A Posteriori Error Estimation for Ordinary Differential Equations

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Estimation of the Global Error

- **ODE initial value problem**

$$\begin{cases} \dot{x} = f(x,t), & 0 < t \le T \\ x(0) = x_0 \end{cases}$$

- **Problem: estimate and control**

$$\left\| x(T) - \hat{x}(T) \right\|$$

- **Why?**
  - **Most codes estimate and control the local error. Propagation of local errors in even a mildly unstable system may lead to a global error that is much larger than the local error.**
  - **As a first step towards the goal of estimating errors due to both discretization and modeling errors**

Related Work and Objectives of This Talk

Related work

– Many methods have been suggested for estimation of the global error. A good survey of basic methods is given in Skeel (1986)

– Methods related to ours (based on the adjoint method) are given by Johnson (1988) and Estep et al. (1995), based mostly on the discontinuous Galerkin method

Objectives of this talk

– To outline a general approach to global error estimation and control which can be applied in conjunction with existing ODE software using local error control, and extended to the estimation and control of model errors (errors due to the use of a reduced or simplified model).

– To present well-justified methodology for initializing the adjoint system

Basic Approach

Estimate the error in the solution coming from several sources

– **Error due to the numerical discretization**

$$\begin{cases} \dot{\hat{x}} = f(\hat{x}, t) + r_1(\hat{x}, t), \qquad 0 < \mathrm{t} \leq \mathrm{T} \\ \hat{x}(0) = x_0 + \mathrm{r}_2 \end{cases}$$

For error estimation, we assume

$$\|r_1\|_\infty < \varepsilon, \|r_2\| < \varepsilon$$

For global error control, we make use of the local error estimate to estimate the perturbations.

– **Propagation of errors by the ODE itself. Condition of the ODE is estimated by a combination of**
  - **Adjoint method**
  - **Small sample statistical method (Kenney and Laub, 1998)**

Error Estimation for a Scalar Derived Function

Given the ODE

$$x' = A(t)x + h(t), x(0) = x_0$$

the perturbed ODE

$$\hat{x}' = a(t)\hat{x} + h(t) + r_1(t), \hat{x}(0) = x_0 + r_2$$

and a scalar derived (output) function

$$g = g(x(T))$$

at the end time T

We wish to estimate the error in the output function as a result of the perturbations

Error Estimation for a Scalar Derived Function

Let

$$e = x - \hat{x}$$

Then

$$\Delta g = g(x(T) - g(\hat{x}(t))) = g_x(x(T))e(T)) + O(\delta^2)$$

The error satisfies

$$e' = A(t)e + r_1(t), e(0) = r_2$$

Thus

$$e(t) = \int_0^t \Phi(t)\Phi^{-1}(s) r_1(s)\,ds + \Phi(t) r_2$$

where Φ is the fundamental solution matrix

Let

$$l = g_x^{\ T}(x(T))$$

Then the error in g satisfies

$$\Delta g = l^T e(T) + O(\delta^2)$$

$$= \int_o^T l^T \Phi(t)\Phi^{-1}(s) r_1(s)\,ds + l^T \Phi(T) r_2 + O(\delta^2)$$

Error Estimation for a Scalar Derived Function

Recall that the error satisfies

$$\Delta g = l^T e(T) + O(\delta^2)$$

$$= \int_o^T l^T \Phi(t)\Phi^{-1}(s) r_1(s)\,ds + l^T \Phi(T) r_2 + O(\delta^2)$$

But $\Phi(T)\Phi^{-1}(s)$ **is too expensive to compute. Thus we compute**

Error Estimation for a Scalar Derived Function

Recall that the error satisfies

$$\Delta g = l^T e(T) + O(\delta^2)$$

$$= \int_o^T l^T \Phi(t)\Phi^{-1}(s) r_1(s)\, ds + l^T \Phi(T) r_2 + O(\delta^2)$$

But $\Phi(T)\Phi^{-1}(s)$ **is too expensive to compute. Thus we compute**

$$l^T \Phi(T)\Phi^{-1}(s)$$

by solving the adjoint ODE

$$\lambda' = -A^T(t)\lambda$$

$$\lambda(T) = l$$

to obtain

$$\lambda^T(s) = l^T \Phi(t)\Phi^{-1}(s)$$

and

$$\lambda^T(0) = l^T \Phi(T)$$

Error Estimation for a Scalar Derived Function

Thus

$$\Delta g = \int_0^T \lambda^T(s) r_1(s) ds + \lambda^T(0) r_2 + O(\delta^2)$$

and the error estimate is given by

$$|\Delta g| \le \|\lambda\|_{L_1} \|r_1\|_\infty + \|\lambda(0)\| \|r_2\| + O(\delta^2)$$

$$\le (\|\lambda\|_{L_1} + \|\lambda(0)\|)\varepsilon + O(\delta^2)$$

The condition number is given by

$$K(\lambda) = \|\lambda(t)\|_{L_1} + \|\lambda(0)\|$$

Error Estimation for the Solution

Our goal is to estimate

$$\|\Delta x(T)\|$$

Although this norm is a scalar, there is a problem with using the previously outlined adjoint approach directly, because g_x depends on Δx

However, if we allow our estimate to have a moderate relative error, we can use the small sample statistical method in combination with the estimate for scalar functions derived earlier.

Basically, we use $\xi = \frac{|l^T z_n|}{E_n}$ for n random vectors z_n to estimate $\|l\|$

where $E_1 = 1, E_2 = \frac{2}{\pi}$, and $E_n \approx \sqrt{\frac{2}{\pi(n - \frac{1}{2})}}$

Two orthogonal random vectors yield an error estimate which is correct to within a factor of 10 with 99% probability

Error Estimation for the Solution

To estimate $\|e(T)\|$, we first select a random vector z uniformly from the unit sphere S_{n-1} . Then we define $g(x) = z^T x$. Solving for λ_z from

$$\lambda_z{}' = -A^T(t)\lambda_z$$

$$\lambda_z(T) = z$$

the condition estimate is given by $\dfrac{1}{E_n} K(\lambda_z)$

For the error estimate, we have

$$\|e(T)\| \approx \frac{1}{E_n}\left|z^T e(T)\right| \le \frac{1}{E_n} K(\lambda_z)\varepsilon$$

For two orthogonal random vectors, we solve the adjoint equation twice to obtain $\lambda_{z_1}, \lambda_{z_2}$. Then the condition number is given by

$$\frac{E_2}{E_n}\left(K(\lambda_{z_1})^2 + K(\lambda_{z_2})^2\right)^{\frac{1}{2}}$$

This resolves a problem noted by Estep regarding the choice of initial values for the adjoint problem, and shows the affect on the accuracy of the error and condition estimates of choosing one versus more random vectors.

Global Error Control

- **Problem: Given a global error tolerance $GTOL$, choose the stepsize so that**

$$\left\| x(T) - \hat{x}(T) \right\| < GTOL$$

- **Traditional way: local error control (error per unit step)**

$$Ch^k \leq LTOL$$

- **Direct method for global error control**

$$GTOL \leq K \cdot LTOL \Rightarrow h_{n+1} \leq \left(\frac{GTOL}{KC} \right)^{\frac{1}{k}}$$

- **Better method for global error control**

$$h_{n+1} \leq \left(\frac{GTOL}{TC \ \left| \lambda(t) \right|} \right)^{\frac{1}{k}}$$

Numerical Results

- **Scalar, linear ODE** $\dot{x} = ax$

$a = 1$

	Tol	10^{-2}	10^{-4}	10^{-6}
original	**Error**	6.7	1.35	0.045
DASPK	**Step**	33	54	73
Global error	**Error**	4×10^{-4}	2.3×10^{-6}	2×10^{-7}
Control	**Step**	81	146	355

$a = -10$

	Tol	10^{-9}	10^{-10}	10^{-12}
original	**Error**	6.3×10^{-11}	3.2×10^{-11}	3.7×10^{-12}
DASPK	**Step**	288	588	557
Global error	**Error**	1.1×10^{-10}	1.8×10^{-12}	8.3×10^{-13}
Control	**Step**	134	225	263

Numerical Results

- **Unstable system**

$$\begin{cases} \dot{y}_1 - \dfrac{y_1}{2(1+t)} + 2t\,y_2 = 0 & t > 0, \\ \dot{y}_2 - \dfrac{y_2}{2(1+t)} - 2t\,y_1 = 0 & t > 0, \\ y_1(0) = 1, \qquad y_2(0) = 0. & \end{cases}$$

	Tol	10^{-2}	10^{-4}	10^{-6}
	Error(y_1 **)**	0.02	8×10^{-3}	5.7×10^{-5}
original	**Error(** y_2 **)**	0.8	0.03	1.3×10^{-3}
DASPK	**Step**	294	568	940
	Error(y_1 **)**	3×10^{-3}	9×10^{-6}	6×10^{-7}
Global error	**Error(** y_2 **)**	5×10^{-3}	1.5×10^{-4}	1.5×10^{-6}
Control	**Step**	767	1472	3613