

WHAT STABILITY SPECTRA DO GENERAL LINEAR METHODS APPROXIMATE?

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Dedicated to the memory of Timo Eirola.

ABSTRACT. We generalize the theory of underlying one-step methods to strictly stable general linear methods (GLMs) solving time-dependent ordinary differential equations (ODEs) that satisfy a global Lipschitz condition. We combine this theory with the Lyapunov and Sacker-Sell spectral stability theory for one-step methods developed in [22, 23, 24] to analyze the Lyapunov stability of a strictly stable GLM solving a time-dependent linear ODE. These results are applied to develop a stability diagnostic for the solution of linear ODEs by strictly stable GLMs.

1. Introduction. 'What do multistep methods approximate?' This question is one that beleaguers many researchers of multistep discretizations of ordinary differential equation (ODE) initial value problems (IVPs) due to the fact that the local truncation error of a k -step multistep method depends on the previous k steps. For autonomous ODEs, two classic papers, [16] and [19], provide an answer to this question by applying invariant manifold theory for maps to relate the numerical solution produced by a multistep method to the flow of the differential equation it is approximating. This facilitates the use of discrete dynamical systems theory which is important in the context of structure preserving methods [17] and time-dependent (nonautonomous) stability theory [22, 23, 24]. The focus of this paper is to use the spirit and technique of [16] and [19] together with invariant manifold theory for nonautonomous difference equations to develop a stability theory for general linear methods (GLMs) solving uniformly exponentially stable, nonautonomous, linear ODEs.

Our contribution in this work is twofold. We first apply invariant manifold theory for nonautonomous difference equations to prove Theorem 3.1. This theorem states that for a strictly stable GLM solving a nonautonomous ODE that satisfies a global

2010 *Mathematics Subject Classification.* Primary: 65L20, 65L07; Secondary: 65Q10.

Key words and phrases. general linear methods, nonautonomous differential equations, Lyapunov exponents, Sacker-Sell spectrum, invariant manifold.

This research was supported in part by NSF grant DMS-1419047.

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Lipshitz condition, there is a time-independent change of variables and a unique one-step method (called the underlying one-step method) so that if the step-size is sufficiently small, then the graph of the one-step method is a global, exponentially attractive, invariant manifold of the discrete-time system resulting from the change of variables. Theorem 3.1 generalizes the technique of characterizing the approximation properties of a GLM by its underlying one-step method to ODEs that are nonautonomous.

The second contribution of this paper is to use Theorem 3.1 and the Lyapunov and Sacker-Sell spectrum based stability theory for one-step methods solving nonautonomous ODE IVPs developed in [22, 23, 24] to prove Theorem 3.3. By stability we shall always be referring to the concept of time-dependent Lyapunov stability unless otherwise specified. Theorem 3.1 states that for all sufficiently small step-sizes the numerical solution by a strictly stable GLM of a nonautonomous linear ODE with Sacker-Sell spectrum bounded above by zero decays at a uniform exponential rate. This provides a way of analyzing the numerical stability of time-dependent linear ODEs that may fail to satisfy a one-sided Lipshitz condition or the uniform decay estimates of AN- and B-stability theory. Subsequently, we apply Theorem 3.3 to develop a stability diagnostic to determine when a strictly stable GLM fails to produce a decaying numerical solution to a linear ODE whose Sacker-Sell spectrum is bounded above by zero.

The use of invariant manifold theory to characterize the approximation properties of a multistep method by an associated one-step method was pioneered in [19] and [16]. The results of [19] were extended to GLMs in [25] using the invariant manifold theory for maps developed in [26]. The techniques used in these works are only rigorously justified for autonomous differential equations which is probably due to the fact that at the time there was not a well-established theory for invariant manifolds of nonautonomous differential and difference equations. This subject has since been one of intensive investigation (see [1, 3, 4, 5, 7]) that we use in the development of our theoretical results.

The stability of the numerical solution of an ODE IVP by a multistep method is a challenging and important problem dating back at least to the investigations by Dahlquist in [8, 9, 10]. For time-dependent trajectories the well-established stability theories (e.g. AN-stability, B-stability, algebraic stability) give conditions on a GLM so that with no step-size restriction it preserves the asymptotic decay of a trajectory that is uniformly decaying. This restricts the analysis to implicit methods and these theories do not provide a way to restrict the step-size for a given convergent or strictly stable GLM solving non-uniformly decaying problems; no obvious analog of linear stability domains exists for time-dependent problems. In this paper we exploit the Lyapunov and Sacker-Sell spectral stability theory for one-step methods developed in [22, 23, 24] to characterize the stability of a strictly stable GLM solving a nonautonomous linear ODE whose Sacker-Sell spectrum is bounded above by zero by analyzing the stability of its underlying one-step method.

The remainder of this paper is organized as follows. In Section 2 we introduce some preliminary notation and cover some background material on the approximation of Lyapunov and Sacker-Sell spectral intervals based on smooth QR decompositions of fundamental matrix solutions. In Section 3.1 we prove an existence theorem (Theorem 3.1) for underlying one-step methods. In Section 3.2 we apply Theorem 3.1 to prove Theorem 3.3 which relates the stability of a strictly stable GLM to the Lyapunov and Sacker-Sell spectrum of its underlying one-step method.

In Section 4 we present the results of two experiments showing how the theory developed in Section 3 can be used as a stability diagnostic for strictly stable GLMs solving linear ODEs. The paper is concluded with some final remarks in Section 5.

2. Preliminaries. In this section we introduce some notation and terminology and state some basic results from the theory of Lyapunov and Sacker-Sell spectra and their approximation using QR based methods. For the remainder of this work we let $\|\cdot\|$ be a norm on \mathbb{R}^d and use the same symbol for the induced matrix norm. We may sometimes drop writing the explicit t dependence of matrices and functions when their time dependence is clear from the context. Whenever we use the word stability we are referring to time-dependent Lyapunov stability. Consider the ODE IVP

$$\begin{cases} \dot{x} = f(x, t) \\ x(t_0) = x_0 \end{cases} \quad (1)$$

where $t_0 \in \mathbb{R}$ and $f : (t_0, \infty) \times \mathbb{R}^d \rightarrow \mathbb{R}^d$. We consider numerical solutions of (1) by a fixed step-size, k -step, s -stage general linear method

$$\begin{cases} G_n = (U \otimes I)X_n + h(C \otimes I)F_n \\ X_{n+1} = (V \otimes I)X_n + h(D \otimes I)F_n \end{cases} \quad (2)$$

where $h > 0$ is the size of the time step (the step-size) with $t_n = t_0 + nh$ and $U = (u_{i,j}) \in \mathbb{R}^{s \times k}$, $V = (v_{i,j}) \in \mathbb{R}^{k \times k}$, $C = (c_{i,j}) \in \mathbb{R}^{s \times s}$, $D = (d_{i,j}) \in \mathbb{R}^{k \times s}$, and $F_n = (f_{n,1}, \dots, f_{n,s})^T \in \mathbb{R}^{ds}$ where $f_{n,i} = f(g_{n,i}, t_n + \xi_i h)$ for some real constants ξ_i and $i = 1, \dots, s$. We also let $G_n = (g_{n,1}^T, \dots, g_{n,s}^T)^T \in \mathbb{R}^{ds}$. The symbol I is the $d \times d$ identity matrix and \otimes denotes the Kronecker matrix product which defines an algebraic operation on matrices $A = (a_{i,j}) \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{p \times q}$ for positive integers m, n, p, q by the rule

$$A \otimes B = \begin{bmatrix} a_{1,1}B & \dots & a_{1,n}B \\ \vdots & \ddots & \vdots \\ a_{m,1}B & \dots & a_{m,n}B \end{bmatrix}$$

An important property of Kronecker products we use in Section 3 is that if A and B are invertible, then $(A \otimes B)^{-1} = (A^{-1} \otimes B^{-1})$. We always consider general linear methods (2) that are in Nordsieck form, that is, the vector $X_n = (x_n^1, \dots, x_n^k)^T \in \mathbb{R}^{dk}$ is such that

$$x_n^i = \sum_{j=0}^p q_{i,j} x^{(j)}(t_n) + \mathcal{O}(h^{p+1}), \quad i = 1, \dots, k, \quad n \geq 0$$

where each $q_{i,j} \in \mathbb{R}$, $x^{(j)}(t)$ denotes the j^{th} derivative of the exact solution $x(t; x_0)$ of (1), and p is the order of the local truncation error of the method. Well-known time-stepping methods such as linear multistep and Runge-Kutta methods are examples of GLMs in addition to many predictor-correct and implicit-explicit methods. A general linear method (2) is said to be strictly stable if 1 is an eigenvalue of V and all the other eigenvalues of V have modulus strictly less than 1. Strict stability is not a particularly stringent hypothesis to place on a GLM since all Runge-Kutta methods are strictly stable as are many popular linear multistep methods such as BDF1-6 and the Adams-Bashforth methods. We refer readers to [18] for an excellent overview of the theory of general linear methods.

Assume that $f(x, t)$ is continuously differentiable. Associated to the solution $x(t; x_0)$ of (1) is the linear variational equation

$$\dot{x} = D(x(t; x_0), t)x \equiv A(t)x, \quad t \geq t_0, \quad D = \frac{\partial}{\partial x}. \quad (3)$$

The stability of the zero solution of (3) in general does not depend on the time-dependent eigenvalues of $A(t)$ which has motivated the development of several alternative stability spectra. The two spectra we consider in this work are the Lyapunov spectrum, first considered in [20], and the Sacker-Sell spectrum, which was first developed in [21].

We say that (3) is uniformly exponentially stable if for any fundamental matrix solution $X(t)$, there exists $K > 0$ and $\alpha > 0$ so that

$$\|X(t)X(s)^{-1}\| \leq Ke^{-\alpha(t-s)}, \quad t \geq s \geq t_0.$$

Analogously, we say that (3) is exponentially stable if for any fundamental matrix solution $X(t)$, there exists $K > 0$ and $\alpha > 0$ so that

$$\|X(t)\| \leq Ke^{-\alpha t}.$$

A sufficient condition for uniform exponential stability of the zero solution is that the Sacker-Sell spectrum is bounded above by zero and a sufficient condition for exponential stability of the zero solution is that the Lyapunov spectrum is bounded above by zero.

Using (3) we can express (1) in linear inhomogeneous form

$$\begin{cases} \dot{x} = A(t)x + N(t) \\ x(t_0) = x_0 \end{cases} \quad (4)$$

where $N(t)$ is bounded. Uniform exponential stability of (3) implies that the solution of (4) is uniformly exponentially stable. A similar implication is not true if is only exponentially stable.

The QR theory for the approximation of the Lyapunov and Sacker-Sell spectrum of (3), developed and analyzed extensively in [12, 13, 14, 15], is based on the construction of a time-dependent orthogonal change of variables. Let $Q(t)$ be a solution of the differential equation

$$\dot{Q}(t) = Q(t)S(Q(t), A(t)), \quad S(Q, A)_{ij} = \begin{cases} (Q^T A Q)_{i,j}, & i > j \\ 0, & i = j \\ -(Q^T A Q)_{i,j}, & i < j \end{cases} \quad (5)$$

where $A(t)$ comes from (3). Under the change of variables $x = Q(t)y$, the system

$$\dot{y} = B(t)y, \quad B = Q^T A Q - Q^T \dot{Q} \quad (6)$$

is such that $B(t)$ is upper triangular for all t . We refer to the system (6) as a corresponding upper triangular system to (3) and the Lyapunov and Sacker-Sell spectra of these two systems coincide. The endpoints of the Sacker-Sell spectrum can be computed using the diagonal of $B(t)$ so long as the coefficient matrix $A(t)$ of (3) is bounded and continuous. To accurately compute the endpoints of the Lyapunov spectrum we must assume in addition that (3) has an integral separation structure; without this additional assumption the Lyapunov spectrum may be unstable with respect to $L^\infty(t_0, \infty)$ perturbations of $A(t)$. The following theorem summarizes how to compute end-points of the Lyapunov and Sacker-Sell spectrum of (3) in terms of the diagonal entries of $B(t)$

Theorem 2.1 (Theorems 2.8, 5.1, 5.5, 6.1 of [12]). *Let $B : (t_0, \infty) \rightarrow \mathbb{R}^{d \times d}$ be bounded, continuous, and upper triangular and let $\Sigma_{ED} = \cup_{i=1}^d [\alpha_i, \beta_i]$ denote the Sacker-Sell spectrum of $\dot{y}(t) = B(t)y(t)$. The endpoints of the spectral intervals are given by*

$$\alpha_i = \liminf_{H \rightarrow 0} \inf_{t \geq t_0} \frac{1}{H} \int_t^{t+H} B_{i,i}(\tau) d\tau, \quad \beta_i = \limsup_{H \rightarrow \infty} \sup_{t \geq t_0} \frac{1}{H} \int_t^{t+H} B_{i,i}(\tau) d\tau, \quad i = 1, \dots, d. \quad (7)$$

Furthermore, there exists $H > 0$ so that if $t - s > H$, then

$$\alpha_i = \inf_{t \geq t_0} \frac{1}{t - s} \int_s^t B_{i,i}(\tau) d\tau, \quad \beta_i = \sup_{t \geq t_0} \frac{1}{t - s} \int_s^t B_{i,i}(\tau) d\tau, \quad i = 1, \dots, d. \quad (8)$$

Assume that $B : (t_0, \infty) \rightarrow \mathbb{R}^{d \times d}$ has an integral separation structure and let $\Sigma_L = \cup_{i=1}^d [\eta_i, \mu_i]$ denote the Lyapunov spectrum of $\dot{y} = B(t)y$. Then the Lyapunov spectrum of $\dot{y}(t) = B(t)y(t)$ is continuous with respect to $L^\infty(t_0, \infty)$ perturbations of $B(t)$ and the endpoints of the Lyapunov spectral intervals are given by

$$\eta_i = \liminf_{t \rightarrow \infty} \frac{1}{t - t_0} \int_{t_0}^t B_{i,i}(\tau) d\tau, \quad \mu_i = \limsup_{t \rightarrow \infty} \frac{1}{t - t_0} \int_{t_0}^t B_{i,i}(\tau) d\tau, \quad i = 1, \dots, d. \quad (9)$$

□

A similar theorem can be proved for discrete-time linear systems (see [6, 27] and [23]) which are in turn used to prove the main results of [23] and Section 3.2 of [22] which are summarized in the following theorem. This result is fundamentally based on the observation that the numerical solution of a nonautonomous linear ODE $\dot{z} = C(t)z$ by a one-step method takes the form $z_{n+1} = \Phi^C(n)z_n$.

Theorem 2.2. *Let $x_{n+1} = \Phi^A(n; h)x_n$ denote the numerical solution to (3) by a one-step method with local truncation error of order $p \geq 1$ with step-size $h > 0$ and initial condition x_0 . Let $\Sigma_L^A = \cup_{i=1}^n [\eta_i^A, \mu_i^A]$ and $\Sigma_{ED}^A = \cup_{i=1}^d [a_i^A, b_i^A]$ denote the Lyapunov and Sacker-Sell spectrum respectively of the discrete nonautonomous difference equation $x_{n+1} = \Phi^A(n; h)x_n$ and let $\Sigma_L = \cup_{i=1}^n [\eta_i, \mu_i]$ and $\Sigma_{ED}^A = \cup_{i=1}^d [a_i, b_i]$ denote the Lyapunov and Sacker-Sell spectrum of (3).*

1. *If the coefficient matrix is bounded and continuous, then for every $\varepsilon > 0$ there exists $h^* > 0$ so that if $h < h^*$, then $|a_i^A - a_i| < \varepsilon$ and $|b_i^A - b_i| < \varepsilon$ for $i = 1, \dots, d$.*
 2. *If (3) has an integral separation structure, then there exists $h^* > 0$ so that if $h < h^*$, then $|a_i^A - a_i| = \mathcal{O}(h^{p+1})$ and $|b_i^A - b_i| = \mathcal{O}(h^{p+1})$ for $i = 1, \dots, d$.*
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We apply Theorem 2.2 in Section 3.2 to prove a stability result for strictly stable GLMs solving nonautonomous, linear ODEs with Sacker-Sell spectrum bounded above by zero.

3. Main Results.

3.1. Nonautonomous invariant manifold reduction. In this section we prove that there exists a unique underlying one-step method for a strictly stable GLM approximating the solution of nonautonomous ODE whose nonlinear part satisfies a global Lipschitz condition. Throughout we consider a strictly stable, k -step, and s -stage general linear method (2) in Nordsieck form that we denote by \mathcal{M} and we

assume that \mathcal{M} has local truncation error of order $p \geq 1$. We let $P \in \mathbb{R}^{k \times k}$ be a matrix so that $E = P^{-1}VP$ is of the form $E = \begin{bmatrix} 1 & \\ & E_{2,2} \end{bmatrix}$ where the eigenvalues of $E_{2,2} \in \mathbb{R}^{k-1 \times k-1}$ all have modulus strictly less than 1 (E may be taken to be e.g. the real Jordan form of V). The main result of this section is the following theorem.

Theorem 3.1. *Consider the following ODE*

$$\dot{x} = A(t)x + N(x, t) \quad (10)$$

where $N(x, t)$ satisfies the Lipschitz condition that there exists $K > 0$ so that for all $x, y \in \mathbb{R}^d$ we have

$$\|N(x, t) - N(y, t)\| \leq K\|x - y\| \quad (11)$$

Assume that $A(t)$ is bounded, $N(0, t) = 0$, $DN(0, t) = 0$, and both $A(t)$ and $N(x, t)$ are C^{p+1} . Then there exists $G > 0$, $\gamma \in (0, 1)$, and $h^* > 0$ so that such that the following conclusions hold.

1. Every numerical solution $\{X_n\}_{n=0}^\infty$ with $X_n \in \mathbb{R}^{dk}$ of (10) by \mathcal{M} using step-size $h \in (0, h^*)$ is the solution of a nonautonomous discrete dynamical system $X_{n+1} = F(X_n, t_n)$.
2. The discrete dynamical system $Y_{n+1} = H(Y_n, t_n) \equiv (P^{-1} \otimes I)F((P \otimes I)Y_n, t_n)$ defined from the change of variables $X_n = (P \otimes I)Y_n$ satisfies that if $h \in (0, h^*)$, then there exists a unique continuous function $\varphi : \mathbb{R}^d \times \mathbb{Z} \rightarrow \mathbb{R}^{d(k-1)}$ whose graph is invariant under the flow of $Y_{n+1} = H(Y_n, t_n)$ and such that for any $Y_0 \in \mathbb{R}^{dk}$, there exists $z_0^1 \in \mathbb{R}^d$ such that the solution $\{Y_n\}_{n=0}^\infty$ of $Y_{n+1} = H(Y_n, t_n)$ using initial value Y_0 satisfies

$$\|Y_n - Z_n\| \leq G\gamma^n, \quad (12)$$

where the sequence $\{Z_n\}_{n=0}^\infty$ is such that $Z_n = ((z_n^1)^T, \varphi(z_n, n)^T)^T$ and $Z_{n+1} = H(Z_n, t_n)$ for all $n \geq 0$.

3. The difference equation $y_{n+1} = H_1(y_n, \varphi(y_n, n), t_n)$ where H_1 denotes the first d components of H defines a one-step approximation to (10) with local truncation error of order p which is referred to as the underlying one-step method of \mathcal{M} .
4. If the derivatives of $f(x, t) = A(t)x + N(x, t)$ are bounded and $h \leq h^*$, then φ is as smooth as $f(x, t)$.

The remainder of this section is dedicated to the proof of Theorem 3.1. The method \mathcal{M} applied to the problem (10) with step-size $h > 0$ takes the form

$$\begin{cases} G_n = (U \otimes I)X_n + h(C \otimes I)M_n G_n + h(C \otimes I)\bar{N}_n \\ X_{n+1} = (V \otimes I)X_n + h(D \otimes I)M_n G_n + h(D \otimes I)\bar{N}_n \end{cases} \quad (13)$$

where $M_n = \text{diag}(A_{n,1}, \dots, A_{n,s}) \in \mathbb{R}^{ds \times ds}$, $\bar{N}_n = (N(g_{n,1}, t_n + \xi_1 h)^T, \dots, N(g_{n,s}, t_n + \xi_s h)^T)^T$, and $A_{n,i} = A(t_n + \xi_i h)$ for $i = 1, \dots, s$. The equation (13) implies that the internal stages G_n satisfy the following algebraic condition

$$G_n = [I - h(C \otimes I)M_n]^{-1}(U \otimes I)X_n + h[I - h(C \otimes I)M_n]^{-1}(C \otimes I)\bar{N}_n. \quad (14)$$

The implicit function theorem, $N(0, t) = 0$, $DN(0, t) = 0$, and the fact that $A(t)$ and $N(x, t)$ are at least C^2 then implies that there exists $h^* > 0$ so that $h \in (0, h^*)$, then

$$X_{n+1} = (V \otimes I)X_n + R(X_n, t_n, h) \quad (15)$$

where the term $R(X, t, h)$ is Lipschitz in X_n with Lipschitz constant $L_R = L_R(h)$ bounded as $L_R(h) \leq hJ'$ for some constant $J' > 0$. Therefore the first conclusion of Theorem 3.1 is proved. Under the change of variables $X_n = (P \otimes I)Y_n$ we have

$$\begin{cases} y_{n+1}^1 = y_n^1 + R_1(Y_n, t_n) \\ y_{n+1}^2 = (E_{2,2} \otimes I)y_n^2 + R_2(Y_n, t_n) \end{cases}, \quad Y_n = ((y_n^1)^T, (y_n^2)^T)^T, \quad y_n^1 \in \mathbb{R}^d, \quad y_n^2 \in \mathbb{R}^{d(k-1)}. \quad (16)$$

where R_1 and R_2 each have Lipschitz constants $L_{R_1} = L_{R_1}(h)$ and $L_{R_2} = L_{R_2}(h)$ bounded by hJ where $J \leq \|P^{-1} \otimes I\|J'\|P \otimes I\|$. The following is an invariant manifold theorem for difference equations of the form (16) and is a restatement of the conclusions of Theorem 3.1, Theorem 3.2, and Theorem 5.1 in [2]. It is included for completeness.

Theorem 3.2. *Consider a system of difference equations of the form*

$$\begin{cases} x_{n+1} = A_n x_n + F_1(t_n, x_n, y_n) \\ y_{n+1} = B_n y_n + F_2(t_n, x_n, y_n) \end{cases} \quad (17)$$

where $x_n \in \mathbb{R}^{d_1}$, $y_n \in \mathbb{R}^{d_2}$, and $n \geq n_0$ such that

$$\begin{aligned} \|\prod_{j=n}^m A_j^{-1}\| &\leq K\beta^{n-m}, \quad n_0 \leq n \leq m \\ \|\prod_{j=m}^n B_j\| &\leq K\alpha^{n-m}, \quad n \geq m \geq n_0 \end{aligned} \quad (18)$$

and

$$\begin{aligned} \|F_1(t_n, x_n, y_n) - F_1(t_n, \tilde{x}_n, \tilde{y}_n)\| &\leq L\|x_n - \tilde{x}_n\| + L\|y_n - \tilde{y}_n\| \\ \|F_2(t_n, x_n, y_n) - F_2(t_n, \tilde{x}_n, \tilde{y}_n)\| &\leq L\|x_n - \tilde{x}_n\| + L\|y_n - \tilde{y}_n\| \end{aligned} \quad (19)$$

for constants $L > 0$, $K \geq 1$ and $0 < \alpha < \beta$ satisfying the following spectral gap conditions

$$0 < L < \frac{\beta - \alpha}{4K}(2 + K - \sqrt{4 + K^2}), \quad c(\alpha + 2KL) < 1 < c(\beta - 2KL) \quad (20)$$

for some $c > 0$. Denote the solution of (17) with the initial condition $z_0 = \begin{bmatrix} x_0 \\ y_0 \end{bmatrix}$ at initial time n_0 as

$$z(n; n_0, x_0, y_0) = \begin{bmatrix} x(n; n_0, x_0, y_0) \\ y(n; n_0, x_0, y_0) \end{bmatrix} \quad (21)$$

Then there exists a unique continuous map $\varphi : \mathbb{R}^{d_1} \times \mathbb{Z} \rightarrow \mathbb{R}^{d_2}$ whose graph is the manifold

$$\mathcal{D} = \{(n, x, \varphi(x, n)) : n \in \mathbb{Z}, x \in \mathbb{R}^{d_1}\}.$$

and \mathcal{D} is invariant under the discrete flow of (17). Additionally, \mathcal{D} is globally exponentially attracting in the sense that for any $z_0 = (x_0, y_0) \in \mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$ there exists $(n_0, w_0, \varphi(w_0, n_0)) \in \mathcal{M}$, $G > 0$ and $\gamma \in (0, 1)$ so that

$$\|z(n; n_0, x_0, y_0) - z(n; n_0, w_0, \varphi(w_0, n_0))\| \leq G\gamma^{n-n_0}, \quad n \geq n_0 \quad (22)$$

□

We now use Theorem 3.2 to complete the proof of Theorem 3.1. There exists $h_1^* > 0$ so that if $h \in (0, h_1^*)$, then X_n satisfies the difference equation (15). The matrix sequence $\{Y_n\}_{n=0}^\infty$ where $Y_n = (P^{-1} \otimes I)X_n$ satisfies the difference equation (16). Since the eigenvalues of $E_{2,2}$ all have modulus strictly less 1 the difference equation satisfied by $\{Y_n\}_{n=0}^\infty$ is of the form (17) for $\alpha < \beta = 1$ and $L = hJ$. Thus, we can choose $c > 0$ and $h^* \in (0, h_1^*)$ so small that the inequalities (20) are satisfied whenever $h \in (0, h^*)$. So, if $h \in (0, h^*)$, then there exists a unique continuous map

$\varphi : \mathbb{R}^d \times \mathbb{Z} \rightarrow \mathbb{R}^{d(k-1)}$, $G > 0$, and $\gamma \in (0, 1)$ such that if Y_n is the solution of (16), then there exists a sequence $\{z_n\}_{n=0}^\infty$ such that

$$z_{n+1} = z_n + R_1(z_n, \varphi(z_n, t_n), t_n), \quad \|Y_n - (z_n, \varphi(z_n, n))^T\| \leq G\gamma^n. \quad (23)$$

which proves the second conclusion of Theorem 3.1. Since \mathcal{M} is of order p the third conclusion follows from the definition of the local truncation error of a GLM in Nordsieck form and the fact that solutions of (16) and (2) are related by the change of variables defined by $P \otimes I$. Conclusion 4 follows from the results of [5].

3.2. Nonautonomous stability of general linear methods. In this section combine the results of Theorems 2.2 and 3.1 to prove a stability result for the solution of (3) by a strictly stable GLM. The main result is the following theorem which shows that if the step-size of a GLM satisfying the hypotheses of Theorem 3.1 solving the linear problem (3) is sufficiently small, then the exponential stability/instability of numerical solutions of (3) found with the GLM are determined by the stability spectra its underlying one-step method approximates. This provides a partial answer to the question posed in the title of this paper.

Theorem 3.3. *Suppose that the coefficient matrix $A(t)$ of the nonautonomous linear ODE (3) is bounded and C^{p+1} . Assume that the method (2) denoted by \mathcal{M} is strictly stable, in Nordsieck form, and has local truncation error of order $p \geq 1$. Let Σ_{SS} denote the Sacker-Sell spectrum of (3).*

1. *If $\Sigma_{SS} \cap [0, \infty) = \emptyset$, then there exists $h^* > 0$, $G > 0$, and $\gamma \in (0, 1)$ so that the numerical solution $\{X_n\}_{n=0}^\infty$ of (3) by \mathcal{M} using step-size $h > 0$ satisfies $\|X_n\| \leq G\gamma^n$ for any initial value $X_0 = (x_0^T, \dots, x_{k-1}^T)^T$ and $h \in (0, h^*)$.*
2. *If $\Sigma_{SS} \cap [0, \infty) \neq \emptyset$, then there exists $h^* > 0$, $G > 0$, and $\gamma > 1$ so that for any $h \in (0, h^*)$, there exists an initial value $X_0 = (x_0^T, \dots, x_{k-1}^T)^T$ so that the numerical solution $\{X_n\}_{n=0}^\infty$ of (3) by \mathcal{M} using step-size h and initial value X_0 satisfies $\|X_n\| \geq G\gamma^n$.*

An analagous result holds for the Lyapunov spectrum of (3) if we assume that the ODE has an integral separation structure.

Proof. We prove the first conclusion since the proof of the second is very similar. Since $A(t)$ is bounded and C^{p+1} and \mathcal{M} is strictly stable, in Nordsieck form and has local truncation error of order $p \geq 1$, we can choose $h_1^* > 0$ so small that the four conclusions of Theorem 3.1 hold for $h < h_1^*$. The first conclusion of Theorem 3.1 implies that $X_{n+1} = F(X_n, t_n)$ for some function F and the second conclusion of 3.1 implies that there exists $G_1 > 0$ and $\gamma_1 \in (0, 1)$ so that

$$\|(P^{-1} \otimes I)X_n - Z_n\| \leq G_1\gamma_1^n, \quad n \geq 0$$

where $Z_n = ((z_n^1)^T, (\varphi(y_n^1, n))^T)^T$ is a solution of $Z_{n+1} = H(Z_n, t_n)$ with H defined as in Theorem 3.1. The third conclusion implies that $z_{n+1}^1 = H_1(z_n^1, \varphi(z_n^1, n), t_n)$, where H_1 is the first d components of H , defines a one-step approximation with local truncation error of order p to $\dot{x} = A(t)x$ with initial condition z_0^1 . We therefore can write $z_{n+1}^1 = H_1(z_n^1, \varphi(z_n^1, n), t_n) \equiv \Phi^A(n)z_n^1$. Theorem 2.2 then implies that there exists $h_2^* > 0$ so that if $h \in (0, h_2^*)$ then the Sacker-Sell spectrum of $z_{n+1} = \Phi^A(n)z_n$ is bounded above by zero and therefore

$$\|z_n^1\| \leq G_2\gamma_2^n, \quad n \geq 0 \quad (24)$$

for some $G_2 > 0$ and $\gamma_2 \in (0, 1)$. By the work in the previous section, there exists $h_2^* > 0$ so that if $h \in (0, h_2^*)$, then $F(X_n, t_n) = \Phi(n)X_n$ and $H(Y_n, t_n) =$

$(P^{-1} \otimes I)\Phi(n)(P \otimes I)Y_n$ where

$$\Phi(n) = (V \otimes I) + h(D \otimes I)M_n[I - h(C \otimes I)M_n]^{-1}$$

and $\Phi(n)$ is bounded and invertible with M_n as defined in Equation (16). Since the graph of φ is invariant under the flow of H and $\Phi(n)$ is bounded and invertible, it follows that $0 = \varphi(y, n)$ if and only if $y = 0$ for all $n \geq 0$. Therefore, since the fourth conclusion of Theorem 3.1 implies that φ is C^{p+1} and since $p \geq 1$ it follows from (24) that there exists $G_3 > 0$ and $\gamma_3 \in (0, 1)$ so that

$$\|Z_n\| \leq G_3\gamma_3^n, \quad n \geq 0$$

If we let $h^* = \max\{h_1^*, h_2^*\}$ and $h \in (0, h^*)$, then

$$\|X_n\| \leq \|(P \otimes I)\| (\|(P^{-1} \otimes I)X_n - Z_n\| + \|Z_n\|) \leq \|(P \otimes I)\| (G_1\gamma_1^n + G_3\gamma_3^n), \quad n \geq 0.$$

The result follows by taking $G = \max\{G_1, G_3\}$ and $\gamma = \max\{\gamma_1, \gamma_3\}$. \square

In the stability theory of ODE IVP solvers it is often the case that a class of test problems is used to characterize the stability of a solver. In [22] and [23] it is shown that the stability of the numerical solution by a one-step method with local truncation error of order $p \geq 1$ of a nonautonomous linear ODE with an integral separation structure and a bounded and sufficiently smooth coefficient matrix can be characterized (approximately to within the supremum of the local truncation error of the method) by the one-step method applied to d scalar test problems of the form $\dot{x} = \lambda(t)x$ where $\lambda(t)$ is the real-valued diagonal element of a matrix $B(t)$ of a corresponding upper triangular system $\dot{y} = B(t)y$ to (3). Theorem 3.3 justifies using such test problems to characterize the stability of strictly stable GLMs solving nonautonomous linear ODEs satisfying the above stated hypotheses by passing to the underlying one-step method.

Theorem 3.3 is an asymptotic result that says that as $h \rightarrow 0$ we can guarantee the exponential decay of the numerical solution of a nonautonomous linear ODE whose Sacker-Sell spectrum lies to the left of zero. It is natural to try and find a subset of AN-stable methods that preserve the asymptotic decay of all such linear ODEs with no restriction on h . The following theorem partially answers this question and says that step-size restriction is essential for the preservation of asymptotic decay by strictly stable linear multistep and Runge-Kutta methods.

Theorem 3.4. *Given any strictly stable and consistent linear multistep method or a convergent Runge-Kutta method \mathcal{M} and any fixed step-size $h > 0$, there exists an asymptotically contracting scalar ODE $\dot{x} = \lambda(t)x$ such that the numerical solution $\{x_n\}_{n=0}^\infty$ becomes unbounded as $n \rightarrow \infty$ for any initial condition $x(0) = x_0 \neq 0$.*

Proof. Let \mathcal{S} denote the linear stability domain of \mathcal{M} and let $\partial\mathcal{S}$ denote its boundary. Since \mathcal{M} is a strictly stable linear multistep method or a convergent Runge-Kutta method it follows that there exists $\delta > 0$ such that $(0, \delta) \notin \mathcal{S} \cup \partial\mathcal{S}$. Consider the ODE $\dot{x} = (D \cos(2\pi\omega t) + L)x \equiv \lambda(t)x$ where $t > 0$, $0 < D + L < \frac{\delta}{2h}$, $L < 0$ and $\omega = 2\pi/h$ and let $x(0) = x_0 \neq 0$. Since $L < 0$ it follows that $\dot{x} = \lambda(t)x$ has Sacker-Sell spectrum bounded above by zero. The equation $D \cos(2\pi\omega t_n) + L = D + L$ implies that the solution of $\dot{x} = \lambda(t)x$ using \mathcal{M} with step-size $h > 0$ is the same as the numerical solution of the ODE $\dot{x} = (D + L)x$. The quantity $h(D + L) \notin \mathcal{S} \cup \partial\mathcal{S}$ since $h(D + L) < \delta/2$. Therefore the numerical solution of $\dot{x} = \lambda(t)x$ by \mathcal{M} using the step-size $h > 0$ becomes unbounded as $n \rightarrow \infty$. \square

The geometric idea behind the proof of Theorem 3.4 is that if the step-size is too large, then $h\lambda(nh + t_0)$ may be outside the classical stability domain too often and destabilize the numerical solution.

In [22, 23], the stability results for one-step methods approximating a nonautonomous linear ODE with Sacker-Sell spectrum bounded above by zero are extended to linear homogeneous problems of the form (4) using the discrete variation of parameters formula. It is challenging to extend the technique developed in this section for analyzing the stability of a strictly stable GLM solving a linear ODE to linear inhomogeneous ODEs since it is unclear what the relationship is between the underlying one-step method of the linear ODE and that of the corresponding linear inhomogeneous equation. It is unlikely that the underlying one-step method is a Runge-Kutta or other classical one-step method and indeed (see [16]) such abstractly defined methods can be 'quite exotic'. This precludes a straightforward application of the discrete variation of parameters formula.

4. Experiments. In this section we apply the results of Section 3 to investigate the stability of the numerical solution of the linear ODE

$$\begin{aligned} \dot{x}(t) &= A(t)x(t), \quad A(t) = QBQ^T + \dot{Q}Q^T, \quad t > 0 \\ B(t) &= \begin{bmatrix} a_1 \cos(t) + b_1 & \beta \\ 0 & a_2 \cos(t) + b_2 \end{bmatrix}, \quad Q(t) = \begin{bmatrix} \cos(\omega t) & -\sin(\omega t) \\ \sin(\omega t) & \cos(\omega t) \end{bmatrix}, \\ &b_2 < b_1 < 0, \quad a_1, a_2, \omega > 0 \end{aligned} \quad (25)$$

by the BDF2 method

$$x_{n+2} - \frac{4}{3}x_{n+1} + \frac{1}{3}x_n = \frac{2}{3}hf(x_{n+2}, t_{n+2}). \quad (26)$$

The BDF2 method is well known to be a 3-step and single stage strictly stable GLM that is AN-stable and has local truncation error of order 2. The ODE (25) has Lyapunov and Sacker-Sell spectrum that is bounded above by zero, the right endpoints of the Lyapunov and Sacker-Sell spectra are equal and given by $b_1 < 0$, and there exists $K > 0$ so that every solution $x(t; x_0)$ of (25) satisfies that $\|x(t; x_0)\| \leq K\|x_0\|e^{b_1 t}$. Although the AN-stability of BDF2 might seem to suggest there should be no stability issues when solving (25), Theorem 3.4 and the results of our experiments below imply that this need not be the case.

We first show how to evaluate the underlying one-step method of a strictly stable GLM indirectly. Theorem 3.3 implies that the exponential stability of a strictly stable GLM solving (25) can be characterized by the Lyapunov or Sacker-Sell spectrum of the underlying one-step method

$$y_{n+1} = H_1(y_n, t_n) \equiv \Phi^A(n)y_n \quad (27)$$

which has local truncation error of the same order. Rather than attempting to directly evaluate the function H_1 we instead make use of (12) to evaluate H_1 indirectly. Let X_0 be some starting values for a GLM satisfying the hypotheses of Section 3.1 applied to solve (3) with step-size $h > 0$ and denote the associated numerical solution as $\{X_n\}_{n=0}^\infty$ where $X_n = (x_n^1, \dots, x_n^k)^T$. For the sequence defined by $Y_n = (P^{-1} \otimes I)X_n$ there exists $G > 0$, $\gamma \in (0, 1)$, and Z_n of the form $Z_n = (z_n, \varphi(z_n, n))^T$ so that

$$\|Y_n - Z_n\| \leq G\gamma^n$$

and $z_{n+1} = H_1(z_n, t_n)$. If we let $P^{-1} = (\bar{p}_{i,j})_{i,j=1}^k$, then the sequence defined component-wise as $w_n := \sum_{j=1}^k \bar{p}_{1,j} x_n^j$ is approximately equal to an output of (27) for sufficiently large values of $n \geq 0$.

We use this technique to approximate the largest discrete Lyapunov exponent of (27) as follows. Given an initial condition $x(0) = x_0$ we use the RK4 Runge-Kutta method to compute x_1 . For $n \geq 2$, we solve the equation (25) for x_{n+2} and set $X_n = (x_n, \dots, x_{n+2})^T$. Using X_n , we form $w_n = \sum_{j=1}^3 q_{1,j} x_{n+j-1}$. Since w_n approximately satisfies (27) we can view it as the first column in a fundamental matrix solution. Suppose that we let $w_n = Q_n R_n$ be a QR factorization where $Q_n \in \mathbb{R}^{d \times d}$ is orthogonal and $R_n \in \mathbb{R}^{d \times 1}$. Under the assumption that (27) has a discrete integral separation structure, the largest (see [11]) discrete Lyapunov exponent μ_{\max} of (27) is typically given by

$$\mu_{\max} = \limsup_{n \rightarrow \infty} \frac{1}{t_n - t_0} \sum_{j=0}^n (R_j)_{1,1} \quad (28)$$

where $(R_n)_{1,1}$ denotes the $(1, 1)$ entry of R_n . We estimate (28) by truncating the limsup as

$$\mu_{\text{appr}}(N_0, N) = \max_{N_0 \leq n \leq N_0 + N} \frac{1}{t_n - t_0} \sum_{j=N_0}^n (R_j)_{1,1}. \quad (29)$$

We approximate the largest discrete Lyapunov exponent μ_{\max} of (27) by (29) and use the sign of $\mu_{\text{appr}}(N_0, N)$ for large values of N_0 and N as a stability diagnostic for the numerical solution of (25) by (26).

h	LTEmean	LTEmax	$\mu_{\text{appr}}(N_f/2, N_f/2)$
$7.5E-1$	$1.37E10$	$1.51E11$	$7.68E-1$
$7.5E-2$	$3.75E-3$	$9.42E-3$	$9.03E-3$
$7.5E-3$	$3.60E-7$	$6.38E-4$	$-9.70E-2$
$7.5E-4$	$1.95E-9$	$6.24E-5$	$9.04E-2$

TABLE 1. Results of an experiment for the solution of (25) using BDF2, $a_1 = a_2 = 1.2$, $b_1 = -0.14$, $b_2 = -0.15$, $\beta = 10.0$, $\omega = 1$, and a final time of $t_f = 40$ for various step-sizes h and the initial condition $x(0) = (1, 0)^T$. LTEmean is the mean local truncation error, LTEmax is the maximum local truncation error, and $\mu_{\text{appr}}(N_f/2, N_f/2)$ is the value of (29) where N_f is the final step of the approximation.

We display the results of our first experiment in Table 1 and Figure 1. For step-sizes $h = 7.5 \cdot 10^{-1}, 7.5 \cdot 10^{-2}$ the method (26) produces numerical solutions to (25) that are growing in norm with approximate largest discrete Lyapunov exponents that are positive. When $h = 7.5 \cdot 10^{-2}$ the local truncation error, which is gradually increasing as shown in Figure 1, remains bounded by 10^{-2} . When $h = 7.5 \cdot 10^{-3}, 7.5 \cdot 10^{-4}$ the method (26) produces a decaying solution to (25) and the approximate largest discrete Lyapunov exponent of (27) is negative. This experiment shows that monitoring the approximate largest discrete Lyapunov exponent of the one-step method (27) can be a more effective tool for controlling the global error and monitoring stability than the local truncation error.

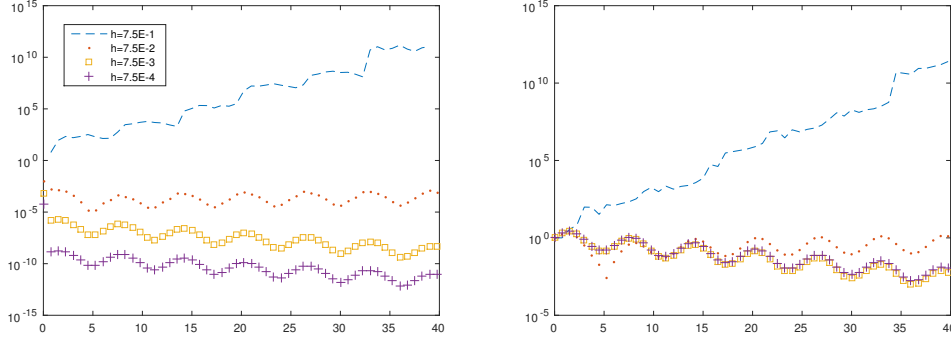


FIGURE 1. Left: Logarithmic plot of the 2-norm of the local truncation error of the numerical solution versus time for various values of h . Right: Logarithmic plot of the 2-norm of the numerical solution versus time for various values of h . The parameter values used were $a_1 = a_2 = 1.2$, $b_1 = -0.14$, $b_2 = -0.15$, $\beta = 10.0$, $\omega = 1$ with a final time of $t_f = 40$ and the initial condition $x(0) = (1, 0)^T$.

$a_1 = a_2 = a$	LTEmean	LTEmax	$\mu_{\text{appr}}(N_f/2, N_f/2)$	τ_{max}
1.15	$5.50E-5$	$4.38E-3$	$-2.33E-2$	1.068
1.45	$1.18E-4$	$5.02E-3$	$-1.69E-3$	1.086
1.75	$2.88E-4$	$5.70E-3$	$1.78E-2$	1.11
2.05	$7.96E-4$	$6.4E-3$	$3.64E-2$	1.23

TABLE 2. Results of an experiment for the solution of (25) using BDF2, using $b_1 = -0.5$, $b_2 = -0.055$, $\beta = 1.0$, $\omega = 1$, and a final time of $t_f = 100$ for various values of $a = a_1 = a_2$ using the step-sizes $h = 0.05$ and the initial condition $x(0) = (1, 0)^T$. LTEmean is the mean local truncation error, LTEmax is the maximum local truncation error, $\mu_{\text{appr}}(N_f/2, N_f/2)$ is the value of (29) where N_f is the final step of the approximation, and τ_{max} is the maximum value of τ_n which denotes the quotient of the local truncation error at time-steps $n+1$ and n .

In Table 2 and Figure 2 we display the results of our second experiment. The results of this experiment are meant to illustrate the difficulty in detecting stability using only point-wise values of the local truncation error. We see that there are no spikes in the local truncation error from one step to the next since τ_{max} is approximately 1 for all values of $a = a_1 = a_2$. Additionally, as the parameter a varies from 1.45 to 1.75, the numerical solution becomes unstable and the ratio between the mean and maximum 2-norm of the local truncation error is 2.44 and 1.14 respectively which are comparable in value to the corresponding ratios when the parameter a varies from 1.15 to 1.45 where there is no loss of stability. This experiment demonstrates that the pointwise local truncation error and its local variation can fail to detect a loss of time-dependent stability.

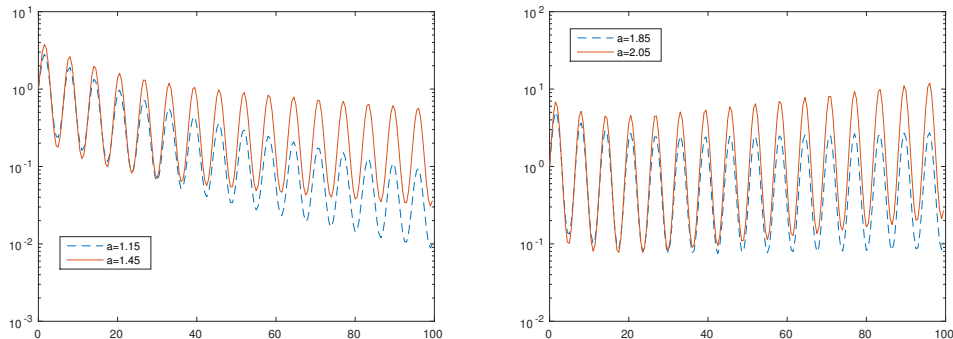


FIGURE 2. Left: Logarithmic plot of the 2-norm of the local truncation error of the numerical solution versus time for various values of h . Right: Logarithmic plot of the 2-norm of the numerical solution versus time for various values of h . The parameter values used were using $b_1 = -0.5$, $b_2 = -.055$, $\beta = 1.0$, $\omega = 1$, and a final time of $t_f = 100$ for various values of $a = a_1 = a_2$ using the step-sizes $h = 0.05$ and the initial condition $x(0) = (1, 0)^T$.

5. Conclusion. In this work we have used invariant manifold theory for nonautonomous difference equations to show that a strictly stable GLM solving a nonautonomous ODE that satisfies a global Lipschitz condition has an underlying one-step methods whenever the step-size is sufficiently small. This result combined with the Lyapunov and Sacker-Sell spectral stability theory for one-step methods developed in [23, 24] and [22] is applied to analyze the stability of a strictly stable GLM solving an nonautonomous, linear ODE whose Sacker-Sell spectrum lies to the left of zero. These theoretical results are then applied to show that sign of the approximate largest discrete Lyapunov exponent of the underlying one-step method of a strictly stable GLM can be a more robust tool than the point-wise values of the local truncation error for monitoring the stability (and hence global error) of the numerical solution of a nonautonomous, linear ODE IVP.

Most step-size selection strategies for the solution of ODE IVPs select step-size based mainly on the local accuracy of the method, which we have shown in Section 4 can lead to stability issues for linear nonautonomous ODEs, even if the method is AN-stable. Our experimental results suggest that the nonautonomous stability theory for GLMs that we have developed can be a useful tool for step-size selection based on stability as well as accuracy (a practical step-size selection algorithm for Runge-Kutta methods based on these ideas can be found in [24]). In future work it remains to show that our results can be extended to variable step-size and variable order GLMs and that the stability theory can be extended to nonlinear ODE IVPs. Interestingly, whereas we have used our nonautonomous results as a practical way of detecting (and hence correcting) an unstable numerical solution, in the abstract of [19] it is stated that "...this result is of theoretical interest; it does not seem to affect the significance of multi-step methods for practical computations". The results of this paper serve as yet another example of how mathematics that is considered theoretical and abstract can one day find a practical application.

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Received xxxx 20xx; revised xxxx 20xx.

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