On the Continuous Realization of Iterative Processes

Moody T. Chu

SIAM Review, Vol. 30, No. 3 (Sep., 1988), 375-387.

Stable URL:
http://links.jstor.org/sici?sici=0036-1445%28198809%2930%3A3%3C375%3AOTCROI%3E2.0.CO%3B2-I

SIAM Review is currently published by Society for Industrial and Applied Mathematics.

SIAM REVIEW
Vol. 30, No. 3, September 1988

ON THE CONTINUOUS REALIZATION OF ITERATIVE PROCESSES*

MOODY T. CHU†

Abstract. Many important mathematical problems are solved by iterative methods. Many of these iterative schemes may be regarded as the discrete realization of certain continuous dynamical systems. This paper summarizes some of the recent developments in the continuous realization of several popular basic iterative methods.

Key words. iterative methods, dynamical systems

AMS(MOS) subject classifications. 65F, 34C, 58F

1. Introduction. The process of successive iterations has been used in a variety of ways to solve many important mathematical problems. Without an attempt to be complete, the following are just a few examples in applications. The Newton methods [15], [30], [37] may be used for solving systems of nonlinear equations; the steepest descent method [19] for solving optimization problems; the power method [16], [23], [31] for finding the eigenvector associated with the largest module eigenvalue; the SVD algorithm [21]–[23] for calculating the singular value decomposition; the QZ algorithm [23], [28] for solving generalized eigenvalue problems; and the linear stationary methods [24], [38], including the Jacobi method, the Gauss–Seidel method, and the SOR method, for solving large and sparse systems of linear algebraic equations.

Over the past few decades numerous researchers have made great efforts and contributions to the description, analysis, and modification for each of the above-mentioned iterative processes. The present paper does not intend to survey the state of the art in that aspect, so only a few general references are cited for each method. Readers should be able to find more detailed discussions and applications from the bibliographies referred to therein.

Recently, continuous versions of various iterative processes have been proposed and studied. Roughly speaking, the continuous method involves systems of differential equations, whereas the discrete method involves systems of difference equations. The subject of the present paper is to examine the differential equation analogues of some of the basic iterative processes.

All the basic iterative methods discussed in this paper can be expressed abstractly in a similar form. That is, each iterative process generates a sequence of points $\{x_\kappa\}$ by

$$x_{\kappa+1} = G_\kappa(x_\kappa), \tag{1.1}$$

where $\{G_\kappa\}$ is a sequence of properly chosen operators. The scheme (1.1) is about the simplest case of the general iterative process [30] defined below.

DEFINITION 1.1. A family of operators $\{G_\kappa\}$, where

$$G_\kappa : D_\kappa \subset (R^n)^{\kappa+p} \to R^n, \qquad \kappa = 0, 1, \cdots, \tag{1.2}$$

defines an iterative process $I = (\{G_\kappa\}, D^*, p)$ with p initial points and with domain $D^* \subset D_0$, if D^* is not empty and if for any point $(x_0, x_{-1}, \cdots, x_{-p+1}) \in D^*$, the

* Received by the editors February 10, 1986; accepted for publication (in revised form) January 9, 1987.

† Department of Mathematics, North Carolina State University, Raleigh, North Carolina 27695-8205.

sequence $\{x_\kappa\}$ generated by

$$x_{\kappa+1} = G_\kappa(x_\kappa, \cdots, x_{-p+1}), \qquad \kappa = 0, 1, \cdots, \tag{1.3}$$

exists, i.e., if $(x_\kappa, \cdots, x_{-p+1}) \in D_\kappa$ for all $\kappa = 0, 1, \cdots$.

DEFINITION 1.2. An iterative process $I = (\{G_\kappa\}, D^*, p)$ is said to be an m-step-method if $p = m$ and if the mappings $\{G_\kappa\}$ are of the form

$$G_\kappa : D_\kappa \subset (R^n)^m \to R^n, \qquad \kappa = 0, 1, \cdots. \tag{1.4}$$

An m-step process is *sequential* if the iterates are generated by

$$x_{\kappa+1} = G_\kappa\{x_\kappa, \cdots, x_{\kappa-m+1}\}, \qquad \kappa = 0, 1, \cdots. \tag{1.5}$$

A sequential m-step process is *stationary* with iteration function G if $G_\kappa = G$, $D_\kappa = D$ for all $\kappa = 0, 1, \cdots$.

It is clear from these definitions that all the basic iterative processes mentioned in this paper are sequential one-step methods. While the Newton method, the Jacobi method, the Gauss–Seidel method, the SOR method, and the power method are stationary processes, the QR algorithm, the steepest descent method, the QZ algorithm, and the SVD algorithm are nonstationary. The secant method is an example of a two-step method. In [37] various multistep methods are proposed in order to obtain higher-order methods for the solution of nonlinear equations. On the other hand, many procedures that are used to accelerate the convergence of the basic linear stationary methods may result in multistep methods. The Chebyshev and conjugate gradient accelerations [24] are just two examples of this kind. Numerical techniques employed to approximate solutions of differential equations often take the form of a sequential, stationary multistep iterative process.

The discussion in this article is presented on a method-by-method basis. The reader will find that some continuous models evaluate exactly the iterates of the corresponding discrete methods, but that others are simply straightforward continuous extentions. In either case, the advantages of considering the differential systems could be as follows:

(a) There are many state-of-the-art numerical techniques available for following the associated solution flows;

(b) The theoretical O.D.E. techniques often offer better understanding about the convergence conditions for the corresponding discrete method;

(c) In contrast to the local properties for some discrete methods, the continuous approach usually offers a global method for solving the underlined problem.

We note that it is a complicated problem to judge whether a more secure but more involved method is superior to a simpler method. Likewise, it is difficult to compare the algorithmic details between the continuous and the discrete methods. In spite of the large amount of variations of iterative procedures, we shall restrict our discussion of continuous realization to the very basic schemes only. We assume that the reader has already learned these basic methods elsewhere, so there is no need to comment on the schemes themselves. Nor do we intend to evaluate the various computational perspectives of the continuous methods, even though in recent years some of these continuous approaches have become more and more appealing and promising [2], [18], [26]. Our primary objective is to summarize a number of connected problems so as to arouse general interest in the various correspondences between iterative methods and dynamical systems.

2. The Newton method. Consider the problem of solving the nonlinear equation

$$f(x)=0, \tag{2.1}$$

where $f: R^n \to R^n$ is a sufficiently smooth function. It has long been known that one cycle of the classical Newton iteration

$$x_{\kappa+1}=x_\kappa-(f'(x_\kappa))^{-1}f(x_\kappa) \tag{2.2}$$

may be regarded as one explicit Euler step with unit steplength applied to the differential system

$$\frac{dx}{ds}=-(f'(x))^{-1}f(x), \qquad x(0)=x_0. \tag{2.3}$$

The solution flow $x(s)$ of (2.3) obviously satisfies the equation $f(x(s))=e^{-s}f(x(0))$. This can be interpreted as follows: the flow always moves in the direction along which the magnitude of $f(x)$ is reduced exponentially. It follows that the solution $x(s)$ of (2.3) either diverges to infinity, converges to a local minimum of f, or converges to a zero of f. From this observation, we can imagine that if x_0 is on the wrong side of a local maximum of the graph of f, then the iterates of (2.2) may diverge. Even though divergence can be avoided by considering Broyden's modification

$$x_{\kappa+1}=x_\kappa-\alpha_\kappa(f'(x_\kappa))^{-1}f(x_\kappa), \tag{2.4}$$

where α_κ is chosen to minimize the norm of $f(x_{\kappa+1})$, the sequence $\{x_\kappa\}$ is still not guaranteed to converge (to a solution of (2.1)).

Let x^* be a solution of (2.1). Suppose that $f'(x^*)$ is nonsingular. It is not difficult to see that the coefficient matrix of the variational equation of (2.3) at x^* is equal to the negative of the identity matrix. It follows that x^* is an asymptotically stable equilibrium point of (2.3). This fact manifests another local convergence property for the Newton method.

The differential system (2.3) can be derived from a topological point of view [25]. Let $f(x_0)=f_0\neq 0$. Let $L=L(f_0)$ be a half-line in R^n

$$L=\{tf_0: t>0\} \tag{2.5}$$

and consider the set $C(x_0)$ which is the connected component of x_0 in $f^{-1}(L)$. If f is sufficiently smooth, then generally $C(x_0)$ will be a smooth one-dimensional submanifold through x_0. It is well known in differential geometry that for $x\in C(x_0)$ the derivative $f'(x)$ maps the tangent space of the manifold $C(x_0)$ at x into that of the manifold L at $f(x)$. Therefore, if the derivative $f'(x)$ is invertible, then the tangent line to $C(x_0)$ at x should be parallel to the vector $(f'(x))^{-1}f(x)$. With some suitable scaling and orientation considerations, we end up with an equation such as (2.3).

Another way to derive the differential system (2.3) is to consider the homotopy equation

$$H(y)=f(x)-tf(x_0)=0, \tag{2.6}$$

where y represents the point (x, t) in R^{n+1}. Suppose that $0\in \mathrm{R}^n$ is a regular value for H. It is well known that the solution set of (2.6) is a one-dimensional sub-

manifold. Differentiating (2.6) with respect to the arc length, denoted by s, yields

$$f'(x)\frac{dx}{ds}-\frac{1}{t}f(x)\frac{dt}{ds}=0, \tag{2.7}$$
$$x(0)=x_0, \qquad t(0)=1.$$

If $f'(x)$ is nonsingular, then (2.7) and (2.3) are almost equivalent. But the regularity of (2.6) also enables us to handle the case when $f'(x)$ is of rank 1 deficiency. Solving system (2.6) is known variously as the continuation method, the Davidenko method, and the homotopy method. It is attractive because of its global and probabilistic features. For general references of the theory and its applications, the reader is referred to [1], [2], [5], [18], [26], [27], [34], [39].

If we formulate an analogous equation of (2.3) for the underdetermined system $H(y)=0$, we get

$$H'(y)\frac{dy}{ds}=-H(y). \tag{2.8}$$

Again, it is easy to see that all solutions of (2.8) will satisfy the equation $H(y(s))=e^{-s}H(y(0))$. Furthermore, it can be shown [36] that the one-dimensional solution set of (2.6) forms an asymptotically stable center manifold with respect to the system (2.8). If we consider the differential system determined from the least square solution of (2.8), i.e.,

$$\frac{dy}{ds}=-H'(y)^{+}H(y), \tag{2.9}$$

where $(H'(y))^{+}$ is the Moore–Penrose generalized inverse of $H'(y)$, then from the well-known fact

$$\text{Range}\,((H')^{+})=\text{Range}\,((H')^{T})=(\text{Kernel}\,(H'))^{\perp} \tag{2.10}$$

we see that the solution flow of (2.9) always moves in the direction that is perpendicular to the one-dimensional kernel space of H'. Note that the zero set of (2.6), in particular, is characterized by its tangent vectors which is in the kernel space of H' since $H'(y(s))\,dy/ds=0$. Thus in summary, we conclude that all solution flows of (2.9) converge globally and perpendicularly to the solution curve of (2.6).

The differential system (2.9) is different from (2.3) only in that the system (2.6) is underdetermined. So it is natural to consider the following Newton-like iteration scheme [20]:

$$y_{\kappa+1}=y_\kappa-(H'(y_\kappa))^{+}H(y_\kappa). \tag{2.11}$$

The resulting point $y_{\kappa+1}$ lies in the hyperplane normal to the tangent vector of the curve $\{y\in R^{n+1};\ H(y)=H(y_\kappa)\}$. Since the tangent vectors form a Lipschitzian vector field [33], we expect that (2.11) can be used to follow the implicitly defined curve of (2.6). In fact, the following theorem which is an analogue of the Kantorovich theorem for the classical Newton method can be established [6].

THEOREM 2.1. *Let $H: D\subset R^{n+1}\to R^n$ be a C^2-function such that*

$$\|H'(z_1)-H'(z_2)\|\leqq\alpha\,\|z_1-z_2\|$$

for every $z_1, z_2\in D$. Suppose $H(y^*)=0$ and $H'(y^*)$ is of full rank. Choose $0<\beta<(3-\sqrt{5})/2$ and define

$$M=\min\{2/(3\alpha\,\|(H')^{+}\|),\,\text{dist}\,(y^*,\delta D)\}.$$

If $0 < r < \beta M$ *is such that for every* y *in the ball* $B(y^*, r)$ *centered in* y^* *with radius* r *we have*

$$\|H(y)\| < \alpha\beta M^2/2,$$

then with any $y_0 \in B(y^*, r) \subset D$, *the scheme* (2.11) *is well-defined and converges geometrically to a solution of* (2.6).

The concept of multistep iterative methods has been proposed to obtain higher order of convergence to the solution of (2.1). A detailed discussion on this topic can be found in [37], which also contains a substantial amount of examples. We note that some of these multistep iterative methods also can be realized from the discretization of the differential system (2.3). As an example, the following iterative scheme [37], known to be in order three of convergence,

$$\begin{aligned} u_\kappa &= (f'(x_\kappa))^{-1} f(x_\kappa), \\ x_{\kappa+1} &= x_\kappa - (\tfrac{1}{2})\{u_\kappa + (f'(x_\kappa - u_\kappa))^{-1} f(x_\kappa)\}, \end{aligned} \tag{2.12}$$

can be regarded as a predictor-corrector method with unit steplength applied to (2.3). More specifically, the predictor is the explicit Euler method and the corrector is the implicit trapezoidal rule.

3. The steepest descent method. Consider the problem of minimizing the scalar-valued function $g: R^n \to R$. As in the Newton method, we may regard one step of the steepest descent method

$$x_{\kappa+1} = x_\kappa - \alpha_\kappa \operatorname{grad} g(x_\kappa) \tag{3.1}$$

as one explicit Euler step with steplength α_κ applied to the differential system

$$\frac{dx}{dt} = -\operatorname{grad} g(x), \qquad x(0) = x_0. \tag{3.2}$$

It is obvious that each strict relative minimizer of the function $g(x)$ is a local attractor of the system (3.2), whereas each strict relative maximizer is a local repeller. Therefore, we may adopt Branin's ideas in [3] to modify (3.2) to

$$\frac{dx}{dt} = (\pm 1) \operatorname{grad} g(x), \tag{3.3}$$

where the sign is changed whenever a critical point of $g(x)$ has been reached or $x(t)$ has moved outside a prescribed domain (say, the feasible domain). Following the solution flows of (3.3) offers a global optimization method. Another advantage is that the path determined from (3.1), which usually is noticed to be highly zigzag in character, is now replaced by a smoother path. Hence, the eccentricity problem becomes less significant.

4. The QR algorithm. Consider the linear algebraic eigenvalue problem

$$Ax = \lambda x, \tag{4.1}$$

where A is an n by n real matrix. Let $X_0 = A$. The unshifted QR algorithm generates a sequence of orthogonally similar matrices $\{X_\kappa\}$ from the scheme

$$X_\kappa = Q_\kappa R_\kappa, \quad X_{\kappa+1} = R_\kappa Q_\kappa, \quad \kappa = 0, 1, \cdots, \tag{4.2}$$

where each Q_κ represents an orthogonal matrix and R_κ an upper triangular matrix. Recently this sequence of matrices has been found [14], [29], [35], [41] to be intimately related to the solution flow of a homogeneous quadratic differential system, known

as the Toda lattice:

$$\frac{dX}{dt}=[X(t),\Pi_0(X(t))]=X(t)\Pi_0(X(t))-\Pi_0(X(t))X(t),\qquad X(0)=X_0, \tag{4.3}$$

where $\Pi_0(X)=(X^-)-(X^-)^T$ and X^- is the strictly lower triangular part of X.

The solution of (4.3) can be expressed as

$$X(t)=Q^T(t)X_0Q(t), \tag{4.4}$$

where $Q(t)$ is an appropriately defined family of orthogonal matrices. When sampled at integer times, this Toda flow gives exactly the same sequence of matrices as the QR algorithm applied to the initial matrix $\exp(X_0)$. The convergence properties of the QR algorithm can thus be explored by techniques from the theory of ordinary differential equations. Listed below are some established results in this respect. Any of these results can be readily interpreted for the dynamics of the QR algorithm. The interested reader may refer to the references for more detailed discussions.

THEOREM 4.1. *The manifold of upper triangular matrices with main diagonal entries in descending order is the stable center manifold of the Toda flow* [7].

THEOREM 4.2. *The Toda flow starting with a real normal matrix converges to a diagonal block matrix where for a real eigenvalue the associated block is of size one by one with that eigenvalue as its element and for complex-conjugate pairs of eigenvalues the associated block is of size two by two with the real part as its diagonal elements and the* (±) *imaginary part as its off-diagonal elements* [8].

THEOREM 4.3. *When the Toda flow is applied to a general real irreducible upper Hessenberg matrix, the solution flow can be only essentially convergent, that is, the solution flow tends to a quasi-upper triangular form* (*which is known as the real-valued version of the Schur theorem*) *but not all elements converge* [9].

Suppose now X_0 is an n by n complex matrix. Let $G(z)$ be an analytic function defined on a domain Ω which contains the spectrum of X_0. The initial value problem

$$\frac{dX}{dt}=[X,\Pi_1(G(X))]=X\Pi_1(G(X))-\Pi_1(G(X))X,\qquad X(0)=X_0, \tag{4.5}$$

with $\Pi_1(X)=(X^-)-(X^-)^*+i\,\mathrm{Im}\,(\mathrm{diag}\,(X))$, where $\mathrm{Im}\,(\mathrm{diag}\,(X))$ means the imaginary part of the diagonal matrix of X and

$$G(X)=\frac{1}{2\Pi i}\int_\Gamma G(\lambda)(\lambda I-X)^{-1}\,d\lambda, \tag{4.6}$$

where Γ is any contour that surrounds the spectrum of X in Ω, is a generalization of (4.3). It is shown in [7], [29] that this generalized Toda flow, when sampled at integer times, gives exactly the same sequence of matrices as the QR algorithm applied to the matrix $\exp(G(X_0))$. Therefore, if X_0 is nonsingular and $G(z)=\ln z$, then the QR algorithm can be completely recovered from the Toda flow. Setting $G(z)=s\ln z$, we obtain the QR power method [42].

We remark that a theory of LU flows as well as Cholesky flows can be developed along the same lines as the theory of Toda flows. The interested reader is referred to the review article [41].

5. The power method. Given a unit vector x_0 in R^n, the power method for a real n by n matrix A generates a sequence of unit vectors $\{x_k\}$ by

$$\begin{aligned} y_{k+1}&=Ax_k,\\ x_{k+1}&=y_{k+1}/\|y_{k+1}\|, \end{aligned} \tag{5.1}$$

for an appropriately chosen vector norm $\| \|$. It is well known that if A has a most dominant eigenvalue in the sense of magnitude, then the sequence $\{x_\kappa\}$, in general, converges to the eigenvector associated with that eigenvalue. This property has then brought about the so-called inverse power method and the Rayleigh quotient iterations [32].

Let B be an n by n real matrix. Suppose that B has a real eigenvalue λ^* that is no less than the real part of any other eigenvalues. Consider the following autonomous differential system on the unit sphere S^{n-1} in R^n:

$$\frac{du}{dt} = Bu - \langle u, Bu \rangle u, \tag{5.2}$$

where $\langle , \rangle$ means the usual inner product in R^n. The system above obviously has equilibrium points only at eigenvectors of B. Indeed, the exact solution of (5.2) with $u(0) = u_0 \in S^{n-1}$ is explicitly known, that is,

$$u(t) = e^{tB}u_0 / \langle e^{tB}u_0, e^{tB}u_0 \rangle^{1/2}. \tag{5.3}$$

From (5.3) it is not difficult to see that the positive semiorbit of (5.2), in general, converges to the eigenvector of B associated with λ^*. Now suppose that A is nonsingular and choose $B = \ln A$. Then (5.3) becomes

$$u(t) = \frac{A^t u_0}{\|A^t u_0\|_2}, \tag{5.4}$$

where by A^t we mean the matrix exponential $e^{t(\ln A)}$. It is now clear that the evaluations of (5.4) at positive integer times correspond precisely to the iterates of the classical power method, whereas the evaluations at negative integer times correspond to the iterates of the inverse power method.

The Rayleigh quotient iteration [31] for a matrix A generates a sequence of unit vectors $\{x_\kappa\}$ from a given unit vector x_0 according to the following scheme:

$$\begin{aligned} &\mu_\kappa = \rho(x_\kappa), \\ &y_{\kappa+1} = (A - \mu_\kappa I)^{-1} x_\kappa, \qquad x_{\kappa+1} = y_{\kappa+1} / \|y_{\kappa+1}\|_2, \end{aligned} \tag{5.5}$$

where $\rho(x) = \langle x, Ax \rangle / \langle x, x \rangle$ is the Rayleigh quotient of x with respect to A. Let $u(t)$ represent the solution of the system (5.2) which now is defined only piece by piece in the way that for all t in the interval $[k, k+1]$, B is chosen to be

$$B = \ln [(A - \rho_\kappa I)^{-1}] \tag{5.6}$$

with $\rho_\kappa = \rho(u(k))$. It then follows that, with $u(t)|_{t=k} = u(k)$,

$$u(k+1) = (A - \rho_\kappa I)^{-1} u(k) / \|(A - \rho_\kappa I)^{-1} u(k)\|. \tag{5.7}$$

In other words, the (piecewise differentiable) solution $u(t)$ of (5.2) with B defined by (5.6), is a continuous extension of the sequence (5.5), provided $x_0 = u(0)$.

Recall that the major subject of the Rayleigh quotient iterations is the speed-up of convergence by making $A - \mu_\kappa I$ nearly singular so that $(A - \mu_\kappa I)^{-1}$ has a most dominant eigenvalue. Given the fact that the two complex-valued functions $\ln [(z - c)^{-1}]$ and $(z - c)^2$ are "qualitatively" similar [4] near the singular point c, we can simulate the dynamics of the Rayleigh quotient iteration by considering the differential system (5.2) with

$$B = B(u) = [(A - \rho(u)I)^T (A - \rho(u)I)]^{-1}. \tag{5.8}$$

Let $\sigma(A)$ denote the spectrum of A. Obviously the resulting differential system (5.2) with B defined by (5.8) becomes singular at any point of the set $\Gamma = \{u \in S^{n-1};\ \rho(u) \in \sigma(A)\}$. But the remaining set $S^{n-1} - \Gamma$ can be shown [10] to be invariant under this system. Furthermore, along any solution flow $u(t)$ on the unit sphere, the residue function $r(t)$ with

$$r(t) = \|(A - \rho(u(t))I)u(t)\| \tag{5.9}$$

is nondecreasing. Using $r(t)$ as the Lyapunov function, we then are able to explore the global dynamics of system (5.2) with B defined by (5.8) as follows [10].

THEOREM 5.1. *Let $E = \{u \in S_{n-1} - \Gamma;\ u$ is an eigenvector of $B(u)\}$. The positive semiorbit of $u(t)$ either*

(a) *approaches the singular set Γ in finite time, or*

(b) *converges to an eigenvector of A as t goes to infinity, or*

(c) *has its w-limit set contained in E.*

Obviously the occurrence of any of the first two cases already provides essential information about eigenvalues of the matrix A. In [10], the set E was further explored and interpreted for real symmetric and normal matrices. The success of this simulation is evidenced by the fact that most of the properties concerning the dynamics of the differential system are almost parallel with those of the classical Rayleigh quotient iterations. The interested reader may refer to [10] and [31] to compare these established results.

A connection between the inverse power method and the Newton method is worth noting [13]. By imposing an additional normalization condition, we can formulate the linear algebraic eigenvalue problem (4.1) as a nonlinear algebraic equation

$$F(x, \lambda) = \begin{bmatrix} \lambda x - Ax \\ v^T x - 1 \end{bmatrix} = 0 \tag{5.10}$$

where the normalization vector v can be chosen in a number of ways but in general depends on x and λ. Solving (5.10) by Newton's method amounts to solving the linear system

$$\begin{bmatrix} \lambda_\kappa I - A, & x_\kappa \\ v_\kappa^T, & 0 \end{bmatrix} \begin{bmatrix} x_{\kappa+1} - x_\kappa \\ \lambda_{\kappa+1} - \lambda_\kappa \end{bmatrix} = -\begin{bmatrix} (\lambda_\kappa I - A)x_\kappa \\ v_\kappa^T x_\kappa - 1 \end{bmatrix} \tag{5.11}$$

or equivalently

$$(\lambda_\kappa I - A)x_{\kappa+1} = -(\lambda_{\kappa+1} - \lambda_\kappa)x_\kappa, \qquad v_\kappa^T x_{\kappa+1} = 1. \tag{5.12}$$

The algorithm is more conveniently formulated as

$$\begin{aligned} &(A - \lambda_\kappa I)y_{\kappa+1} = x_\kappa, \\ &x_{\kappa+1} = y_{\kappa+1}/(v_\kappa^T y_{\kappa+1}), \\ &\lambda_{\kappa+1} = \lambda_\kappa + 1/v_\kappa^T y_{\kappa+1}. \end{aligned} \tag{5.13}$$

From (5.13), we see that Newton's method applied to the nonlinear equation (5.10) is equivalent to the inverse power method.

6. The SVD algorithm. It is well known that the singular value decomposition (SVD) of a matrix A is closely related to the Schur decomposition of the symmetric matrix A^TA. So Golub and Kahan [21] proposed the following algorithm for the

computation of the SVD of an m by $n (m \geqq n)$ real matrix A:

(a) Use a sequence of Householder transformations to reduce A to upper bidiagonal form, that is,

$$U_B^T A V_B = \left| \frac{B}{0} \right|, \tag{6.1}$$

where B is an n by n upper bidiagonal matrix.

(b) Apply a sequence of implicit-shift QR steps to the tridiagonal matrix $B^T B$ to compute the SDV of B.

We are interested in a continuous analogue of the iteration that is taking place in part (b). Toward this end, we consider the one-parameter family of matrices

$$Y(t) = U(t) B V(t), \tag{6.2}$$

where $U(t)$ and $V(t)$ are families of orthogonal matrices to be specified so that $Y(t)$ maintains the bidiagonal form for all t. Differentiating (6.2) with respect to t yields

$$\frac{dY}{dt} = YN - MY, \tag{6.3}$$

where, due to the orthogonality of U and V, the two matrices

$$\begin{aligned} M(t) &= -\left(\frac{dU(t)}{dt}\right) U^T(t), \\ N(t) &= V^T(t)\left(\frac{dV(t)}{dt}\right) \end{aligned} \tag{6.4}$$

are necessarily skew-symmetric. It is clear from (6.3) and (6.4) that $Y(t)$, $U(t)$, and $V(t)$ will be unambiguously determined from the specifications of $M(t)$ and $N(t)$. In [11], the following definitions are introduced:

$$\begin{aligned} M(t) &= \Pi_0(Y(t)Y^T(t)), \\ N(t) &= \Pi_0(Y^T(t)Y(t)). \end{aligned} \tag{6.5}$$

In this case, (6.2) becomes a system of autonomous, homogeneous cubic differential equations

$$\begin{aligned} \frac{dy_{i,i}}{dt} &= y_{i,i}(y_{i,i+1}^2 - y_{i-1,i}^2) \quad \text{for } n \geqq i \geqq 1, \\ \frac{dy_{i,i+1}}{dt} &= y_{i,i+1}(y_{i+1,i+1}^2 - y_{i,i}^2) \quad \text{for } n-1 \geqq i \geqq 1, \end{aligned} \tag{6.6}$$

where we denote $y_{0,1} = y_{n,n+1} = 0$.

The asymptotic behavior of $Y(t)$ defined by (6.6), as well as the corresponding $U(t)$ and $V(t)$, can be understood from the theory of the Toda lattice. Indeed, $V(t)$ and $U^T(t)$ correspond to the matrix $Q(t)$ in (4.4) if $X(t)$ in (4.3) is replaced by $Y^T(t)Y(t)$ and $Y(t)Y^T(t)$, and X_0 is replaced by $B^T B$ and BB^T, respectively. It follows from Theorem 4.2 that both $U(t)$ and $V(t)$ converge to constant matrices, say $U(t) \to U_*$ and $V(t) \to V_*$, and $X(t)$ converges to a diagonal matrix, say $X(t) \to \Sigma$, as t goes to plus infinity. The matrix B then has a singular value decomposition:

$$B = U_* \Sigma V_*^T. \tag{6.7}$$

We conclude that the system (6.6) is related to part (b) of the Golub–Kahan SVD algorithm almost in the same way as the Toda lattice is related to the QR algorithm.

7. The QZ algorithm. The development of the QZ algorithm is based on the generalized Schur decomposition theorem [28], that is, given any two matrices A and B, there exist unitary matrices Q and Z such that QAS and QBZ both are upper triangular. The algorithm is designed deliberately to accomplish the following two tasks for real matrices:

(a) Use orthogonal transformations to reduce simultaneously A to upper Hessenberg form and B to upper triangular form.
(b) Apply a QR-analogue algorithm to reduce A iteratively to upper quasi-triangular form while the triangularity of B is preserved.

A differential system whose solution is an analogue of the iteration taking place in (b) can be developed. The approach is similar to that discussed in the previous section. We shall assume, henceforth, that A is upper Hessenberg and that B is upper triangular and nonsingular. Consider simultaneously the two one-parameter families of matrices

$$\begin{aligned} X(t) &= Q(t)AZ(t), \\ Y(t) &= Q(t)BZ(t), \end{aligned} \tag{7.1}$$

where $Q(t)$ and $Z(t)$ are orthogonal matrices to be specified with $Q(0) = Z(0) = I$. Differentiating (7.1) with respect to t will yield equations similar to (6.3) and (6.4). In order to maintain the upper Hessenberg form for $X(t)$ and the upper triangular form for $Y(t)$ for all t, some extra conditions must be imposed on the matrices $Q(t)$ and $Z(t)$. In [12], the solutions of the following two initial value problems were found to fulfill these requirements:

$$\begin{aligned} \frac{dQ(t)}{dt} &= -M(t)Q(t), \qquad Q(0) = I, \\ \frac{dZ(t)}{dt} &= Z(t)N(t), \qquad Z(0) = I, \end{aligned} \tag{7.2}$$

where $M(t)$ and $N(t)$ are two tridiagonal, skew-symmetric matrices defined by

$$\begin{aligned} M(t) &= \Pi_0(X(t)Y^{-1}(t)), \\ N(t) &= \Pi_0(Y^{-1}(t)X(t)). \end{aligned} \tag{7.3}$$

In this case, $X(t)$ and $Y(t)$ correspond to solution flows of the autonomous system

$$\begin{aligned} \frac{dX}{dt} &= X\Pi_0(Y^{-1}X) - \Pi_0(XY^{-1})X, \\ \frac{dY}{dt} &= Y\Pi_0(Y^{-1}X) - \Pi_0(XY^{-1})Y, \\ X(0) &= A, \qquad Y(0) = B. \end{aligned} \tag{7.4}$$

The system (7.4) is again closely related to the Toda lattice. Indeed, the matrices $Q^T(t)$ and $Z(t)$ defined by (7.2) correspond, respectively, to the cases when the Toda lattice (4.3) is applied to the matrices $X(t)Y^{-1}(t)$ and $Y^{-1}(t)X(t)$ with initial values AB^{-1} and $B^{-1}A$. It follows from the theory of the Toda lattice that under suitable conditions both $X(t)$ and $Y(t)$ converge to constant upper triangular matrices. In

other words, the solution to (7.2) offers a continuous approximation to the generalized Schur decomposition of the pencil $\{A, B\}$. It is amazing that all the plane rotations involved in the QZ algorithm to maintain certain matrix structures are now implicitly retained in following the flow defined by (7.4).

8. The linear stationary methods. Most of the basic linear stationary methods for solving the linear system

$$Ax = b, \tag{8.1}$$

where A is a real n by n nonsingular matrix and $b \in \mathbb{R}^n$, may be expressed in the form

$$x_{\kappa+1} = Gx_\kappa + c, \qquad \kappa = 0, 1, 2, \cdots, \tag{8.2}$$

where G is the real n by n iteration matrix for the method and c is an associated known vector. In general, the above quantities are related by

$$G = I - Q^{-1}A, \qquad c = Q^{-1}b \tag{8.3}$$

for some nonsingular matrix Q which is called a splitting matrix. It is clear that x^* is a fixed point to the iteration (8.2) if and only if x^* is the unique solution to (8.1). A necessary and sufficient condition for convergence of (8.2) is that the spectral radius $p(G) < 1$.

We may regard (8.2) as one Euler step with unit stepsize applied to the linear differential system

$$\frac{dx}{dt} = (G - I)x + c = (-Q^{-1}A)x + c. \tag{8.4}$$

But then we only need the assumption that all eigenvalues of $G - I$ have negative real parts to ensure that the unique solution x^* of (8.1) is a global attractor to all flows of (8.4). This requirement obviously is much weaker than that for the general iterative scheme (8.2). In fact, given a nonsingular matrix A, there always exists a nonsingular matrix Q such that the spectrum of the product $Q^{-1}A$ is equal to any prescribed set of n nonzero real numbers. In our case, we certainly want to control these numbers to be positive (to ensure convergence), nearly equal (to avoid stiffness) and relatively large (to reach the steady state faster).

Solving (8.4) by a numerical method amounts to a new iterative scheme. For example, if the trapezoidal rule

$$x_{\kappa+1} = x_\kappa + (h/2)(f_\kappa + f_{\kappa+1}) \tag{8.5}$$

with stepsize h is applied to solve (8.4), then due to the linearity of (8.4) we obtain

$$x_{\kappa+1} = [I - (h/2)(G - I)]^{-1}[I + (h/2)(G - I)]x_\kappa + [I - (h/2)(G - I)]^{-1}hc. \tag{8.6}$$

We remark that implicit schemes like (8.6) are not practical in general because of the involvement of the inverse. But it is interesting to note that the iteration matrix in (8.6) is precisely the (1, 1)-pair Padé approximation of the matrix $\exp[(h/2)(G - I)]$. If all eigenvalues of $G - I$ have negative real parts, then the iteration (8.6) converges for all $h > 0$. Solving the differential system (8.4) by higher-order methods, such as the Adams method or the Runge–Kutta method, usually results in highly complicated multistep iterative schemes.

Chebyshev and conjugate gradient acceleration are two special methods of a general procedure, known as polynomial acceleration [24], for accelerating the rates of convergence for the basic iterative scheme (8.1). These methods generate a sequence

of vectors $\{x_n\}$ by using a three-term relation:

$$\begin{aligned} x_1 &= \beta_1(Gx_0 + c) + (1-\beta_1)x_0, \\ x_{\kappa+1} &= \alpha_{\kappa+1}\{\beta_{\kappa+1}(Gx_\kappa + c) + (1-\beta_{\kappa+1})x_\kappa\} + (1-\alpha_{\kappa+1})x_{\kappa-1}, \end{aligned} \tag{8.7}$$

where α_κ, β_κ are properly defined real numbers. By rearranging terms in (8.7), we realize that this relation can be expressed as

$$\begin{aligned} x_1 &= x_0 + \beta_1 f_0, \\ x_{\kappa+1} &= \alpha_{\kappa+1}x_\kappa + (1-\alpha_{\kappa+1})x_{\kappa-1} + \alpha_{\kappa+1}\beta_{\kappa+1}f_\kappa, \end{aligned} \tag{8.8}$$

with $f_\kappa = (G - I)x_\kappa + c$. In other words, the polynomial acceleration procedure described in (8.7) can be regarded as the application of the explicit, variable coefficient two-step method (8.8) to the differential system (8.4). This observation is especially true for the Chebyshev acceleration since β_κ is a constant and α_κ converges to a constant as κ goes to infinity.

The context of a "higher order of accuracy" method may be different from that of a "higher order of convergence" method. The former follows the solution curve of (8.4) carefully (and hence may be slower) which eventually leads to the desired solution of (8.1). The latter, in constrast, may be of fairly low order in the sense of solving the differential equation. As an example, it can be shown easily that the scheme (8.8) can be of order one only.

REFERENCES

[1] E. ALLGOWER, *A survey of homotopy method for smooth mappings*, in Numerical Solution of Nonlinear Equations, Lecture Notes in Math. 878, 1980, pp. 1–29.

[2] E. ALLGOWER AND K. GEORG, *Simplicial and continuations methods for approximating fixed points and solutions to systems of equations*, SIAM Rev., 22 (1980), pp. 28–85.

[3] T. H. BRANIN, JR., *Widely convergent method for finding multiple solutions of simultaneous nonlinear equations*, IBM J. Res. Develop., 16 (1972), pp. 504–522.

[4]. T. BRAUER AND J. NOHEL, *Qualitative Theory of Ordinary Differential Equations*, W. A. Benjamin, New York, 1969.

[5] S. N. CHOW, J. MALLET-PARET, AND J. A. YORKE, *Finding zeros of maps: homotopy methods that are constructive with probability one*, Math. Comp., 32 (1978), pp. 887–899.

[6]. M. T. CHU, *On a numerical treatment for the curve tracing of the homotopy method*, Numer. Math., 42 (1983), pp. 323–329.

[7] ———, *The generalized Toda flow, the QR algorithm and the center manifold theorem*, SIAM J. Algebraic Discrete Methods, 5 (1984), pp. 187–210.

[8] ———, *On the global convergence of the Toda lattice for real normal matrices and its applications to the eigenvalue problems*, SIAM J. Math. Anal., 15 (1984), pp. 98–103.

[9] ———, *Asymptotic analysis of the Toda lattice on diagonalizable matrices*, Nonlinear Anal. Theory Methods Appl., 9 (1985), pp. 193–201.

[10] ———, *Curves on S^{n-1} that lead to eigenvalues or their means of a matrix*, SIAM J. Algebraic Discrete Methods, 7 (1986), pp. 425–432.

[11] ———, *A differential equation approach to the singular value decomposition of bidiagonal matrices*, Linear Algebra Appl., 80 (1986), pp. 71–79.

[12] ———, *A continuous approximation to the generalized Schur's decomposition*, Linear Algebra Appl., 78 (1986), pp. 119–132.

[13] L. COLLATZ, *Functional Analysis and Numerical Mathematics*, Academic Press, New York, 1966.

[14] P. DEIFT, T. NANDA, AND C. TOMEI, *Differential equations for the symmetric eigenvalue problem*, SIAM J. Numer. Anal., 20 (1983), pp. 1–22.

[15] J. E. DENNIS, JR. AND J. MORÉ, *Quasi-Newton methods, motivation and theory*, SIAM Rev., 19 (1977), pp. 46–89.

[16] D. K. FADDEEV AND V. N. FADDEEVA, *Computational Methods of Linear Algebra*, W.H. Freeman, San Francisco, 1963.

[17] J. D. F. FRANCIS, *The QR transformation, a unitary analogue to the LR transformation, Parts* I *and* II, Comput. J., 4 (1961), pp. 265–273, 332–345.
[18] C. B. GARCIA AND W. I. ZANGWILL, *Pathways to Solutions, Fixed Points, and Equilibria*, Prentice–Hall, Englewood Cliffs, NJ, 1981.
[19] K. GEORG, *Numerical integration of the Davidenko equation*, in Numerical Solution of Nonlinear Equations, Lecture Notes in Math. 878, 1980, pp. 128–161.
[20] P. E. GILL, W. MURRAY, AND M. H. WRIGHT, *Practical Optimization*, Academic Press, London, 1981.
[21] G. H. GOLUB AND W. KAHAN, *Calculating the singular values and pseudoinverse of a matrix*, SIAM J. Numer. Anal., 2 (1965), pp. 205–224.
[22] G. H. GOLUB AND C. REINSCH, *Singular value decomposition and least square solutions*, Numer. Math., 14 (1970), pp. 134–151.
[23] G. H. GOLUB AND C. F. VAN LOAN, *Matrix Computations*, Johns Hopkins University Press, Baltimore, MD, 1983.
[24] L. A. HAGEMAN AND D. M. YOUNG, *Applied Iterative Methods*, Academic Press, New York, 1981.
[25] M. W. HIRSCH AND S. SMALE, *On algorithms for solving* $f(x) = 0$, Commun. Pure Appl. Math., 32 (1979), pp. 281–312.
[26] R. B. KEARFORT, *A derivative-free arc continuation method and a bifurcation technique*, in Numerical Solution of Nonlinear Equations, Lecture Notes in Math. 878, 1980, pp. 182–198.
[27] H. B. KELLER, *Global homotopies and Newton methods*, in Recent Advances in Numerical Analysis, C. de Boor and G. Golub, eds., Academic Press, New York, 1978, pp. 73–94.
[28] C. B. MOLER AND G. W. STEWART, *An algorithm for the generalized matrix eigenvalue problems*, SIAM J. Numer. Anal., 10 (1973), pp. 241–256.
[29] T. NANDA, *Isospectral flows on band matrices*, Ph.D. thesis, New York University, New York, 1982.
[30] J. M. ORTEGA AND W. C. RHEINBOLDT, *Iterative Solution of Nonlinear Equations in Several Variables*, Academic Press, New York, 1970.
[31] B. N. PARLETT, *The Rayleigh quotient iteration and some generalizations for nonnormal matrices*, Math. Comp., 28 (1974), pp. 679–693.
[32] ———, *The Symmetric Eigenvalue Problem*, Prentice–Hall, Englewood Cliffs, NJ, 1978.
[33] W. C. RHEINBOLDT, *Solution fields of nonlinear equations and continuation methods*, SIAM J. Numer. Anal., 17 (1980), pp. 221–237.
[34] W. V. RHEINBOLDT AND J. V. BURKARDT, *Algorithm* 596, *A program for a locally parameterized continuation process*, ACM Trans. Math. Software, 9 (1983), pp. 236–241.
[35] W. W. SYMES, *The QR algorithm and scattering for the finite nonperiodic Toda lattice*, Phys. D, 4 (1982), pp. 275–280.
[36] K. TENABE, *Continuous Newton-Raphson method of solving an underdetermined system of nonlinear equations*, Nonlinear Anal. Theory Methods Appl., 3 (1979), pp. 495–503.
[37] J. F. TRAUB, *Iterative Methods for the Solution of Equations*, Prentice–Hall, Englewood Cliffs, NJ, 1964.
[38] K. S. VARGA, *Matrix Iterative Analysis*, Prentice–Hall, Englewood Cliffs, NJ, 1962.
[39] H. J. WACKER, *Continuation Methods*, Academic Press, New York, 1978.
[40] D. S. WATKINS, *Understanding the QR algorithm*, SIAM Rev., 24 (1982), pp. 427–440.
[41] ———, *Isospectral flows*, SIAM Rev., 26 (1984), pp. 379–391.
[42] J. H. WILKINSON, *The Algebraic Eigenvalue Problem*, Clarendon Press, Oxford, 1965.
[43] J. H. WILKINSON AND C. REINSCH, *Handbook for Automatic Computation, Vol.* 2, *Linear Algebra*, Springer-Verlag, New York, 1971.