Portugal. Math. (N.S.)
Vol. 68, Fasc. 4, 2011, 431–475
DOI 10.4171/PM/1901

Portugaliae Mathematica

Newton's method and secant methods: A longstanding relationship from vectors to matrices

Marlliny Monsalve and Marcos Raydan*

(Communicated by Luis Nunes Vicente)

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 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 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.

Mathematics Subject Classification (2010). Primary 34G20, 49M15, 90C53; Secondary 15A24.

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

*Partially supported by the Scientific Computing Center at UCV.

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 method has been proposed to solve specific problems, secant methods have also 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, and in practice this difference in speed of convergence is 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 the secant method. 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.

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 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** $k = 0, 1, \ldots$ **do**
3: Solve $F'(X_k)S_k = -F(X_k)$
4: $X_{k+1} = X_k + S_k$
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.

On the other hand, a suitable secant method can also be obtained for solving nonlinear problems. For example, in the well-known scalar case, $f : \mathbb{C} \to \mathbb{C}$, the secant method can be written as follows:

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

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 [143], a full investigation is included on the historical development of the secant method.

For different scenarios, from vector problems to matrix problems, we will discuss in this review specialized Newton 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 [57].

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 $J \in \mathrm{Lip}_\gamma\big(N(x_*, r)\big)$. Then there exists $\varepsilon > 0$ such that for all $x_0 \in N(x_*, \varepsilon)$ 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*

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

Here, we introduce the notation $J \in \mathrm{Lip}_{\gamma}\big(N(x_*, r)\big)$ 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 nonsingular, 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 books by Bertsekas [16], Conn et al. [42], Fletcher [70], and Nocedal and Wright [139]. 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 [5]. A historical review about the convergence analysis of Newton's method can be found in [140].

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 [25]. 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}

$$\hat{\boldsymbol{M}}_k(x) = F(x_k) + A_k(x - x_k). \tag{4}$$

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 $F(x_{k-1}) = \hat{\boldsymbol{M}}_k(x_{k-1})$. 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 $\hat{\boldsymbol{M}}_k(x_k) = F(x_k)$ and the next iterate, x_{k+1}, is the one that satisfies $\hat{\boldsymbol{M}}_k(x_{k+1}) = 0$. 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 [28], and later analyzed by Dennis [53]. 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 [57], [70]. 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., [29], [57], [128], [139], [179].

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** $k = 0, 1, \ldots$ **do**
3: Solve $A_k s_k = -F(x_k)$ ▷ 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 [57].

Theorem 2.2. *Under the same hypothesis of Theorem* 2.1*, there exist positive constants* ε *and* δ *such that if* $\|x_0 - x_*\|_2 \leq \varepsilon$ *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 [57]. 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 [55], [56], [57]. 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., [66], [80], [115], [166], [171], [176]. 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 convergence rate faster than q-superlinear; see for example [67], [88]. In the scalar case, the relationship between the convergence rate of Newton's method and that of the secant method has been characterized [152].

As in the case of Newton's method, the secant-type methods have also been extended and analyzed for solving nonlinear problems in Hilbert spaces; see e.g. [77], [156]. Newton's method has been extended for solving nonsmooth systems of nonlinear equations [38], [98], [129], [155], and has been combined with interior point methods [78]. Similarly, the secant-type methods have also been extended for nonsmooth problems [37], [121], [130], [145], and have been combined with inexact schemes and nonstandard globalization strategies [20], [73].

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 approximates 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 [32], 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 [123]. See [36] 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 [144], who developed such a combined scheme for solving two point boundary value problems, and was later generalized and formalized by Dembo et al. [51]. The inexact Newton method has been associated with globalization strategies [59], nonsmooth problems [129], and Krylov subspace methods [11], [27].

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 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 [57], [139], and solving optimization subproblems as in the trust region approach [42]. 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 [47] 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 [71]. These very successful methods, also called 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 [56], [57]. The most successful ones are the DFP, the BFGS, and the SR1 methods. All these methods belong to the family described by (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. [57], [139]. As in the Newton method, it is always possible to guarantee that d_k is a descent direction, and as before, the direction can be obtained inexactly [72]. The secant methods for unconstrained optimization have also been extended for nonsmooth problems [37], [121], [130].

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,

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

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 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 [22]. 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 [16], [70], [139] for details.

As it usually happens, the earliest reference of an SQP algorithm was concerned with the extension of Newton's method [177], and later SQP-type methods were developed to extend the secant method. The first secant-SQP method was introduced by García-Palomares and Mangasarian [75]. Further extensions and convergence analysis (local and global) for SQP-Newton's method can be found for example in [43], [61], [148], and for SQP-secant methods in [24], [31], [58], [72], [87], [147], [170]. 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 [79], [164], [168], and a diagonalized multiplier version of the SQP-secant method was discussed in [169]. See also Tapia [170] for optional extensions of the secant method for solving (9), El-Bakry et al. [61] for the application of a Newton interior-point methods for nonlinear programming problems, and Boggs et al. [23] for a special treatment of the large-scale case. A quasi-Newton interior-point method for nonlinear programming has also been analyzed in [127], and the connection of the trust-region globalization strategy with SQP-type methods has received special attention; see e.g. [33], [54], [60].

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 problems 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 [3], and an inexact Newton version is introduced in [144]. Later on, as it usually happens, quasi-Newton methods were introduced for solving TPBVP; see e.g. [86]. For a general discussion on the numerical solution of TPBVP; see [6]. Some other classical differential equation problems have also been attacked by Newton-type methods which are not related to discretization schemes; see e.g. [167].

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 [120], and after been extended in several ways, it was recently analyzed by Gander and Vandewalle [74]. In [74], the authors observed the connection of the parareal method with multiple shooting, as analyzed by Chartier and Phillipe [34], for which q-quadratic convergence can be established since the multiple shooting method can be viewed as Newton's method. In [74], they also analyze a variant first proposed by Baffico et al. [7] 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 [87], [109], [174]. Moreover, SQP-type extensions have been proposed where the control variables receive a special treatment [58], [116].

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 [93], [161].

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 [146] 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:

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

where the normalization $\|x\|_2 = 1$ is included. Then Newton's method or the so-called projected Newton 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 method. If the normalization is not included, then local q-quadratic convergence is immediately obtained. Surprisingly, it is

established in Tapia and Whitley [171] 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 [171] 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 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 [10]. See [166] 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], [124].

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 $\phi := \{\phi_1, \ldots, \phi_n\}$. The first effective algorithm, based on the alternating theorem, was proposed by Remez in 1934 [153]. 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 [40], [138]; see also [173]. For additional details on this topic see [39], and also [149].

3. Matrix problems

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

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

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 matrix 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 [35], [36]. 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. [21], [90], [94], [103], [132], whereas the general case, $p > 2$, has been recently considered, see e.g. [17], [49], [50], [81], [104], [105], [162]. Computing the square root ($p = 2$) of a given matrix is useful for solving some boundary value problems [158] and also appears in the modelling of flow problems [126]; and the general case ($p > 2$) appears associated with Markov processes [82] among other applications. For a complete discussion on matrix p-th roots see [95].
- *Matrix sign function*. The sign of a matrix extends naturally the concept of the sign of a complex number [113]. Given a matrix A with no pure imaginary eigenvalues, the sign of A is given by

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

where $A^{1/2}$ is the principal square root of A, that will be fully described later. See [95] 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 [101]. A practical property states that the sign of a matrix A is a square root of the identity that commutes with A [111]. This property motivates to consider $F(X) = X^2 - I$, 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 [117]. Riccati equations arise naturally in control problems [4], [12], [15], [45], [2], [131], [154].
- *Quadratic equations.* Given the matrices A, B, and C, the quadratic matrix equation $AX^2 + BX + C = 0$ arises in control theory [45], [48], [97] and also in the solution of Markov processes [118], [18]. 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 [62], [63], [64], [84], [107], [136], [151], [178].
- *Matrix logarithm and matrix exponential.* For computing the logarithm of a given matrix A [41], [110], 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 [96], [133], 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 difficult linear matrix problems is the so-called Sylvester equation [165], that appears, e.g., in the solution of control theory problems [45]:

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

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 [125]. 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 [165]. For a full description of the theoretical properties of Sylvester equations see [45], [99]. 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. [9], [46], [76], [102], [108], [134] and the references therein.

As we mentioned before, whenever a Newton method is proposed, it is possible to define a secant scheme. Recently some authors have developed secant methods for nonlinear matrix problems that inherit, 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 as the step S_k and the map-difference Y_k. Therefore, 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 [135], [137]:

Algorithm 3 General secant method for matrix problems

Given $X_{-1} \in \mathbb{C}^{n\times n}$, $X_0 \in \mathbb{C}^{n\times n}$
Set $S_{-1} = X_0 - X_{-1}$
Set $Y_{-1} = F(X_0) - F(X_{-1})$
Solve $A_0 S_{-1} = Y_{-1}$ ▷ for A_0
for $k = 0, 1, \ldots$ until convergence **do**
    Solve $A_k S_k = -F(X_k)$ ▷ for S_k
    Set $X_{k+1} = X_k + S_k$
    Set $Y_k = F(X_{k+1}) - F(X_k)$
    Solve $A_{k+1} S_k = Y_k$ ▷ for A_{k+1}
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

Given $X_{-1} \in \mathbb{C}^{n\times n}$, $X_0 \in \mathbb{C}^{n\times n}$
Set $S_{-1} = X_0 - X_{-1}$
Set $Y_{-1} = F(X_0) - F(X_{-1})$
Solve $B_0 Y_{-1} = S_{-1}$ ▷ for B_0
for $k = 0, 1, \ldots$ until convergence **do**
    Set $S_k = -B_k F(X_k)$
    Set $X_{k+1} = X_k + S_k$
    Set $Y_k = F(X_{k+1}) - F(X_k)$
    Solve $B_{k+1} Y_k = S_k$ ▷ for B_{k+1}
end for

Solving a secant equation 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. [77], [156]), 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 $F'(X) \in \mathrm{Lip}_\gamma\big(N(X_*, r)\big)$, 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. In contrast to the standard convergence theory for Newton's method and secant methods when solving nonlinear vector problems, for matrix problems it is not enough to choose the initial matrices sufficiently close to the solution to ensure convergence; see e.g. [95], [137]. The convergence properties of most methods discussed in the next subsections will depend on a specialized choice of the initial matrices.

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 non-singular matrix and C is any other matrix such that $B + C$ is invertible then

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

Consequently, forcing Step 3 in Algorithm 1 yields

$$-X_k^{-1}H_kX_k^{-1} = -(X_k^{-1} - A)$$
$$H_k = X_k - X_kAX_k,$$

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 the Schulz method [159] which was first introduced 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 [89], it is a numerical stable scheme [163], 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) [89], [95], [141], [163].

A secant method has also been defined to find the root of (16) [137]. For that, let us consider the general secant method applied to (16)

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

that after several algebraic manipulations can be reduced to

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

which avoids the inverse matrix calculations per iteration associated with iteration (18). Notice the resemblance between (19) and the Schulz method for solving the same problem. The method described in (19), denoted as the secant-Schulz method, can be written as a fixed point iteration for a suitable map, and it has been established in [137] that the Fréchet derivative of this iteration map has bounded powers. Therefore, the secant-Schulz method generates a stable iteration. It has also been established that it converges locally and q-superlinearly to the inverse of A, from $X_{-1} = \alpha A^*/\|A\|_2^2$ and $X_0 = \beta A^*/\|A\|_2^2$, with $\alpha, \beta \in (0, 1]$. Moreover, when A has no inverse, it converges locally and q-superlinearly to $A\dagger$; see

[137] for details. It is also important to note that the q-superlinear convergence implies the well-known Dennis-Moré condition [55], [57]

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

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 behavior of the secant-Schulz and the Newton–Schulz iterative methods for computing the inverse of the symmetric and positive definite matrices `poisson` and `gcdmat` from the Matlab gallery with $n = 400$. In both cases, since the matrices A to be considered are symmetric and PD, we have chosen $X_{-1} = \alpha I$ with $0 < \alpha \leq 1/\|A\|_2$ and $X_0 = A^*/\|A\|_2^2$ for the secant-Schulz, and the same X_0 for the Newton–Schulz to guarantee the convergence for both methods [135], [137]. Using a fixed value of α we report the number of required iterations (Iter), the relative residual $\left(\|F(X_k)\|_F/\|A\|_F\right)$ and the relative error $(\|X_k - X_*\|_F/\|X_*\|_F)$ at convergence. We also show average results for the secant-Schulz method using 100 different random values of α in the interval $(0, 1/\|A\|_2]$. For this experiment and for all upcoming experiments, we stop the process when

$$\|F(X_k)\|_F/\|A\|_F \leq 0.5 \times 10^{-12}. \tag{20}$$

The results are reported in Table 1, and the semilog of the relative residual and the relative error using $\alpha = 1/\|A\|_2$ are showed in Figure 1. Concerning the average results, using the matrix `poisson`, we also noted that in 51 cases the secant-Schulz method required more iterations than the Newton–Schulz method, and both methods required the same number of iterations for all the other cases. A

Table 1. Performance of the secant-Schulz and the Newton–Schulz methods for finding the inverse of $A =$ `gallery('poisson',20)` and $A =$ `gallery('gcdmat',n)` when $n = 400$, $X_{-1} = \alpha I$, $X_0 = A^*/\|A\|_2^2$ and $\alpha = 1/\|A\|_2$. Average results for secant-Schulz with $X_{-1} = \alpha I$, for 100 different random values of α.

Method	`poisson`			`gcdmat`		
	Iter	$\frac{\|F(X_k)\|_F}{\|A\|_F}$	$\frac{\|X_k - X_*\|_F}{\|X_*\|_F}$	Iter	$\frac{\|F(X_k)\|_F}{\|A\|_F}$	$\frac{\|X_k - X_*\|_F}{\|X_*\|_F}$
Newton–Schulz	21	5.28e-16	4.58e-15	35	5.71e-17	2.03e-13
Secant-Schulz	21	6.11e-16	1.60e-15	30	1.05e-13	5.65e-10
Average results for Secant-Schulz using 100 different values of α						
Secant-Schulz	22.48	4.81e-14	3.22e-12	32.56	6.39e-14	3.42e-10

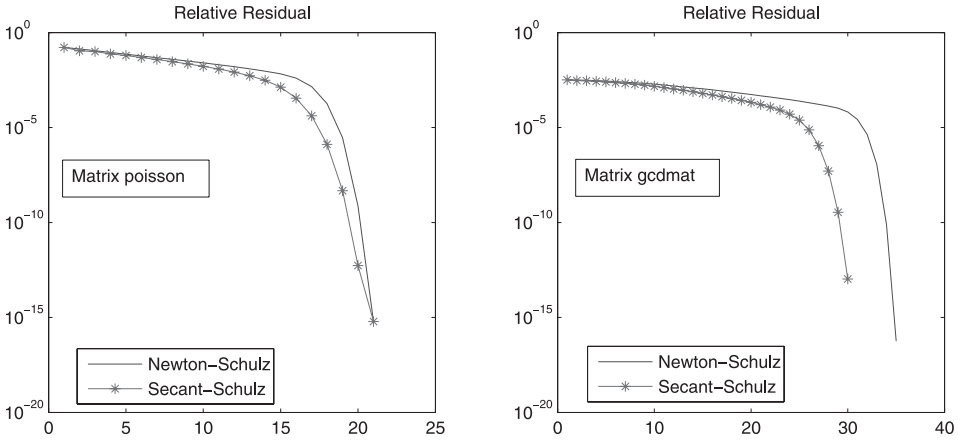

Figure 1. Semilog of the relative residual for matrices `poisson` (left) and `gdcmat` (right) associated with Table 1 and $\alpha = 1/\|A\|_2$.

similar behavior has been observed frequently. Nevertheless, for the matrix `gcdmat` we observed that for 8 cases the Newton–Schulz method required less iterations than the secant-Schulz method, for 7 cases both methods required the same number of iterations, and in 85 cases the secant-Schulz method required less iterations than the Newton–Schulz method.

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 [92], [99]. 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

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

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ 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 $\Lambda^{1/2} = \operatorname{diag}(\sqrt{\lambda_1}, \sqrt{\lambda_2}, \ldots, \sqrt{\lambda_2})$ and so $A^{1/2} = W\Lambda^{1/2}W^{-1}$. For details see [95]. The special interest in $A^{1/2}$ is based on the role it plays for several applica-

tions, e.g., Markov processes [82], [106], [175], modelling of flow problems [126], and applications related to the logarithm of a matrix [41], [110].

Newton's method and specialized versions of it, for computing the principal square root of a matrix, has received significant attention for many years [82], [90], [94], [103], [132], [160]. 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** $k = 0, 1, \ldots$ **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**

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, and 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 $m > 0$; see [90].

In order to avoid the solution of a Sylvester equation per iteration, several variants of Newton's method have emerged. In [90], [94], [95] 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 $AX_k = X_k A$ and $X_k S_k = S_k X_k$ for all $k \geq 0$ [90]. 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 $S_k = \frac{1}{2}[AX_k^{-1} - X_k]$, and two simplified variants of Newton's method are obtained:

$$\text{(I)} : Y_{k+1} = \frac{1}{2}[Y_k + Y_k^{-1}A] \tag{21}$$

$$\text{(II)} : Z_{k+1} = \frac{1}{2}[Z_k + AZ_k^{-1}]. \tag{22}$$

In Higham [90], it is established that if A is diagonalizable and no real eigenvalue of A is in $\mathbb{R}^-$, then the sequence of matrices generated by (21), or (22), 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 conditions hold

$$\frac{1}{2}|1-(\lambda_j/\lambda_i)^{1/2}| \leq 1 \qquad \text{for } 1 \leq i,j \leq n, \tag{23}$$

where the λ_i's are the eigenvalues of A. If A is symmetric and positive definite (SPD), (23) is equivalent to $\kappa_2(A) \leq 9$ [90]. Due to these restrictive conditions the schemes given by (21) and (22) are of little 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 [94]. We now present some of the most relevant Newton-type stable options:

- Denman and Beavers [52] propose a specialized iteration for Riccati equations, that reduced to the square root problem produces the following coupled scheme:

$$Y_{k+1} = \frac{1}{2}[Y_k + Z_k^{-1}] \qquad Z_{k+1} = \frac{1}{2}[Z_k + Y_k^{-1}], \tag{24}$$

  from $Y_0 = A$ and $Z_0 = I$. Iteration (24) 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 [94]. 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 [94] analyzes the following coupled variant that combines the Denman-Beaver scheme with the Schulz method for the matrix inverse problem

$$P_{k+1} = \frac{1}{2}P_k[3I - Q_kP_k], \qquad Q_{k+1} = \frac{1}{2}Q_k[3I - P_kQ_k], \tag{25}$$

  from $P_0 = A$ and $Q_0 = I$. The coupled iteration (25) 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 $\|\text{diag}(A-I, A-I)\| < 1$ holds for any consistent matrix norm; see [94], [111] for details.

- Meini [132] 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

$$Y_{k+1} = -Y_kZ_k^{-1}Y_k, \qquad Z_{k+1} = Z_k + 2Y_{k+1}, \tag{26}$$

from $Y_0 = I - A$ and $Z_0 = 2(I + A)$. The coupled iteration (26) is stable and has the property that Y_k converges to 0 while Z_k converges q-quadratically to $4A^{1/2}$.

- Iannazzo [103] presents and analyzes the following iteration that requires one matrix inverse per iteration

$$X_{k+1} = X_k + H_k, \qquad H_{k+1} = -\frac{1}{2} H_k X_{k+1}^{-1} H_k, \tag{27}$$

from $X_0 = A$ and $H_0 = \frac{1}{2}(I - A)$. Iteration (27) 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

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

Now, we will establish the q-superlinear convergence of iteration (28). Let us assume that A is *diagonalizable*, that is, there exists a nonsingular matrix V such that

$$V^{-1} A V = \Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n), \tag{29}$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of A. If we define $D_k = V^{-1} X_k V$ then we have from (28) that

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

If we choose X_{-1} and X_0 such that $D_{-1} = V^{-1} X_{-1} V$ and $D_0 = V^{-1} X_0 V$ are diagonal matrices, then all successive D_k are also diagonal, 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 $k \geq 0$, 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 generated by* (28) *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, $\mathrm{Re}(\sqrt{\lambda_i})$, 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

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

and hence, from (35)

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

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 $1 \le i \le n$, such that $\tilde{c}_k^i > 0$ for all k, $\lim_{k\to\infty} \tilde{c}_k^i = 0$, and

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

Using (37) we now obtain in the Frobenius norm

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

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

$$\begin{aligned} \|X_{k+1} - A^{1/2}\|_F &= \|VV^{-1}(X_{k+1} - A^{1/2})VV^{-1}\|_F \le \kappa_F(V)\|D_{k+1} - \Lambda^{1/2}\|_F \\ &\le \kappa_F(V)\sqrt{n}\hat{c}_k \|D_k - \Lambda^{1/2}\|_F \le \kappa_F(V)^2 \sqrt{n}\hat{c}_k \|X_k - A^{1/2}\|_F, \end{aligned}$$

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

Remark 3.2. 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 $A^{1/2}$.

Remark 3.3. The matrix V that appears in the diagonalization of A, equation (29), is not available. Fortunately, it is only required for theoretical purposes. In practice, when using algorithm (28) the matrix V is not required.

It is worth pointing out that if X_k commutes with A in (28), we obtain a simplified version of Algorithm 3 given by

$$\begin{aligned} X_{k+1} &= X_k - (X_k - X_{k-1})(X_k - X_{k-1})^{-1}(X_k + X_{k-1})^{-1}(X_k^2 - A) \\ &= (X_k + X_{k-1})^{-1}\big((X_k + X_{k-1})X_k - (X_k^2 - A)\big) \\ &= (X_k + X_{k-1})^{-1}(X_{k-1}X_k + A). \end{aligned} \tag{39}$$

Notice the resemblance between (39) and (21). Both iterations are very attractive from a computational point of view, but using similar arguments to the ones

used by Higham in [90], our next result shows that (39) is an unstable iteration unless the eigenvalues of A satisfy a restrictive condition.

Theorem 3.4. *Let $A \in \mathbb{C}^{n\times n}$ be diagonalizable as in* (29). *Let us assume that A has no nonpositive real eigenvalues, all iterates X_k generated by* (39) *are well defined, and $X_k A = A X_k$ for all $k \geq 0$. If*

$$\frac{1}{2}|1 - (\lambda_j/\lambda_i)^{1/2}| \leq 1 \qquad \text{for } 1 \leq i, j \leq n, \tag{40}$$

then (39) *is a stable iteration.*

Proof. Let $\hat{X}_k \approx X_k$ such that $\hat{X}_k = X_k + \Delta_k$ for some Δ_k error matrix. Our goal is to prove that Δ_{k+1} is uniformly bounded when condition (40) holds. Using similar arguments to the ones used by Higham in section 3 of [90] we have that

$$\Delta_{k+1} = (X_k + X_{k-1})^{-1}[X_{k-1}\Delta_k + \Delta_{k-1}X_k - (\Delta_k + \Delta_{k-1})X_{k+1}] + O(\|\Delta\|^2),$$

where $\Delta = \max\{\Delta_k, \Delta_{k-1}\}$. Using the notation given by (29), it follows that $D_k = V^{-1}X_k V$. Let $\tilde{\Delta}_k = V^{-1}\Delta_k V$. Hence, each element $\tilde{\delta}_{ij}^{(k+1)}$ of $\tilde{\Delta}_{k+1}$ can be written as

$$\tilde{\delta}_{ij}^{(k+1)} = \frac{\tilde{\delta}_{ij}^{(k)} d_{k-1}^i + \tilde{\delta}_{ij}^{(k-1)} d_k^j - (\tilde{\delta}_{ij}^{(k)} + \tilde{\delta}_{ij}^{(k-1)}) d_{k+1}^j}{d_k^i + d_{k-1}^i} + O(\|\Delta\|^2), \tag{41}$$

where $1 \leq i, j \leq n$ and $d_k^i = (D_k)_{ii}$. Since d_k^i converges to λ_i, we have that (41) can also be written as

$$\begin{aligned}\tilde{\delta}_{ij}^{(k+1)} &= \frac{1}{2\lambda_i^{1/2}}[\tilde{\delta}_{ij}^{(k)}\lambda_i^{1/2} + \tilde{\delta}_{ij}^{(k-1)}\lambda_j^{1/2} - (\tilde{\delta}_{ij}^{(k)} + \tilde{\delta}_{ij}^{(k-1)})\lambda_j^{1/2}] + O(\|\Delta\|^2) \\ &= \frac{1}{2}[1 - (\lambda_j/\lambda_i)^{1/2}]\tilde{\delta}_{ij}^{(k)} + O(\|\Delta\|^2). \end{aligned} \tag{42}$$

Note that, if $\frac{1}{2}|1 - (\lambda_j/\lambda_i)^{1/2}| \leq 1$ then $\tilde{\delta}_{ij}^{(k+1)}$ remains bounded, and the result is established. □

We now present some numerical experiments to illustrate the behavior of the specialized secant method (Algorithm 3), the Denman and Beavers (DB) iteration (24), and Meini's iteration (26). We stop all considered algorithms when (20) holds. First, we consider the matrix `dorr` from the Matlab gallery with $n = 10$ and $\theta = 10^{-7}$. These values were chosen as in [132]. This matrix is row diagonal

Table 2. Performance of the secant method and Newton methods for finding the square root of $A = \texttt{gallery('dorr',n,}\theta\texttt{)}$ when $n = 10$, $\theta = 10^{-7}$, and α and β are random positive values generated with `rand('state',1)`.

Method	Iter	$\|F(X_k)\|_F/\|A\|_F$	$\|X_k - X_*\|_F/\|X_*\|_F$
DB	**	**	**
Meini	20	1.58e-13	3.62e-07
Secant	8	2.3e-14	5.66e-09

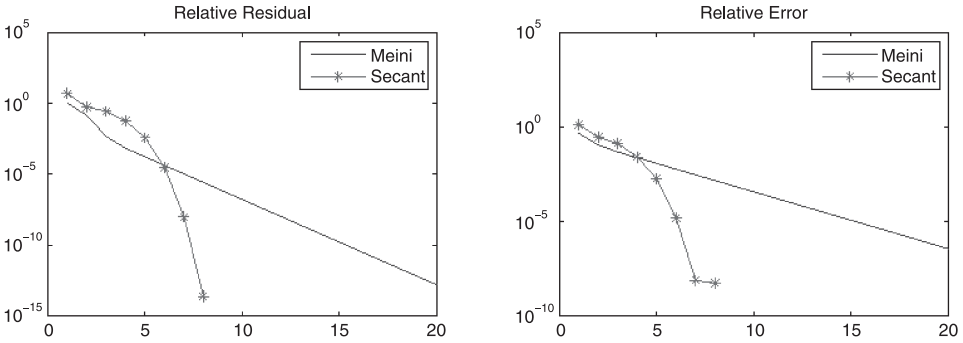

Figure 2. Semilog of the relative residual (left) and the relative error (right) associated with Table 2.

dominant, tridiagonal, ill-conditioned for small value of the input argument θ, and all its eigenvalues are nonnegative. The initial matrices which guarantee convergence for the used methods are $X_{-1} = \alpha I$ and $X_0 = \beta A$ for secant method (according to Theorem 3.1) where $\alpha > 0$ and $\beta > 0$. For the DB iteration we use $Y_0 = A$ and $Z_0 = I$, and for Meini's iteration $Y_0 = I - A$ and $Z_0 = 2(I + A)$ are used; see [52], [132] for details. The symbol (**) means that the algorithm does not converge. The results are reported in Table 2. We can observe that DB does not achieve convergence (to be precise, the norm of the residual diverges to infinity). Meini's iteration converges, but it requires more than twice as many iteration as the secant method, see Figure 2.

We now consider a problem described in [132]. For this example, A is the following Frobenius matrix

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

Table 3. Performance of the secant method and Newton methods for finding the square root of a Frobenius matrix with $p(x) = (x-2)(x-5)\left((x+1)^2+\varepsilon\right)$ for different values of ε, and for $n = 4$.

ε	Method	Iter	$\|F(X_k)\|_F/\|A\|_F$	$\|X_k - X_*\|_F/\|X_*\|_F$
10^{-2}	DB	11	1.32e-14	6.47e-15
	Meini	10	4.99e-13	7.78e-14
	Secant	29	1.25e-12	2.94e-11
10^{-4}	DB	14	3.4e-13	1.03e-12
	Meini	12	4.46e-07	3.96e-09
	Secant	50	3.38e-11	9.94e-10
10^{-6}	DB	71	4.55e-11	1.74e-10
	Meini	13	0.74108	0.0338
	Secant	30	1.51e-07	6.74e-08
10^{-8}	DB	55	1.86e-09	2.93e-09
	Meini	1	0.902	0.999
	Secant	58	5.86e-04	3.55e-05

where p_i with $3 \le i \le 0$ are the coefficients of $p(x) = (x-2)(x-5)\left((x+1)^2+\varepsilon\right)$ which is the characteristic polynomial of A. In this case A has two complex conjugate eigenvalues $-1 \pm i\sqrt{\varepsilon}$. 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 [132], we report the iteration at which the minimal value of $\|F(X_k)\|_F/\|A\|_F$ is reached. We use the same initial matrices as in the previous experiment.

We can see in Table 3 that for all values of ε the DB iteration achieves the lowest relative residual norm. On the other hand, Meini's iteration for $\varepsilon = 10^{-6}$ and $\varepsilon = 10^{-8}$ has the worst performance and for these cases the secant method reduces considerably the relative 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 $S = \operatorname{sign}(A) = A(A^2)^{-1/2}$, 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 [95]: $S^2 = I$, i.e., $S^{-1} = S$; $AS = SA$; and if A is SPD then $S = I$. Moreover, if A is a square matrix with no pure imaginary eigenvalues, and B is a block matrix defined as

$$\begin{bmatrix} 0 & A \\ I & 0 \end{bmatrix}, \tag{43}$$

then

$$\operatorname{sign}(B) = \begin{bmatrix} 0 & A^{1/2} \\ A^{-1/2} & 0 \end{bmatrix}. \tag{44}$$

For a proof of this last property see [94], and for additional properties of the matrix sign function see [95], [113]. Each method studied on the previous section to find the square root of a given matrix A can be used to find $S = \operatorname{sign}(A)$. 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 methods (21–22) to $F(X) = X^2 - I$, that yields:

$$X_{k+1} = \frac{1}{2}[X_k + X_k^{-1}]. \tag{45}$$

Iteration (45) from $X_0 = A$ was originally proposed by Roberts [154]; and it is stable and q-quadratically convergent to $\operatorname{sign}(A)$. Once again, to avoid the inverse matrix required per iteration, this scheme can be combined with the Schulz method, to produce the so-called Newton–Schulz method

$$X_{k+1} = \frac{1}{2} X_k[3I - X_k^2] \tag{46}$$

from $X_0 = A$. Iteration (46) converges q-quadratically to $S^{-1} = S$, if $\|I - A^2\| < 1$ for any consistent matrix norm. Iteration (46) is equivalent to the direct application of Newton's method to $F(X) = X^{-2} - I$ [135]. As we mentioned before, iteration (45) is q-quadratically convergent, however its initial convergence behavior can be slow [91], [112]. To reduce the number of initial iterations, a scaling in (45) can be introduced 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., [8], [30], [91]. A commonly used scaling is given by

$$\mu_k = 1/|\det(X_k)|^{1/n}, \tag{47}$$

that can be computed inexpensively during the matrix inverse calculation in (45). Finally, it is worth mentioning that Kenney and Laub [111] present a family of iterations to compute the sign of a matrix based on Padé approximation techniques [26].

Once again, we can use the fact that $S = \operatorname{sign}(A)$ is one of the square roots of the identity matrix to propose a secant method (28) for computing a root of $F(X) = X^2 - I$. Note that, all iterates X_k commute with the identity matrix I,

Table 4. Performance of Newton, scaled Newton, and secant for finding the sign of $A = \texttt{gallery('orthog',n,2)}$ and $A = \texttt{gallery('fiedler',1:n)}$ when $n = 150$, $\alpha = 1.0$ and $\beta = 1.5$.

Method	ortho			fiedler		
	Iter	$\frac{\|F(X_k)\|_F}{\|A\|_F}$	$\frac{\|X_k - X_*\|_F}{\|X_*\|_F}$	Iter	$\frac{\|F(X_k)\|_F}{\|A\|_F}$	$\frac{\|X_k - X_*\|_F}{\|X_*\|_F}$
Newton	3	5.18e-15	5.12e-15	19	9.1e-18	1.68e-9
Newton (scaled)	3	5.18e-15	5.12e-15	16	1.5e-17	1.68e-9
Secant	3	6.42e-14	9.12e-15	17	2.59e-14	1.68e-9

so it is possible to use iteration (39) instead of (28). Finally, the secant iteration to compute the sign of A can be written as

$$X_{k+1} = (X_k + X_{k-1})^{-1}(X_{k-1}X_k + I), \tag{48}$$

from $X_{-1} = \alpha A$, $X_0 = \beta A$ where $\alpha, \beta > 0$. For these initial matrices and using similar arguments as in the proof of Theorem 3.1, it is possible to guarantee q-superlinear convergence of (48) to the sign of A. Moreover, (48) is a stable iteration because all the eigenvalues of I are equal to one, and therefore they satisfy the restrictive conditions (23).

In the following experiment we illustrate the performance of the Newton iteration (45), the scaled Newton iteration (45) and (47), and also the secant iteration (48) to compute the sign of the symmetric matrices `orthog` and `fiedler` from the Matlab gallery. As far as we know there is no scaled version of the secant method. For this experiment we fix $n = 150$, $\alpha = 1.0$, and $\beta = 1.5$. A similar behavior of the secant method is observed for any other positive values of α and β. Once again we stop the algorithms when (20) holds.

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 $\beta_1, \beta_2, \ldots, \beta_n$ 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 $\arg(z) = \arctan(b/a)$.

Different ideas have been recently proposed to compute $A^{1/p}$; see e.g. [17], [49], [100], [104], [172], [162]. We now describe the most relevant schemes which relate

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

$$\sum_{i=0}^{p-1} X_k^{p-1-i} S_k X_k^i = A - X_k^p. \tag{49}$$

Equation (49) represents the step 3 of Algorithm 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 (49) per iteration, several simplified versions of Newton's method have been considered. 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 [100], [104], but in the general case convergence to $A^{1/p}$ cannot be guaranteed [162]. Unfortunately, in general it is numerically unstable [162]. There are some other simplified iterations based on the commutativity of A with X_0 that are numerically stable; see e.g. [49].

Bini et al. [17] 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 [104] 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 $A^{1/2}$.

As far as we know, there are no matrix secant methods based on Algorithms 3 and 4 for computing the matrix p-th root when $p > 2$. Nevertheless, a low-cost scheme has been recently developed for large-scale matrix p-th root calculations, which satisfies a weak secant equation [50].

3.5. Riccati equations. Let us now consider

$$F(X) = XA + A^T X - XBB^T X + C^T C, \tag{50}$$

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 [45], [131] and dynamical systems [4], among others.

Several applications require a symmetric positive semidefinite stabilizing solution of (50). 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., [45], [117] 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., [45], [117], [131] and references therein. However it is a common approach, in the large and sparse case, to use Newton's method to find a solution of (50), e.g., [13], [14], [83], [114], [157]. As usual, the general Newton 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

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** $k = 0, 1, \ldots$ until convergence **do**
3: **Set** $\mathscr{A}_k = A - BB^T X_k$
4: **Solve** $\mathscr{A}_k^T X_{k+1} + X_{k+1}\mathscr{A}_k = -C^T QC - X_k BB^T X_k$ ▷ for X_{k+1}
5: **end for**

Algorithm 6 has been known in the literature as the Kleinman iteration for CARE [114]. 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 [14], [68]. For another approach suitable for small and medium size problems which is based on the sign function see Byers [30].

A quasi-Newton scheme has also been developed for solving CARE, that obtains a reduction in the computational cost of the linear algebra involved [142]. However, the scheme proposed in [142] approximates the Fréchet derivative using finite differences, and so it cannot be considered as a secant method. So far, there are no matrix secant methods based on Algorithms 3 and 4 for Riccati equations.

3.6. Rational equations. We consider the following rational matrix equation

$$X \pm A^* X^{-p} A = Q, \tag{51}$$

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 (51) requires maximal (minimal) Hermitian positive definite solutions.

A maximal solution of (51) 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 (51) see [64], [65], [178]. Rational equations appear in the analysis of stationary Gaussian reciprocal processes over a finite interval [69], in the field of optimal control theory [64], and it is related to an algebraic Riccati equation of the type arising in Kalman filter theory [119]. 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

$$X_{k+1} \pm L_k^* X_{k+1} L_k = Q \pm 2L_k^* A, \tag{52}$$

where $L_k = X_k^{-1} A$. Notice that at every iteration of (52) 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 matrices and mild assumptions the q-quadratic convergence of (52) has been established [84].

To avoid the inverse at each iteration in (52), 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 [136]. This simplified iteration is given by

$$X_{k+1} = 2X_k - X_k A^{-*}(I - X_k)A^{-1} X_k. \tag{53}$$

The method indicated by (53) is clearly inexpensive. Notice that it only requires to compute A^{-1} at the beginning of the process. Starting with $X_0 = AA^*$, iteration (53) converges q-linearly to the minimal solution of (51) [136]. For different values of p, there are some other iterative schemes that posses q-linear convergence to extremal solutions of (51) which are not based on Newton's method, but instead on fixed points iterations [62], [63], [84], [107], [150], [178]. So far, there are no matrix secant methods based on Algorithms 3 and 4, for solving rational equations.

4. Conclusions

Newton's method has been omnipresent in the development of applied mathematics and scientific computing; and whenever a Newton 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 illustrate their practical performance together with the best available specialized Newton method. Our preliminary numerical experiments show the expected q-quadratic and q-superlinear convergence for Newton's method and secant methods respectively, and indicate that for solving nonlinear matrix problems the secant methods have interesting properties that remain to be fully understood.

Acknowledgements. We thank an anonymous referee and also Daniel Szyld and Bruno Iannazzo for many constructive comments and suggestions.

References

[1] P.-A. Absil, R. Sepulchre, P. Van Dooren, and R. Mahony, Cubically convergent iterations for invariant subspace computation. *SIAM J. Matrix Anal. Appl.* **26** (2004), 70–96. Zbl 1075.65049 MR 2112852

[2] F. A. Aliev and V. B. Larin, Generalized Lyapunov equation and factorization of matrix polynomials. *Systems Control Lett.* **21** (1993), 485–491. Zbl 0794.93075 MR 1249927

[3] H. A. Antosiewicz, Newton's method and boundary value problems. *J. Comput. System Sci.* **2** (1968), 177–292. Zbl 0164.17302 MR 0243734

[4] A. C. Antoulas, *Approximation of large-scale dynamical systems*. SIAM, Philadelphia 2005. Zbl 1112.93002 MR 2155615

[5] I. K. Argyros, Convergence and applications of Newton-type iterations. Springer, New York 2008. Zbl 1153.65057 MR 2428779

[6] U. M. Ascher, R. M. M. Mattheij, and R. D. Russell, *Numerical solution of boundary value problems for ordinary differential equations*. Prentice Hall, Englewood Cliffs, NJ, 1988. Zbl 0671.65063 MR 1000177

[7] L. Baffico, S. Bernard, Y. Maday, G. Turinici and G. Zérah, Parallel-in-time molecular-dynamics simulations. *Phys. Rev. E* **66** (2002), 057701.

[8] A. Y. Barraud, Investigations autour de la fonction signe d'une matrice: application à l'équation de Riccati. *RAIRO Automat. Syst. Anal. Control* **13** (1979), 335–368. Zbl 0424.93062 MR 557961

[9] R. H. Bartels and G. W. Stewart, Algorithm 432, solution of the matrix equation $AX + XB = C$ [F4]. *Comm. ACM* **15** (1972), 820–826.

[10] S. Batterson and J. Smillie, Rayleigh quotient iteration for nonsymmetric matrices. *Math. Comp.* **55** (1990), 169–178. Zbl 0701.65027 MR 1023041

[11] S. Bellavia and B. Morini, A globally convergent Newton-GMRES subspace method for systems of nonlinear equations. *SIAM J. Sci. Comput.* **23** (2001), 940–960. Zbl 0998.65053 MR 1860971

[12] P. Benner, *Contributions to the numerical solution of algebraic Riccati equations and related eigenvalue problems*. Logos Verlag, Berlin 1997. Zbl 0896.65047

[13] P. Benner and R. Byers, An exact line search method for solving generalized continuous-time algebraic Riccati equations. *IEEE Trans. Automat. Control* **43** (1998), 101–107. Zbl 0908.93026 MR 1604269

[14] P. Benner, J.-R. Li, and T. Penzl, Numerical solution of large-scale Lyapunov equations, Riccati equations, and linear-quadratic optimal control problems. *Numer. Linear Algebra Appl.* **15** (2008), 755–777. Zbl 1212.65245 MR 2464169

[15] P. Benner and E. S. Quintana-Ortí, Solving stable generalized Lyapunov equations with the matrix sign function. *Numer. Algorithms* **20** (1999), 75–100. Zbl 0940.65035 MR 1688781

[16] D. P. Bertsekas, *Nonlinear programming*. 2nd ed., Athena Scientific, Belmont, MA, 1999. Zbl 1015.90077

[17] D. A. Bini, N. J. Higham, and B. Meini, Algorithms for the matrix *p*th root. *Numer. Algorithms* **39** (2005), 349–378. Zbl 1103.65046 MR 2134331

[18] D. A. Bini, G. Latouche, and B. Meini, *Numerical methods for structured Markov chains*. Oxford University Press, Oxford 2005. Zbl 1076.60002 MR 2132031

[19] D. A. Bini, B. Iannazzo, and F. Poloni, A fast Newton's method for a nonsymmetric algebraic Riccati equation. *SIAM J. Matrix Anal. Appl.* **30** (2008), 276–290. Zbl 1166.15300 MR 2399580

[20] E. G. Birgin, N. Krejić, and J. M. Martínez, Globally convergent inexact quasi-Newton methods for solving nonlinear systems. *Numer. Algorithms* **32** (2003), 249–260. Zbl 1034.65032 MR 1989368

[21] A. Björck and S. Hammarling, A Schur method for the square root of a matrix. *Linear Algebra Appl.* **52/53** (1983), 127–140. Zbl 0515.65037 MR 0709347

[22] P. T. Boggs and J. W. Tolle, Sequential quadratic programming. In *Acta Numerica 1995*, Cambridge Univ. Press, Cambridge 1995, 1–51. Zbl 0828.65060 MR 1352470

[23] P. T. Boggs, A. J. Kearsley, and J. W. Tolle, A practical algorithm for general large scale nonlinear optimization problems. *SIAM J. Optim.* **9** (1999), 755–778. Zbl 0986.90077 MR 1692773

[24] P. T. Boggs, J. W. Tolle, and P. Wang, On the local convergence of quasi-Newton methods for constrained optimization. *SIAM J. Control Optim.* **20** (1982), 161–171. Zbl 0494.65036 MR 646946

[25] C. Brezinski, A classification of quasi-Newton methods. *Numer. Algorithms* **33** (2003), 123–135. Zbl 1030.65053 MR 2005557

[26] C. Brezinski and J. Van Iseghem, A taste of Padé approximation. In *Acta Numerica 1995*, Cambridge Univ. Press, Cambridge 1995, 53–103. Zbl 0827.41010 MR 1352471

[27] P. N. Brown and Y. Saad, Convergence theory of nonlinear Newton-Krylov algorithms. *SIAM J. Optim.* **4** (1994), 297–330. Zbl 0814.65048 MR 1273761

[28] C. G. Broyden, A class of methods for solving nonlinear simultaneous equations. *Math. Comp.* **19** (1965), 577–593. Zbl 0131.13905 MR 0198670

[29] C. G. Broyden, J. E. Dennis, Jr., and J. J. Moré, On the local and superlinear convergence of quasi-Newton methods. *J. Inst. Math. Appl.* **12** (1973), 223–245. Zbl 0282.65041 MR 0341853

[30] R. Byers, Solving the algebraic Riccati equation with the matrix sign function. *Linear Algebra Appl.* **85** (1987), 267–279. Zbl 0611.65027 MR 869359

[31] R. H. Byrd, R. A. Tapia, and Y. Zhang, An SQP augmented Lagrangian BFGS algorithm for constrained optimization. *SIAM J. Optim.* **2** (1992), 210–241. Zbl 0773.90065 MR 1158838

[32] A. Cauchy, Méthodes générales pour la résolution des systèmes d'équations simultanées. *C. R. Acad. Sci. Par.* **25** (1847), 536–538. http://gallica.bnf.fr/ark:/12148/bpt6k90190w/f406

[33] M. R. Celis, J. E. Dennis, and R. A. Tapia, A trust region strategy for nonlinear equality constrained optimization. In *Numerical optimization 1984*, SIAM, Philadelphia 1985, 71–82. Zbl 0566.65048 MR 802084

[34] P. Chartier and B. Philippe, A parallel shooting technique for solving dissipative ODEs. *Computing* **51** (1993), 209–236. Zbl 0788.65079 MR 1253404

[35] J.-P. Chehab and J. Laminie, Differential equations and solution of linear systems. *Numer. Algorithms* **40** (2005), 103–124. Zbl 1086.65026 MR 2189162

[36] J.-P. Chehab and M. Raydan, Implicit and adaptive inverse preconditioned gradient methods for nonlinear problems. *Appl. Numer. Math.* **55** (2005), 32–47. Zbl 1078.65049 MR 2152980

[37] X. Chen, Superlinear convergence of smoothing quasi-Newton methods for nonsmooth equations. *J. Comput. Appl. Math.* **80** (1997), 105–126. Zbl 0881.65042 MR 1455748 (99a:90182)

[38] X. Chen, Z. Nashed, and L. Qi, Convergence of Newton's method for singular smooth and nonsmooth equations using adaptive outer inverses. *SIAM J. Optim.* **7** (1997), 445–462. Zbl 0871.65047 MR 1443628

[39] E. W. Cheney, *Introduction to approximation theory*. 2nd ed., Chelsea Publishing, New York 1982. Zbl 0535.41001 MR 1656150

[40] E. W. Cheney and A. A. Goldstein, Newton's method for convex programming and Tchebycheff approximation. *Numer. Math.* **1** (1959), 253–268. Zbl 0113.10703 MR 0109430

[41] S. H. Cheng, N. J. Higham, C. S. Kenney, and A. J. Laub, Approximating the logarithm of a matrix to specified accuracy. *SIAM J. Matrix Anal. Appl.* **22** (2001), 1112–1125. Zbl 0989.65057 MR 1825853

[42] A. R. Conn, N. I. M. Gould, and P. L. Toint, *Trust-region methods*. SIAM, Philadelphia 2000. Zbl 0958.65071 MR 1774899

[43] D. Cores and R. A. Tapia, Perturbation lemma for the Newton method with application to the SQP Newton method. *J. Optim. Theory Appl.* **97** (1998), 271–280. Zbl 0907.90217 MR 1625076

[44] T. Damm and D. Hinrichsen, Newton's method for a rational matrix equation occurring in stochastic control. *Linear Algebra Appl.* **332/334** (2001), 81–109. Zbl 0982.65050 MR 1839427

[45] B. N. Datta, *Numerical methods for linear control systems*. Elsevier Academic Press, Amsterdam 2004. Zbl 1079.65072 MR 2260346

[46] B. N. Datta and Y. Saad, Arnoldi methods for large Sylvester-like observer matrix equations, and an associated algorithm for partial spectrum assignment. *Linear Algebra Appl.* **154/156** (1991), 225–244. Zbl 0734.65037 MR 1113144

[47] W. C. Davidon, Variable metric method for minimization. *SIAM J. Optim.* **1** (1991), 1–17. Zbl 0752.90062 MR 1094786

[48] G. J. Davis, Numerical solution of a quadratic matrix equation. *SIAM J. Sci. Statist. Comput.* **2** (1981), 164–175. Zbl 0467.65021 MR 622713

[49] B. De Abreu, M. Monsalve and M. Raydan, Specialized hybrid Newton schemes for matrix pth roots. *Appl. Math. Sci.* (*Ruse*) **2** (2008), no. 49, 2401–2424. Zbl 1188.65059 MR 2480458

[50] B. De Abreu and M. Raydan, Residual methods for the large-scale matrix p-th root and some related problems. *Appl. Math. Comput.* **217** (2010), 650–660. Zbl 1200.65032 MR 2678578

[51] R. S. Dembo, S. C. Eisenstat, and T. Steihaug, Inexact Newton methods. *SIAM J. Numer. Anal.* **19** (1982), 400–408. Zbl 0478.65030 MR 650059

[52] E. D. Denman and A. N. Beavers, Jr., The matrix sign function and computations in systems. *Appl. Math. Comput.* **2** (1976), 63–94. Zbl 0398.65023 MR 0393075

[53] J. E. Dennis, Jr., On the convergence of Broyden's method for nonlinear systems of equations. *Math. Comp.* **25** (1971), 559–567. Zbl 0277.65030 MR 0295560

[54] J. E. Dennis, Jr., M. El-Alem, and M. C. Maciel, A global convergence theory for general trust-region-based algorithms for equality constrained optimization. *SIAM J. Optim.* **7** (1997), 177–207. Zbl 0867.65031 MR 1430563

[55] J. E. Dennis, Jr. and J. J. Moré, A characterization of superlinear convergence and its application to quasi-Newton methods. *Math. Comp.* **28** (1974), 549–560. Zbl 0282.65042 MR 0343581

[56] J. E. Dennis, Jr. and R. B. Schnabel, Least change secant updates for quasi-Newton methods. *SIAM Rev.* **21** (1979), 443–459. Zbl 0424.65020 MR 545880

[57] J. E. Dennis, Jr. and R. B. Schnabel, *Numerical methods for unconstrained optimization and nonlinear equations*. Classics Appl. Math. 16, SIAM, Philadelphia 1996. Zbl 0847.65038 MR 1376139

[58] J. E. Dennis, M. Heinkenschloss, and L. N. Vicente, Trust-region interior-point SQP algorithms for a class of nonlinear programming problems. *SIAM J. Control Optim.* **36** (1998), 1750–1794. Zbl 0921.90137 MR 1632552

[59] S. C. Eisenstat and H. F. Walker, Globally convergent inexact Newton methods. *SIAM J. Optim.* **4** (1994), 393–422. Zbl 0814.65049 MR 1273766

[60] M. El-Alem, A robust trust-region algorithm with a nonmonotonic penalty parameter scheme for constrained optimization. *SIAM J. Optim.* **5** (1995), 348–378. Zbl 0828.65063 MR 1330201

[61] A. S. El-Bakry, R. A. Tapia, T. Tsuchiya, and Y. Zhang, On the formulation and theory of the Newton interior-point method for nonlinear programming. *J. Optim. Theory Appl.* **89** (1996), 507–541. Zbl 0851.90115 MR 1393361

[62] S. M. El-Sayed, An algorithm for computing positive definite solutions of the nonlinear matrix equation $X + A^*X^{-1}A = I$. *Int. J. Comput. Math.* **80** (2003), 1527–1534. Zbl 1049.65033 MR 2031600

[63] S. M. El-Sayed and A. M. Al-Dbiban, A new inversion free iteration for solving the equation $X + A^*X^{-1}A = Q$. *J. Comput. Appl. Math.* **181** (2005), 148–156. Zbl 1072.65060 MR 2146416

[64] J. C. Engwerda, On the existence of a positive definite solution of the matrix equation $X + A^TX^{-1}A = I$. *Linear Algebra Appl.* **194** (1993), 91–108. Zbl 0798.15013 MR 1243822

[65] J. C. Engwerda, A. C. M. Ran, and A. L. Rijkeboer, Necessary and sufficient conditions for the existence of a positive definite solution of the matrix equation $X + A^*X^{-1}A = Q$. *Linear Algebra Appl.* **186** (1993), 255–275. Zbl 0778.15008 MR 1217209

[66] J. A. Ezquerro and M. A. Hernández, On a convex acceleration of Newton's method. *J. Optim. Theory Appl.* **100** (1999), 311–326. Zbl 0915.90235 MR 1673435

[67] J. A. Ezquerro and M. A. Hernández, On the application of a fourth-order two-point method to Chandrasekhar's integral equation. *Aequationes Math.* **62** (2001), 39–47. Zbl 0990.45002 MR 1849138

[68] F. Feitzinger, T. Hylla, and E. W. Sachs, Inexact Kleinman–Newton method for Riccati equations. *SIAM J. Matrix Anal. Appl.* **31** (2009), 272–288. Zbl 1191.49033 MR 2496419

[69] A. Ferrante and B. C. Levy, Hermitian solutions of the equation $X = Q + NX^{-1}N^*$. *Linear Algebra Appl.* **247** (1996), 359–373. Zbl 0876.15011 MR 1412761

[70] R. Fletcher, *Practical methods of optimization*. 2nd ed., John Wiley & Sons Ltd., Chichester 1987. Zbl 0905.65002 MR 955799

[71] R. Fletcher and M. J. D. Powell, A rapidly convergent descent method for minimization. *Comput. J.* **6** (1963), 163–168. Zbl 0132.11603 MR 0152116

[72] R. Fontecilla, Inexact secant methods for nonlinear constrained optimization. *SIAM J. Numer. Anal.* **27** (1990), 154–165. Zbl 0688.65048 MR 1034926

[73] A. Friedlander, M. A. Gomes-Ruggiero, D. N. Kozakevich, J. M. Martínez, and S. A. Santos, Solving nonlinear systems of equations by means of quasi-Newton methods with a nonmonotone strategy. *Optim. Methods Softw.* **8** (1997), 25–51. Zbl 0893.65032 MR 1488086

[74] M. J. Gander and S. Vandewalle, Analysis of the parareal time-parallel time-integration method. *SIAM J. Sci. Comput.* **29** (2007), 556–578. Zbl 1141.65064 MR 2306258

[75] U. M. Garcia Palomares and O. L. Mangasarian, Superlinearly convergent quasi-Newton algorithms for nonlinearly constrained optimization problems. *Math. Programming* **11** (1976), 1–13. Zbl 0362.90103 MR 0434445

[76] G. H. Golub, S. Nash, and C. Van Loan, A Hessenberg-Schur method for the problem $AX + XB = C$. *IEEE Trans. Automat. Control* **24** (1979), 909–913. Zbl 0421.65022 MR 566448

[77] M. A. Gomes-Ruggiero and J. M. Martínez, The column-updating method for solving nonlinear equations in Hilbert space. *RAIRO Modél. Math. Anal. Numér.* **26** (1992), 309–330. Zbl 0752.65047 MR 1153004

[78] M. D. González-Lima and F. Montes de Oca, A Newton-like method for nonlinear system of equations. *Numer. Algorithms* **52** (2009), 479–506. Zbl 1181.65072 MR 2563953

[79] J. Goodman, Newton's method for constrained optimization. *Math. Programming* **33** (1985), 162–171. Zbl 0589.90065 MR 808908

[80] M. Grau-Sánchez, Improvements of the efficiency of some three-step iterative like-Newton methods. *Numer. Math.* **107** (2007), 131–146. Zbl 1123.65037 MR 2317831

[81] F. Greco and B. Iannazzo, A binary powering Schur algorithm for computing primary matrix roots. *Numer. Algorithms* **55** (2010), 59–78. Zbl 1202.65053 MR 2679750

[82] C.-H. Guo and N. J. Higham, A Schur–Newton method for the matrix pth root and its inverse. *SIAM J. Matrix Anal. Appl.* **28** (2006), 788–804. Zbl 1128.65030 MR 2262981

[83] C.-H. Guo and P. Lancaster, Analysis and modification of Newton's method for algebraic Riccati equations. *Math. Comp.* **67** (1998), 1089–1105. Zbl 0903.65047 MR 1459388

[84] C.-H. Guo and P. Lancaster, Iterative solution of two matrix equations. *Math. Comp.* **68** (1999), 1589–1603. Zbl 0940.65036 MR 1651757

[85] C.-H. Guo and A. J. Laub, On the iterative solution of a class of nonsymmetric algebraic Riccati equations. *SIAM J. Matrix Anal. Appl.* **22** (2000), 376–391. Zbl 0973.65025 MR 1780190

[86] W. E. Hart and S. O. W. Soul, Quasi-Newton methods for discretized non-linear boundary problems. *J. Inst. Math. Appl.* **11** (1973), 351–359. Zbl 0259.65074

[87] M. Heinkenschloss, Projected sequential quadratic programming methods. *SIAM J. Optim.* **6** (1996), 373–417. Zbl 0861.49025 MR 1387332

[88] M. A. Hernández, M. J. Rubio, and J. A. Ezquerro, Secant-like methods for solving nonlinear integral equations of the Hammerstein type. *J. Comput. Appl. Math.* **115** (2000), 245–254. Zbl 0944.65146 MR 1747223

[89] B. Héron, F. Issard-Roch, and C. Picard, *Analyse numé*rique. Dunod, Paris 1999.

[90] N. J. Higham, Newton's method for the matrix square root. *Math. Comp.* **46** (1986), 537–549. Zbl 0614.65045 MR 829624

[91] N. J. Higham, Computing the polar decomposition—with applications. *SIAM J. Sci. Statist. Comput.* **7** (1986), 1160–1174. Zbl 0607.65014 MR 857788

[92] N. J. Higham, Computing real square roots of a real matrix. *Linear Algebra Appl.* **88/89** (1987), 405–430. Zbl 0625.65032 MR 882456

[93] N. J. Higham, *Accuracy and stability of numerical algorithms*. SIAM, Philadelphia 1996. Zbl 0847.65010 MR 1368629

[94] N. J. Higham, Stable iterations for the matrix square root. *Numer. Algorithms* **15** (1997), 227–242. Zbl 0884.65035 MR 1475179

[95] N. J. Higham, *Functions of matrices*. SIAM, Philadelphia 2008. Zbl 1167.15001 MR 2396439

[96] N. J. Higham, The scaling and squaring method for the matrix exponential revisited. *SIAM Rev.* **51** (2009), 747–764. Zbl 1178.65040 MR 2563832

[97] N. J. Higham and H.-M. Kim, Numerical analysis of a quadratic matrix equation. *IMA J. Numer. Anal.* **20** (2000), 499–519. Zbl 0966.65040 MR 1795295

[98] T. Hoheisel, C. Kanzow, B. S. Mordukhovich and H. Phan, Generalized Newton's method based on graphical derivatives. *Nonlinear Anal.*, to appear.

[99] R. A. Horn and C. R. Johnson, *Topics in matrix analysis*. Cambridge University Press, Cambridge 1991. Zbl 0729.15001 MR 1091716

[100] W. D. Hoskins and D. J. Walton, A faster, more stable method for computing the pth roots of positive definite matrices. *Linear Algebra Appl.* **26** (1979), 139–163. Zbl 0407.65017 MR 535683

[101] J. L. Howland, The sign matrix and the separation of matrix eigenvalues. *Linear Algebra Appl.* **49** (1983), 221–232. Zbl 0507.15007 MR 688386

[102] D. Y. Hu and L. Reichel, Krylov-subspace methods for the Sylvester equation. *Linear Algebra Appl.* **172** (1992), 283–313. Zbl 0777.65028 MR 1168508

[103] B. Iannazzo, A note on computing the matrix square root. *Calcolo* **40** (2003), 273–283. Zbl 1117.65059 MR 2025713

[104] B. Iannazzo, On the Newton method for the matrix pth root. *SIAM J. Matrix Anal. Appl.* **28** (2006), 503–523. Zbl 1113.65054 MR 2255340

[105] B. Iannazzo, A family of rational iterations and its application to the computation of the matrix pth root. *SIAM J. Matrix Anal. Appl.* **30** (2008), 1445–1462. Zbl 1176.65054 MR 2486848

[106] R. B. Israel, J. S. Rosenthal, and J. Z. Wei, Finding generators for Markov chains via empirical transition matrices, with applications to credit ratings. *Math. Finance* **11** (2001), 245–265. Zbl 0987.60086 MR 1822778

[107] I. G. Ivanov, V. I. Hasanov, and B. V. Minchev, On matrix equations $X \pm A^*X^{-2}A = I$. *Linear Algebra Appl.* **326** (2001), 27–44. Zbl 0979.15007 MR 1815949

[108] K. Jbilou, Low rank approximate solutions to large Sylvester matrix equations. *Appl. Math. Comput.* **177** (2006), 365–376. Zbl 1095.65041 MR 2234524

[109] C. T. Kelley and E. W. Sachs, Solution of optimal control problems by a pointwise projected Newton method. *SIAM J. Control Optim.* **33** (1995), 1731–1757. Zbl 0841.49013 MR 1358092

[110] C. Kenney and A. J. Laub, Padé error estimates for the logarithm of a matrix. *Internat. J. Control* **50** (1989), 707–730. Zbl 0685.65036 MR 1017754

[111] C. Kenney and A. J. Laub, Rational iterative methods for the matrix sign function. *SIAM J. Matrix Anal. Appl.* **12** (1991), 273–291. Zbl 0725.65048 MR 1089159

[112] C. Kenney and A. J. Laub, On scaling Newton's method for polar decomposition and the matrix sign function. *SIAM J. Math. Anal. Appl.* **13** (1992), 688–706. Zbl 0754.65043 MR 1168017

[113] C. S. Kenney and A. J. Laub, The matrix sign function. *IEEE Trans. Automat. Control* **40** (1995), 1330–1348. Zbl 0830.93022 MR 1343800

[114] D. Kleinman, On an iterative technique for Riccati equation computations. *IEEE Trans. Automat. Control* **13** (1968), 114–115.

[115] J. Kou, Y. Li, and X. Wang, A family of fifth-order iterations composed of Newton and third-order methods. *Appl. Math. Comput.* **186** (2007), 1258–1262. Zbl 1119.65037 MR 2316746

[116] F.-S. Kupfer and E. W. Sachs, Numerical solution of a nonlinear parabolic control problem by a reduced SQP method. *Comput. Optim. Appl.* **1** (1992), 113–135. Zbl 0771.49010 MR 1195632

[117] P. Lancaster and L. Rodman, *Algebraic Riccati equations*. Oxford University Press, Oxford 1995. Zbl 0836.15005 MR 1367089

[118] G. Latouche and V. Ramaswami, *Introduction to matrix analytic methods in stochastic modeling*. SIAM, Philadelphia 1999. Zbl 0922.60001 MR 1674122

[119] B. C. Levy, R. Frezza, and A. J. Krener, Modeling and estimation of discrete-time Gaussian reciprocal processes. *IEEE Trans. Automat. Control* **35** (1990), 1013–1023. Zbl 0709.60043 MR 1065037

[120] J.-L. Lions, Y. Maday, and G. Turinici, Résolution d'EDP par un schéma en temps "pararéel". *C. R. Acad. Sci. Paris Sér. I Math.* **332** (2001), 661–668. Zbl 0984.65085 MR 1842465

[121] V. L. R. Lopes and J. M. Martínez, On the convergence of quasi-Newton methods for nonsmooth problems. *Numer. Funct. Anal. Optim.* **16** (1995), 1193–1209. Zbl 0860.65038 MR 1374972

[122] L. Z. Lu, Newton iterations for a non-symmetric algebraic Riccati equation. *Numer. Linear Algebra Appl.* **12** (2005), 191–200. Zbl 1164.65386 MR 2125630

[123] F. Luengo, M. Raydan, W. Glunt, and T. L. Hayden, Preconditioned spectral gradient method. *Numer. Algorithms* **30** (2002), 241–258. Zbl 1027.90110 MR 1927505

[124] E. Lundström and L. Eldén, Adaptive eigenvalue computations using Newton's method on the Grassmann manifold. *SIAM J. Matrix Anal. Appl.* **23** (2001/02), 819–839. Zbl 0999.65019 MR 1896820

[125] A. M. Lyapunov, *The general problem of the stability of motion*. Taylor & Francis Ltd., London 1992. Zbl 0786.70001 MR 1229075

[126] A. J. Majda and E. G. Tabak, A two-dimensional model for quasigeostrophic flow: comparison with the two-dimensional Euler flow. *Phys. D* **98** (1996), 515–522. Zbl 0899.76105 MR 1422288

[127] H. J. Martinez, Z. Parada, and R. A. Tapia, On the characterization of Q-superlinear convergence of quasi-Newton interior-point methods for nonlinear programming. *Bol. Soc. Mat. Mexicana* (3) **1** (1995), 137–148. Zbl 0853.65061 MR 1387657

[128] J. M. Martínez, A family of quasi-Newton methods for nonlinear equations with direct secant updates of matrix factorizations. *SIAM J. Numer. Anal.* **27** (1990), 1034–1049. Zbl 0702.65053 MR 1051122

[129] J. M. Martínez and L. Q. Qi, Inexact Newton methods for solving nonsmooth equations. *J. Comput. Appl. Math.* **60** (1995), 127–145. Zbl 0833.65045 MR 1354652

[130] J. M. Martínez and M. C. Zambaldi, Least change update methods for nonlinear systems with nondifferentiable terms. *Numer. Funct. Anal. Optim.* **14** (1993), 405–415. Zbl 0801.65049 MR 1229666

[131] V. L. Mehrmann, *The autonomous linear quadratic control problem*. Lecture Notes in Control and Inform. Sci. 163, Springer-Verlag, Berlin 1991. Zbl 0746.93001 MR 1133203

[132] B. Meini, The matrix square root from a new functional perspective: theoretical results and computational issues. *SIAM J. Matrix Anal. Appl.* **26** (2004), 362–376. Zbl 1087.15019 MR 2124152

[133] C. Moler and C. Van Loan, Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later. *SIAM Rev.* **45** (2003), 3–49. Zbl 1030.65029 MR 1981253

[134] M. Monsalve, Block linear method for large scale Sylvester equations. *Comput. Appl. Math.* **27** (2008), 47–59. Zbl 1161.65032 MR 2393283

[135] M. Monsalve, Esquemas tipo Newton y cuasi-Newton en la solución de problemas no lineales en espacio de matrices. PhD thesis, Departmento de Computación, Universidad Central de Venezuela, Caracas 2008.

[136] M. Monsalve and M. Raydan, A new inversion-free method for a rational matrix equation. *Linear Algebra Appl.* **433** (2010), 64–71. Zbl 1191.65043 MR 2645065

[137] M. Monsalve and M. Raydan, A secant method for nonlinear matrix problems. In *Numerical linear algebra in signals, systems and control*, Lecture Notes in Electrical Engineering 80, Springer, New York 2011, Chapter 19.

[138] F. D. Murnaghan and J. W. Wrench, Jr., The determination of the Chebyshev approximating polynomial for a differentiable function. *Math. Tables Aids Comput.* **13** (1959), 185–193. Zbl 0112.08002 MR 0105790

[139] J. Nocedal and S. J. Wright, *Numerical optimization*. Springer Series in Operations Research, Springer-Verlag, New York 1999. Zbl 0930.65067 MR 1713114

[140] J. M. Ortega and W. C. Rheinbolt, *Iterative solution of nonlinear equations in several variables*. Classics Appl. Math. SIAM, Philadelphia 2000. Zbl 0949.65053 MR 1744713

[141] V. Pan and R. Schreiber, An improved Newton iteration for the generalized inverse of a matrix, with applications. *SIAM J. Sci. Statist. Comput.* **12** (1991), 1109–1130. Zbl 0733.65023 MR 1114976

[142] P. Pandey, Quasi-Newton methods for solving algebraic Riccati equations. In *Proceedings of the 1992 American Control Conference*, Chicago 1992, 654–658.

[143] J. M. Papakonstantinou, Historical development of the BFGS secant method and its characterization properties. PhD thesis, Rice University, Houston 2009. http://www.caam.rice.edu/tech_reports/2009/TR09-43.pdf

[144] V. Pereyra, Accelerating the convergence of discretization algorithms. *SIAM J. Numer. Anal.* **4** (1967), 508–533. Zbl 0265.65043 MR 0221726

[145] R. Pérez and V. L. R. Lopes, Recent applications and numerical implementation of quasi-Newton methods for solving nonlinear systems of equations. *Numer. Algorithms* **35** (2004), 261–285. Zbl 1049.65043 MR 2072974

[146] G. Peters and J. H. Wilkinson, Inverse iteration, ill-conditioned equations and Newton's method. *SIAM Rev.* **21** (1979), 339–360. Zbl 0424.65021 MR 535118

[147] M. J. D. Powell, The convergence of variable metric methods for nonlinearly constrained optimization calculations. In *Nonlinear programming 3*, Academic Press, New York 1978, 27–63. Zbl 0464.65042 MR 507858

[148] M. J. D. Powell, Algorithms for nonlinear constraints that use Lagrangian functions. *Math. Programming* **14** (1978), 224–248. Zbl 0383.90092 MR 0469283

[149] M. J. D. Powell, *Approximation theory and methods*. Cambridge University Press, Cambridge 1981. Zbl 0453.41001 MR 604014

[150] M. A. Ramadan, Necessary and sufficient conditions for the existence of positive definite solutions of the matrix equation $X + A^T X^{-2} A = I$. *Int. J. Comput. Math.* **82** (2005), 865–870. Zbl 1083.15020 MR 2185641

[151] M. A. Ramadan and N. M. El-Shazly, On the matrix equation $X + A^{\mathrm{T}} \sqrt[m]{X^{-1}} A = I$. *Appl. Math. Comput.* **173** (2006), 992–1013. Zbl 1089.65037 MR 2207992

[152] M. Raydan, Exact order of convergence of the secant method. *J. Optim. Theory Appl.* **78** (1993), 541–551. Zbl 0795.65026 MR 1240435

[153] E. Y. Remez, Sur le calcul effectif des polynômes d'approximation de Tschebycheff. *C.R. Acad. Sci. Paris* **199** (1934), 337–340. JFM 60.0212.01 Zbl 0010.01702

[154] J. D. Roberts, Linear model reduction and solution of the algebraic Riccati equation by use of the sign function. *Internat. J. Control* **32** (1980), 677–687. Zbl 0463.93050 MR 595962

[155] S. M. Robinson, Newton's method for a class of nonsmooth functions. *Set-Valued Anal.* **2** (1994), 291–305. Zbl 0804.65062 MR 1285835

[156] E. W. Sachs, Broyden's method in Hilbert space. *Math. Programming* **35** (1986), 71–82. Zbl 0598.90080 MR 842635

[157] N. R. Sandell, Jr., On Newton's method for Riccati equation solution. *IEEE Trans. Automatic Control* **19** (1974), 254–255. Zbl 0278.65096 MR 0421798

[158] B. A. Schmitt, An algebraic approximation for the matrix exponential in singularly perturbed boundary value problems. *SIAM J. Numer. Anal.* **27** (1990), 51–66. Zbl 0689.65056 MR 1034920

[159] G. Schulz, Iterative Berechnung der reziproken Matrix. *Z. Angew. Math. Mech.* **13** (1933), 57–59. JFM 59.0535.04

[160] L. S. Shieh, S. R. Lian and B. C. Mcinnis, Fast and stable algorithms for computing the principal square root of a complex matrix. *IEEE Trans. Automat. Control* **32** (1987), 820–822. Zbl 0626.65042

[161] R. D. Skeel, Iterative refinement implies numerical stability for Gaussian elimination. *Math. Comp.* **35** (1980), 817–832. Zbl 0441.65027 MR 572859

[162] M. I. Smith, A Schur algorithm for computing matrix pth roots. *SIAM J. Matrix Anal. Appl.* **24** (2003), 971–989. Zbl 1040.65038 MR 2003316

[163] T. Söderström and G. W. Stewart, On the numerical properties of an iterative method for computing the Moore-Penrose generalized inverse. *SIAM J. Numer. Anal.* **11** (1974), 61–74. Zbl 0241.65038 MR 0341843

[164] J. Stoer and R. A. Tapia, On the characterization of q-superlinear convergence of quasi-Newton methods for constrained optimization. *Math. Comp.* **49** (1987), 581–584. Zbl 0632.90052 MR 906190

[165] J. J. Sylvester, Sur l'equation en matrices $px = xq'$. *C.R. Acad. Sci. Paris* **99** (1884), 67–71, 115–116. JFM 16.0108.03

[166] D. B. Szyld, Criteria for combining inverse and Rayleigh quotient iteration. *SIAM J. Numer. Anal.* **25** (1988), 1369–1375. Zbl 0665.65031 MR 972460

[167] R. A. Tapia, An application of a Newton-like method to the Euler-Lagrange equation. *Pacific J. Math.* **29** (1969), 235–246. Zbl 0176.41401 MR 0250479

[168] R. A. Tapia, Newton's method for problems with equality constraints. *SIAM J. Numer. Anal.* **11** (1974), 174–196. Zbl 0244.65036 MR 0348590

[169] R. A. Tapia, Diagonalized multiplier methods and quasi-Newton methods for constrained optimization. *J. Optimization Theory Appl.* **22** (1977), 135–194. Zbl 0336.65034 MR 0459641

[170] R. Tapia, On secant updates for use in general constrained optimization. *Math. Comp.* **51** (1988), 181–202. Zbl 0657.90088 MR 942149

[171] R. A. Tapia and D. L. Whitley, The projected Newton method has order $1 + \sqrt{2}$ for the symmetric eigenvalue problem. *SIAM J. Numer. Anal.* **25** (1988), 1376–1382. Zbl 0674.65012 MR 972461

[172] J. S. H. Tsai, L. S. Shieh, R. E. Yates, Fast and stable algorithms for computing the principal nth root of a complex matrix and the matrix sector function. *Comput. Math. Appl.* **15** (1988), 903–913. Zbl 0653.65031 MR 0950036

[173] L. Veidinger, On the numerical determination of the best approximations in the Chebyshev sense. *Numer. Math.* **2** (1960), 99–105. Zbl 0090.33702 MR 0139889

[174] L. N. Vicente, On interior-point Newton algorithms for discretized optimal control problems with state constraints. *Optim. Methods Softw.* **8** (1998), 249–275. Zbl 0903.49020 MR 1623241

[175] F. V. Waugh and M. E. Abel, On fractional powers of a matrix. *J. Amer. Statist. Assoc.* **62** (1967), 1018–1021. MR 0219228

[176] S. Weerakoon and T. G. I. Fernando, A variant of Newton's method with accelerated third-order convergence. *Appl. Math. Lett.* **13** (2000), 87–93. Zbl 0973.65037 MR 1791767

[177] R. B. Wilson, A simplicial algorithm for concave programming. PhD Thesis, Harvard Business School, Boston 1963.

[178] X. Zhan, Computing the extremal positive definite solutions of a matrix equation. *SIAM J. Sci. Comput.* **17** (1996), 1167–1174. Zbl 0856.65044 MR 1404867

[179] Y. Zhang and R. P. Tewarson, Quasi-Newton algorithms with updates from the preconvex part of Broyden's family. *IMA J. Numer. Anal.* **8** (1988), 487–509. Zbl 0661.65061 MR 975609

Received December 28, 2010; revised September 15, 2011

M. Monsalve, Departamento de Computación, Facultad de Ciencias, Universidad Central de Venezuela, Ap. 47002, Caracas 1041-A, Venezuela

E-mail: marlliny.monsalve@ciens.ucv.ve

M. Raydan, Departamento de Cómputo Científico y Estadística, Universidad Simón Bolívar, Ap. 89000, Caracas 1080-A, Venezuela

E-mail: mraydan@usb.ve