{-1} \right] \\ Z_{k+1} &= \frac{1}{2} \left[Z_k + Y_k^{-1} \right] , \end{aligned} \tag{23}$$

from $Y_0 = A$ and $Z_0 = I$. Iteration (23) is stable and has the property that Y_k converges to $A^{1/2}$ and Z_k converges to $A^{-1/2}$, both q-quadratically [91]. The main criticism is that it requires the inverse of two distinct matrices per iteration.

- To avoid the inverse of two matrices per iteration, Higham [91] analyzes the following coupled variant that combines the Denman-Beaver scheme with Schulz method for

the matrix inverse problem

$$
\begin{aligned}
P_{k+1} &= \frac{1}{2} P_k [3I - Q_k P_k] \\
Q_{k+1} &= \frac{1}{2} Q_k [3I - P_k Q_k],
\end{aligned}
\tag{24}
$$

from $P_0 = A$ and $Q_0 = I$. The coupled iteration (24) is also stable, and has the property that P_k converges to $A^{1/2}$ whereas Q_k converges to $A^{-1/2}$, both q-quadratically, whenever the condition $\|diag(A - I, A - I)\| < 1$ holds [91].

- Meini [126] presents the following coupled iteration that avoids additional conditions on the matrix A for convergence, while requiring a matrix inverse (instead of two) per iteration

$$
\begin{aligned}
Y_{k+1} &= -Y_k Z_k^{-1} Y_k \\
Z_{k+1} &= Z_k + 2Y_{k+1},
\end{aligned}
\tag{25}
$$

from $Y_0 = I - A$ and $Z_0 = 2(I + A)$. The coupled iteration (25) is stable and has the property that Y_k converges to 0 while Z_k converges q-quadratically to $4A^{1/2}$.

- Iannazzo [99] presents and analyzes the following iteration that requires one matrix inverse per iteration

$$
\begin{aligned}
X_{k+1} &= X_k + H_k \\
H_{k+1} &= -\frac{1}{2} H_k X_{k+1}^{-1} H_k,
\end{aligned}
\tag{26}
$$

from $X_0 = A$ and $H_0 = \frac{1}{2}(I - A)$. Iteration (26) is stable and the sequence X_k converges q-quadratically to $A^{1/2}$, without additional conditions.

On the other hand, it is possible to develop a secant method to find a square root of a given matrix A. Applying Algorithm 3 to $F(X) = X^2 - A$, we obtain

$$
X_{k+1} = X_k - (X_k - X_{k-1})(X_k^2 - X_{k-1}^2)^{-1}(X_k^2 - A),
\tag{27}
$$

and from (27), if X_k commutes with A, we obtain a simplified version of Algorithm 3 given by

$$
\begin{aligned}
X_{k+1} &= X_k - (X_k - X_{k-1})(X_k - X_{k-1})^{-1}(X_k + X_{k-1})^{-1}(X_k^2 - A) \\
&= (X_k + X_{k-1})^{-1}((X_k + X_{k-1})X_k - (X_k^2 - A)) \\
&= (X_k + X_{k-1})^{-1}(X_{k-1}X_k + A).
\end{aligned}
\tag{28}
$$

Notice the resemblance between (28) and (20). Both iterations are very attractive from a computational point of view, but using similar arguments to the ones used by Higham in [87], it can be established that (28) is an unstable iteration unless the eigenvalues of A satisfy the condition (22). Therefore iteration (28) should be avoided.

Now, we will establish q-superlinear convergence of iteration (27) without assuming commutativity. Let us assume that A is *diagonalizable*, that is, there exists a nonsingular matrix V such that

$$V^{-1}AV = \Lambda = diag(\lambda_1, \lambda_2, \cdots, \lambda_n), \tag{29}$$

where $\lambda_1, \lambda_2, \cdots, \lambda_n$ are the eigenvalues of A. If we define $D_k = V^{-1}X_kV$ then we have from (27) that

$$
\begin{aligned}
D_{k+1} &= D_k - V^{-1}(X_k - X_{k-1})VV^{-1}(X_k^2 - X_{k-1}^2)VV^{-1}(X_k^2 - A)V \\
&= D_k - (D_k - D_{k-1})(D_k^2 - D_{k-1}^2)^{-1}(D_k^2 - \Lambda).
\end{aligned}
\tag{30}
$$

If we choose X_{-1} and X_0 such that $D_{-1} = V^{-1}X_{-1}V$ and $D_0 = V^{-1}X_0V$ are diagonal matrices, then all successive D_k are diagonal too, and (30) can be written as

$$D_{k+1} = D_k - (D_k + D_{k-1})^{-1}(D_k^2 - \Lambda) = (D_k + D_{k-1})^{-1}[D_{k-1}D_k + \Lambda]. \tag{31}$$

Note that we can write (31) as n uncoupled scalar secant iterations for computing the square roots of λ_i, for $1 \le i \le n$, given by

$$d_{k+1}^i = \frac{d_k^i d_{k-1}^i + \lambda_i}{d_{k-1}^i + d_k^i}, \tag{32}$$

where $d_k^i = (D_k)_{ii}$. From (32) we have that

$$d_{k+1}^i \pm \sqrt{\lambda_i} = \frac{(d_k^i \pm \sqrt{\lambda_i})(d_{k-1}^i \pm \sqrt{\lambda_i})}{d_{k-1}^i + d_k^i}, \tag{33}$$

and so

$$\frac{d_{k+1}^i - \sqrt{\lambda_i}}{d_{k+1}^i + \sqrt{\lambda_i}} = \left(\frac{d_k^i - \sqrt{\lambda_i}}{d_k^i + \sqrt{\lambda_i}}\right)\left(\frac{d_{k-1}^i - \sqrt{\lambda_i}}{d_{k-1}^i + \sqrt{\lambda_i}}\right). \tag{34}$$

Applying (34) recursively it follows that

$$\frac{d_{k+1}^i - \sqrt{\lambda_i}}{d_{k+1}^i + \sqrt{\lambda_i}} = \left(\frac{d_0^i - \sqrt{\lambda_i}}{d_0^i + \sqrt{\lambda_i}}\right)^{f_k} \left(\frac{d_{-1}^i - \sqrt{\lambda_i}}{d_{-1}^i + \sqrt{\lambda_i}}\right)^{f_{k-1}}, \tag{35}$$

where $f_{k+1} = f_k + f_{k-1}$ for $k \ge 0$, and $f_{-1} = f_0 = 1$. Notice that $\{f_k\}$ is a Fibonacci sequence that appears quite frequently in the analysis of secant methods. We are now ready to establish our convergence result.

Theorem 3.1 *Let $A \in \mathbb{C}^{n \times n}$ be a diagonalizable matrix as in (29). Let us assume that A has no nonpositive real eigenvalues, and that all iterates X_k are well defined. If $X_{-1} = \alpha I$; $\alpha > 0$ and $X_0 = \beta I$; $\beta > 0$ then the sequence $\{X_k\}$ converges q-superlinearly to $A^{1/2}$.*

Proof. From (31) and (32) it is enough to study the convergence of $\{d_k^i\}$ to the square root $\sqrt{\lambda_i}$ for all $1 \leq i \leq n$. Since none of the eigenvalues of A is real and nonpositive then we can choose $\sqrt{\lambda_i}$ such that its real part, $Re(\sqrt{\lambda_i})$, is positive for $1 \leq i \leq n$. On the other hand, since $d_{-1}^i = \alpha > 0$ and $d_0^i = \beta > 0$ then for each i

$$\left| \frac{d_{-1}^i - \sqrt{\lambda_i}}{d_{-1}^i + \sqrt{\lambda_i}} \right| < 1 \ \ \text{and} \ \ \left| \frac{d_0^i - \sqrt{\lambda_i}}{d_0^i + \sqrt{\lambda_i}} \right| < 1,$$

and hence, from (35)

$$\lim_{k \to \infty} d_k^i = \lambda_i^{1/2}, \ \ Re(\lambda_i^{1/2}) > 0.$$

Therefore,

$$\lim_{k \to \infty} X_k = V\Lambda^{1/2}V^{-1} = A^{1/2},$$

and the convergence is established. Now, to prove the local q-superlinear convergence, consider (33) that can be written as

$$e_{k+1}^i = c_k^i e_k^i e_{k-1}^i, \tag{36}$$

where $e_k^i = d_k^i - \lambda_i^{1/2}$ and $c_k^i = 1/(d_{k-1}^i + d_k^i)$. Notice that c_k^i tends to $1/(2\lambda_i^{1/2})$ when k goes to infinity, and so it is bounded for k sufficiently large. From (36) we conclude that each scalar secant iteration (32) converges locally and q-superlinearly to $\lambda_i^{1/2}$. Therefore, equivalently, there exists a sequence $\{\tilde{c}_k^i\}$, for each $1 \leq i \leq n$, such that $\tilde{c}_k^i > 0$ for all k, $\lim_{k \to \infty} \tilde{c}_k^i = 0$, and

$$|e_{k+1}^i| \leq \tilde{c}_k^i |e_k^i|. \tag{37}$$

Using (37) we now obtain in the Frobenius norm

$$\|D_{k+1} - \Lambda^{1/2}\|_F^2 = \sum_{i=1}^n (e_{k+1}^i)^2 \leq \sum_{i=1}^n (\tilde{c}_k^i)^2 (e_k^i)^2 \leq n\hat{c}_k^2 \sum_{i=1}^n (e_k^i)^2 \leq n\hat{c}_k^2 \|D_k - \Lambda^{1/2}\|_F^2, \tag{38}$$

where $\hat{c}_k = \max_{1 \leq i \leq n}\{\tilde{c}_k^i\}$. Finally, we have that

$$\|X_{k+1} - A^{1/2}\|_F = \|VV^{-1}(X_{k+1} - A^{1/2})VV^{-1}\|_F \leq \kappa_F(V)\|D_{k+1} - \Lambda^{1/2}\|_F$$

$$\leq \kappa_F(V)\sqrt{n}\hat{c}_k\|D_k - \Lambda^{1/2}\|_F \leq \kappa_F(V)^2\sqrt{n}\hat{c}_k\|X_k - A^{1/2}\|_F,$$

where $\kappa_F(V)$ is the Frobenius condition number of V. Hence, $\{X_k\}$ converges locally and q-superlinearly to $A^{1/2}$. $\qquad\square$

Remark. If all the eigenvalues of A have positive real part, then we can choose either $X_{-1} = \alpha A$ or $X_0 = \beta A$ or both, for $\alpha > 0$ and $\beta > 0$, and using the same arguments as in Theorem 3.1 guarantee the q-superlinear convergence of $\{X_k\}$ to $A^{1/2}$.

Now we present some numerical experiments to compare our specialized secant method (Algorithm 3) with the DM iteration (23) and Meini's iteration (25). We stop all considered

algorithms when the Frobenius norm of the residual is less than $0.5D - 12$, and we report the number of required iterations (Iter), and the norm of the residual ($\|F(X_k)\|_F$) when the process is stopped. The symbol (**) means that the algorithm accomplished the maximum number of iterations. First, we consider the matrix `dorr` from the Matlab gallery. This matrix is row diagonal dominant, tridiagonal, and ill-conditioned for small value of the input argument θ. For this experiment we use $n = 10$ and $\theta = 10^{-7}$. These values were chosen as in [126]. The results are reported in Table 2. We can observe that DB does not

Method	Iter	$\|F(X_k)\|_F$
DB	**	13.62
Meini	22	1.27e-13
Secant	10	2.08e-13

Table 2: Performance of the secant method and Newton methods for finding the square root of $A =$ `gallery('dorr',n,`θ`)` when $n = 10$, $\theta = 10^{-7}$, $X_{-1} = I$, and $X_0 = A/\|A\|_F$.

achieve convergence. Meini's iteration converges, but it requires more than twice as many iteration as the secant method.

Now, we consider a problem described in [126]. For this example, A is the following Frobenius matrix

$$A = \begin{pmatrix} -p_3 & -p_2 & -p_1 & -p_0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

where p_i with $3 \leq i \leq 0$ are the coefficients of $p(x) = (x - 2)(x - 5)((x + 1)^2 + \epsilon)$ which is the characteristic polynomial of A. In this case A has two complex conjugate eigenvalues $-1 \pm i\sqrt{\epsilon}$. For small values of ϵ, these eigenvalues tend to be real and negative, and therefore the matrix $A^{1/2}$ is ill-conditioned. In this experiment we take different values of ϵ and, following [126], we report the iteration at which the minimal value of $\|F(X_k)\|_F$ is reached. Since A has two eigenvalues with negative real part we choose $X_{-1} = 5^{-10}I$ and $X_0 = 2I$.

We can see in Table 3 that for all values of ϵ the DB iteration achieves the lowest residual norm. On the other hand, the Meini's iteration for $\epsilon = 10^{-6}$ and $\epsilon = 10^{-8}$ has the worst performance and for this cases the secant method reduces considerably the residual norm in spite of the ill-conditioning of $A^{1/2}$.

3.3   Sign of a matrix

Let us now consider the application of Newton's method for computing the sign of a matrix. Let us recall that $S = sign(A) = A(A^2)^{-1/2}$, where $A^{1/2}$ is the principal square root of A. The following is a list of the most important properties of the matrix sign function, that play a role when defining iterative schemes to compute S [92]: $S^2 = I$, i.e., $S^{-1} = S$; $AS = SA$; and if A is SPD then $S = I$. Moreover, if A is a square matrix with

ϵ	Method	Iter	$\|F(X_k)\|_F$
	DB	11	9.67e-14
10^{-2}	Meini	10	1.09e-11
	Secant	19	5.24e-11
	DB	18	6.07e-12
10^{-4}	Meini	12	5.6e-6
	Secant	21	1.55e-7
	DB	33	6.73e-10
10^{-6}	Meini	13	11.28
	Secant	41	8.62e-8
	DB	35	2.21e-8
10^{-8}	Meini	1	15.78
	Secant	47	2.1e-3

Table 3: Performance of the secant method and Newton methods for finding the square root of the Frobenius matrix with $p(x) = (x-2)(x-5)((x+1)^2 + \epsilon)$ for different values of ϵ, $n = 4$, $X_{-1} = 5^{-10}I$, and $X_0 = 2I$.

no pure imaginary eigenvalues, and B is a block matrix defined as

$$\begin{bmatrix} 0 & A \\ I & 0 \end{bmatrix}, \tag{39}$$

then

$$sign(B) = \begin{bmatrix} 0 & A^{1/2} \\ A^{-1/2} & 0 \end{bmatrix}. \tag{40}$$

For a proof of this last property, see [91], and for additional properties of the matrix sign function, see [92, 108]. The previous list of properties indicates that $S = sign(A)$ is the square root of the identity matrix that commutes with A. Hence, each method studied on the previous section to find the square root of a given matrix A can be used to find $S = sign(A)$. For example, to apply Newton's method it suffices to start from $X_0 = A$, that obviously commutes with A, and apply one of the simplified Newton's methods (20 - 21) to $F(X) = X^2 - I$, that yields:

$$X_{k+1} = \frac{1}{2}[X_k + X_k^{-1}]. \tag{41}$$

Iteration (41) from $X_0 = A$ was originally proposed by Roberts [148]; and it is stable and q-quadratically convergent to $sign(A)$. It is referred quite frequently as Roberts method. Once again, to avoid the inverse matrix required per iteration, this scheme can be combined with Schulz method, to produce the so-called Newton-Schulz method:

$$X_{k+1} = \frac{1}{2}X_k[3I - X_k^2], \tag{42}$$

from $X_0 = A$. Iteration (42) converges q-quadratically to $S^{-1} = S$, if $\|I - A^2\| < 1$. Iteration (42) is equivalent to the direct application of Newton's method to $F(X) =$

$X^{-2} - I$ [129]. As we mentioned before, iteration (41) is q-quadratically convergent, however its initial convergence behavior can be slow [88, 107]. To reduce the number of initial iterations of (41), Higham [88] introduces a scaling in (41) replacing X_k by $\mu_k X_k$ with $\mu_k \in \mathbb{R}^+$. Several ways to choose the parameter μ_k has been proposed, see e.g., [7, 28, 88]. Finally, it is worth mentioning that Kenney and Laub [106] present a family of iterations to compute the sign of a matrix based on Padé approximation techniques [23].

Once again, we can use the fact that $S = sign(A)$ is one of the square roots of the identity matrix to propose a secant method (27) for computing a root of $F(X) = X^2 - I$. Note that, all iterates X_k commute with the identity matrix I, so it is possible to use iteration (28) instead of (27). Finally, the secant iteration to compute the sign of A can be written as

$$X_{k+1} = (X_k + X_{k-1})^{-1}(X_{k-1}X_k + I). \tag{43}$$

with $X_{-1} = \alpha A$, $X_0 = \beta A$ and $\alpha, \beta > 0$. For these initial guesses and using similar arguments as in the proof of Theorem 3.1, it is possible to guarantee q-superlinear convergence of (43) to the sign of A. Moreover, (43) is a stable iteration because all the eigenvalues of I are equal to one, and therefore they satisfy the condition (22).

In the following experiment we compare the performance of the Newton iteration (41) with the secant iteration (43) to compute the sign of the symmetric matrix 'orthog' from the Matlab gallery. For this experiment we fix $n = 150$ and the internal parameter $\theta = 2$. In our implementation we stop the algorithms when $\|F(X_k)\|_F \leq 0.5D - 14$ or when 30 iterations are reached.

Table 4: Performance of secant and Newton methods for finding the sign of $A = $ gallery('orthog',n,2) when $n = 150$, $X_{-1} = 0.5 * A$, $X_0 = 0.5 * A$ and $Y_0 = A$.

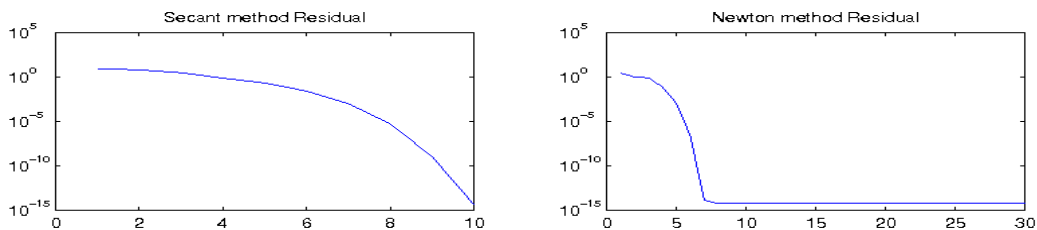| Method	Iter	$\|F(X_k)\|_F$
Secant method	9	4.16e-15
Newton-method	30	2.76e-14

Figure 2: Semilog of the residual associated with Table 4.

3.4 p-th root

We now consider $F(X) = X^p - A$, where $p \in \mathbb{N}$ and $p \geq 2$, to find a p-th root of A. As for $p = 2$, there is a special interest in the principal p-th root of A that will be denoted by $X_* = A^{1/p}$. If A has no real eigenvalue in $\mathbb{R}^-$, then $A^{1/p}$ is the unique matrix that satisfies:

1. $F(A^{1/p})=0$.

2. Let $\beta_1, \beta_2, \cdots, \beta_n$ be the eigenvalues of $A^{1/p}$ and $Z = \{z : -\pi/p < arg(z) < \pi/p\}$. Then for $A^{1/p}$ it holds that $\beta_i \in Z$ for all i, where z is a complex number, $z = a + ib$, and $arg(z) = \arctan(b/a)$.

Several recent ideas have been proposed to compute $A^{1/p}$, see e.g., [16, 47, 96, 100, 155, 156, 159]. We now describe the most relevant schemes related to Newton's method. The general form of this method for computing a p-th root of A is $X_{k+1} = X_k + S_k$ where S_k solves

$$\sum_{i=0}^{p-1} X_k^{p-1-i} S_k X_k^i = A - X_k^p. \tag{44}$$

Equation (44) represents the step 3 of Algorithms 1, and it was obtained using the Taylor expansion of $F(X) = X^p - A$. This equation is a generalized Sylvester equation in the matrix variable S_k. To avoid the significant computational cost of solving (44) per iteration, several simplified versions of Newton's method have been considered for solving the matrix p-root problem. The standard simplified Newton iteration can be obtained assuming that A commutes with X_0, which in turn implies that $AX_k = X_k A$ and $S_k X_k = X_k S_k$ for all k. Under this assumption Newton's method can be written as

$$X_{k+1} = \frac{1}{p}[(p-1)X_k + X_k^{(1-p)} A].$$

This simplified iteration converges to the unique positive definite root of A when A is SPD [96, 100], but in the general case convergence to $A^{1/p}$ cannot be guaranteed [159]. Unfortunately, in general it is numerically unstable [159]. There are some other simplified iterations based on the commutativity of A with X_0 that are numerically stable, see e.g. [47].

Bini et al. [16] present a Newton-type method to compute $A^{-1/p}$ instead of $A^{1/p}$, which is also q-quadratically convergent and numerically stable. This specialized method requires a trustable scheme for computing $A^{1/2}$, and so it can be applied only for $p > 2$. Similarly, Iannazzo [100] presents two different Newton-type iterations to compute $A^{1/p}$, and once again they are q-quadratically convergent and numerically stable, but they also require a trustable scheme for computing $A^{1/2}$.

3.5 Riccati equations

Let us now consider

$$F(X) = XA + A^T X - XBB^T X + C^T C, \tag{45}$$

with $A \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times r}, C \in \mathbb{R}^{q \times n}$, and $r, q \ll n$. The equation $F(X) = 0$ is known as Continuous-time Algebraic Riccati Equation (CARE) and plays an important role in control theory problems [43] and dynamical systems [3], among others.

Several applications require a symmetric positive semidefinite stabilizing solution of (45). The solution X_* is stabilizing if the matrix $A - BB^T X_*$ is stable, i.e, if its eigenvalues lie in the open left half plane, see e.g., [43, 112] for details. Since the $n \times n$ solution X_* is symmetric, it is customary to represent it in a factored form $X_* = YY^T$. There is an extensive literature concerning numerical methods for the solution of CARE; e.g., [43, 112] and references therein. However it is a common approach to use Newton's method to find a solution of (45), e.g., [12, 13, 80, 109, 136, 151]. As usual, the general Newton's iteration is given by $X_{k+1} = X_k - F'(X_k)^{-1} F(X_k)$, that after the standard Taylor expansion can be written as

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Algorithm 6 Newton's method for CARE

1: Given $X_0 \in \mathbb{R}^{n \times n}$ such that $X_0 = X_0^T$ and $A - BB^T X_0$ is stable.
2: **for** $k = 0, 1, \cdots$ until convergence **do**
3:     **Set** $\mathcal{A}_k = A - BB^T X_k$
4:     **Solve** $\mathcal{A}_k^T X_{k+1} + X_{k+1} \mathcal{A}_k = -C^T QC - X_k BB^T X_k$ $\triangleright$ for X_{k+1}
5: **end for**

Algorithm 6 has been known in the literature as the Kleinman iteration for CARE [109]. Notice that the Lyapunov equation (step 4) must be solved at every iteration. Recently for large scale problems the Kleinman iteration is combined with Alternating Direction Implicit (ADI) iterations for solving the Lyapunov equations [13, 66]. For another approach suitable for small and medium size problems which is based on the sign function, see Byers [28].

A quasi-Newton scheme has also been developed for solving CARE, that obtains a reduction in the computational cost of the linear algebra involved [136].

3.6 Rational equations

We consider the following rational matrix equation

$$X \pm A^* X^{-p} A = Q, \tag{46}$$

where A is a nonsingular $n \times n$ matrix, Q is an $n \times n$ Hermitian positive definite matrix, p is a positive integer and A^* represents the conjugate transpose of A. Equation (46) requires maximal (minimal) Hermitian positive definite solutions. A maximal solution of (46) denoted by X_+ satisfies that $X_+ > X$ for any Hermitian solution X, where $A > B$ ($A \geq B$) means that $A - B$ is a positive definite (semidefinite) matrix, which is the well-known Löwner ordering for Hermitian matrices. A minimal solution X_- can be defined similarly. For additional comments concerning the existence of solutions for (46) see [62, 63, 174]. Rational equations appear in the analysis of stationary Gaussian reciprocal processes over a finite interval [67], in the field of optimal control theory [62], and it is related to an algebraic Riccati equation of the type arising in Kalman filter theory [114].

When $p = 1$ a Newton's method has been already developed, and after a standard Taylor expansion and simple manipulations it can be written as

$$X_{k+1} \pm L_k^* X_{k+1} L_k = Q \pm 2L_k^* A, \qquad (47)$$

where $L_k = X_k^{-1} A$. Notice that at every iteration of (47) the inverse of a matrix needs to be computed, and a discrete Sylvester equation (also known as Stein equation) needs to be solved for X_{k+1}. From suitable initial guesses and mild assumptions the q-quadratic convergence of (47) has been established [81].

To avoid the inverse per iteration in (47), when $p = 1$, $Q = I$ and using the plus sign, a simplified variant based on the Newton-Schulz scheme (17) has been recently proposed and analyzed [130]. This simplified iteration is given by

$$X_{k+1} = 2X_k - X_k A^{-*}(I - X_k)A^{-1}X_k. \qquad (48)$$

The method indicated by (48) is clearly inexpensive. Notice that it only requires to compute A^{-1} at the beginning of the process. From $X_0 = AA^*$, iteration (48) converges q-linearly to the minimal solution of (46) [130]. For different values of p, there are some other iterative schemes that posses q-linear convergence to extremal solutions of (46) which are not based on Newton's method but instead they are based on fixed points iterations [60, 61, 81, 102, 144, 174].

4   Conclusions

Newton's method has been omnipresent in the development of applied mathematics and scientific computing; and whenever a Newton's method is applicable to a general nonlinear problem a suitable secant method can also be obtained for the same problem. In this work we present a condensed review of this longstanding relationship in different and sometimes unexpected scenarios. In our presentation, we also emphasize that Newton's method has been rediscovered several times through history for solving specialized vector and matrix problems.

In the space of matrices we discuss and further analyze a recent interpretation of the classical secant method. In the special case of computing the inverse, the square root, and the sign of a given matrix, we fully analyze the specialized versions that emerge from this interpretation of the secant method, and compare their practical performance with the best available specialized Newton's method. Our preliminary numerical experiments show the expected q-superlinear convergence and indicate that, for solving nonlinear matrix problems, these secant schemes have interesting properties that remain to be fully understood.

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