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A survey of shadowing methods for numerical solutions of ordinary differential equations

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Abstract

A *shadow* is an exact solution to a set of equations that remains close to a numerical solution for a long time. Shadowing can thus be used as a form of backward error analysis for numerical solutions to ordinary differential equations. This survey introduces the reader to shadowing with a detailed tour of shadowing algorithms and practical results obtained over the last 15 years.

Keywords: Shadowing; Validated computing; ODEs; IVPs

1. Introduction

An *initial value problem* (IVP) for an *ordinary differential equation* (ODE) is [5]

$$\mathbf{y}'(t) = \mathbf{f}\big(\mathbf{y}(t)\big), \tag{1}$$

$$\mathbf{y}(t_0) = \mathbf{y}_0. \tag{2}$$

An *autonomous* ODE such as (1) contains no explicit dependence on t. If $\mathbf{y}(t; t_0, \mathbf{y}_0)$ is the solution of (1), (2), we let the *time-h solution operator* φ_h be

$$\varphi_h(\mathbf{u}) \equiv \mathbf{y}(h; 0, \mathbf{u}). \tag{3}$$

Let $\tilde{\varphi}_h$ be a numerical approximation to φ_h computed by some numerical method for small h, and let $\mathbf{y}_{i+1} = \tilde{\varphi}_{h_i}(\mathbf{y}_i)$ define a sequence of discrete points representing approximations to $\mathbf{y}(t_{i+1}; t_0, \mathbf{y}_0)$ where

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$t_{i+1} = t_i + h_i$ [37]. We call this sequence a *pseudo-trajectory*. The natural first question to ask about pseudo-trajectories is how accurately they approximate the exact solution. Since the *forward error* $\|\mathbf{y}_i - \mathbf{y}(t_i; t_0, \mathbf{y}_0)\|$ can in general grow exponentially [27, §§8.1.2, 8.3.6], more sophisticated methods of error analysis must be used to gain insight into the value of the numerical solution.

Backward error analysis is a general term applied to methods of error analysis that relate the pseudo-trajectory to the exact solution of a nearby problem [23,46]. *Defect based* backward error analysis requires a piecewise differentiable interpolant $\mathbf{u}(t)$ of the pseudo-trajectory, and then defines the *defect* as $\delta(t) = \mathbf{u}'(t) - \mathbf{f}(\mathbf{u}(t))$. If for some input tolerance ε we can show that $\|\delta(t)\| \leqslant \varepsilon$ wherever $\mathbf{u}'(t)$ is defined over the whole of the interpolated solution, then the interpolated solution is the exact solution to an ε-close problem (see, for example, [26,23]), namely $\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t)) + \delta(t)$.

Defect-based and other backward error analysis methods modify (1) but leave (2) untouched. In contrast, shadowing [54,52] is a method of backward error analysis in which (1) remains fixed while (2) is allowed to change. In other words, a *shadow* $\bar{\mathbf{y}}(t)$ is an exact solution to (1) remaining close to the pseudo-trajectory $\mathbf{u}(t)$, but having slightly different initial conditions:

$$\bar{\mathbf{y}}'(t) = \mathbf{f}\big(\bar{\mathbf{y}}(t)\big), \qquad \big\|\bar{\mathbf{y}}(t) - \mathbf{u}(t)\big\| < \varepsilon,$$

for a nontrivial duration of time t including $t = t_0$. Shadowing is thus best applied to systems in which the governing equations are extremely well-known, and virtually all error is introduced by imprecise knowledge of initial conditions and/or by numerical error in the computation of the solution. It is less applicable to systems in which the mathematics only approximately model the truth. For example, shadowing is an appropriate measure of error for the gravitational n-body problem, because the equations of motion are extremely well-understood, and an exact solution of the model very closely approximates the behaviour of a real system under the assumed conditions of the model, whereas the initial conditions for the system are often not known precisely. Conversely, shadowing is an inappropriate measure of error for a weather simulation, because the models are known to be only rough approximations of the real processes involved, and so having a numerical solution that closely follows an exact solution of such an approximate model is of dubious value.

1.1. Motivation

Many physical systems under active study today can be modelled using ODEs; however, many of them display *sensitive dependence on initial conditions*, which means that two solutions that are initially close to each other tend to diverge exponentially with time. Since numerical methods introduce small errors that produce a pseudo-trajectory rather than an exact solution, it is virtually guaranteed that a pseudo-trajectory of such an ODE will diverge exponentially away from the exact solution with the same initial conditions. Although this is widely recognized, its impact on the qualitative properties of a pseudo-trajectory is not well understood.

Even when the mathematical model corresponds extremely closely to reality, real systems undergo external perturbations, so one could argue that numerical errors can be grouped into the same category as external perturbations [22,23]. However, numerical errors may be biased in qualitatively different ways than natural perturbations, and may introduce biases into the numerical solution that cause it to behave in a nonphysical manner. For example, (i) many physical perturbations do not appreciably change the energy of the system, whereas spurious energy dissipation can be a major problem in long numerical integrations of conservative systems. Although symplectic integrators [6,57] and other types of conservative