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NUMERICAL TECHNIQUES FOR ORDINARY DIFFERENTIAL EQUATIONS

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General numerical methods for ordinary differential equation (ODE) initial-value problems are surveyed, with emphasis on second-order ODE's. Issues include truncation and roundoff error, stability, and starting/stopping. For nonstiff systems, predictor-corrector Adams methods, with variable step and order, are best overall.

I. INTRODUCTION

Much literature and software is devoted to initial-value problems for ODE systems. Most of it addresses first-order systems,

$$\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}) \quad (\dot{\mathbf{y}} \equiv d\mathbf{y}/dt).$$

Here, a crucial consideration is *stiffness*, which means the presence of one or more strongly damped (*not* oscillatory) modes.

Second-order ODE systems, which can be written

$$\ddot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}, \dot{\mathbf{y}}) \quad (\ddot{\mathbf{y}} \equiv d^2\mathbf{y}/dt^2),$$

can always be reduced to first-order systems and solved as such, and often are, but they can also be treated directly. Stiffness, defined via the equivalent first-order system, can occur only if the $\dot{\mathbf{y}}$-dependence contributes strong damping. The *special problem* [$\mathbf{y}$ absent, $\ddot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$] is often treated by special methods.

II. SUMMARY OF METHODS FOR SECOND-ORDER PROBLEMS

Many types of methods have been developed for second-order ODE initial-value problems.[1,2] What follows is a partial list.

Runge–Kutta methods include the classical Nyström formulas (for the special problem). Fehlberg developed imbedded formula pairs for the general problem with easy local-error estimates.

Linear multistep methods include the explicit Störmer formulas and the implicit Cowell formulas, which are special and exist at all orders; the fourth-order Cowell formula is Numerov's method. The implicit Adams methods (general; all orders) have been generalized to second-order ODE's.[1,3,4] Numerous other methods of particular orders occur in the literature. A framework for analyzing

the order and stability of linear multistep formula pairs (one for $\mathbf{y}$ and one for $\dot{\mathbf{y}}$) is given by Addison and Enright.[5]

Extrapolation methods integrate over each major step with several smaller step sizes and extrapolate to the limit of zero step size. Recent work by Deuflhard is noteworthy.[6]

Hybrid methods, combining the features of Runge–Kutta and multistep formulas, have been studied. Examples include a method of De Vogelaere and a sequence of methods by Dyer[7] (special).

Taylor-series methods may be useful if the function $\mathbf{f}$ is amenable to symbolic differentiation to arbitrary degrees.

Exponential fitting methods invole setting coefficients of a multistep formula so as to make it exact when the solution is a given exponential (real or complex) or trigonometric polynomial. Bettis and others have studied fitting methods for orbit problems.

Multirevolution methods (Petzold et al.) can be highly effective when a single high-frequency oscillation is present.

Multirate methods attempt to use different step sizes for different groups (fast vs slow) of ODE components.

As a simple example, consider the explicit leapfrog formula,

$$\mathbf{y}_{n+1} - 2\mathbf{y}_n + \mathbf{y}_{n-1} = h^2\mathbf{f}_n \quad [\mathbf{f}_n \equiv \mathbf{f}(t_n, \mathbf{y}_n)],$$

with constant step size $h = t_{k+1} - t_k$. If $\mathbf{f}$ is general or if $\dot{\mathbf{y}}$ values are needed, one must also advance $\dot{\mathbf{y}}$, for example by

$$\dot{\mathbf{y}}_{n+1} = \dot{\mathbf{y}}_n + h\mathbf{f}_n \quad \text{(explicit Euler)}.$$

Contrast this with the (implicit) Numerov formula,

$$\mathbf{y}_{n+1} - 2\mathbf{y}_n + \mathbf{y}_{n-1} = (h^2/12)(\mathbf{f}_{n+1} + 10\mathbf{f}_n + \mathbf{f}_{n-1}).$$

Along with this, if necessary, one advances $\dot{\mathbf{y}}$ with, for example,

$$\dot{\mathbf{y}}_{n+1} = \dot{\mathbf{y}}_n + (h/2)(\mathbf{f}_{n+1} + \mathbf{f}_n)(\text{Trapezoid Rule}).$$

An algebraic system for $\mathbf{y}_{n+1}$ (and possibly $\dot{\mathbf{y}}_{n+1}$) must somehow be solved, either (a) analytically, (b) by a Newton iteration (appropriate only in the stiff case), or (c) by simple iteration (predictor-corrector). For special $\mathbf{f}$, the latter would be given by

$$\mathbf{y}_{n+1}^{(m+1)} = 2\mathbf{y}_n - \mathbf{y}_{n-1} + (h^2/12)[\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}^{(m)}) + 10\mathbf{f}_n + \mathbf{f}_{n-1}].$$

III. NUMERICAL ISSUES

Truncation Error

Although definitions vary, the idea of *local truncation error* (L.T.E.) is simple. It is the difference between the computed $\mathbf{y}_{n+1}$ and the exact $\mathbf{y}(t_{n+1})$ when the step is

taken with all earlier data (up through $\mathbf{y}_n$) exact. A given method generally satisfies

$$\text{L.T.E.} = 0(h^p) \quad \text{as} \quad h \to 0,$$

with p determined by relations among the method coefficients. The *global error* (G.E.) is the actual error in $\mathbf{y}_n$ after n steps, assuming only that the starting values are sufficiently accurate. A typical convergence theorem for a method for $\ddot{\mathbf{y}} = \mathbf{f}$ says that if L.T.E. $= 0(h^{q+2})$, then G.E. $= 0(h^q)$ as $h \to 0$ with $t_n = t_0 + nh$ fixed $(n \to \infty)$. Two powers of h are lost as L.T.E. accumulates to G.E. because the method resembles a double-summation process.

In practice, modern ODE solvers always estimate the L.T.E. and then vary h in order to meet a prescribed bound on L.T.E. If methods of different orders are available, the L.T.E.'s at nearby orders are also estimated, and q is varied accordingly.

Other error issues studied are (a) numerical growth/damping, and (b) phase error (dispersion) for oscillatory solutions.

Roundoff Error

Machine roundoff subjects each computed $\mathbf{y}_n$ to an error of at least $\pm u\mathbf{y}_n$, where u = the machine unit roundoff. Adding bounds on these errors to the convergence theorem gives a result of the form

$$\|\text{G.E.}\| \leq Bh^q + Aun^r \quad (A, B = \text{problem-dependent constants}).$$

In a rigorous bound r is 2, but cancellation of roundoff errors tends to give a smaller value. Since $n \propto 1/h$, this bound has a positive minimum as h varies. Reducing r reduces this minimum, but there is always a finite limit to the accuracy of the computed solution. It is clear that an orbiting particle can be reliably tracked only over thousands or perhaps millions of orbits at most.

Stability

A fundamental stability concept in ODE methods is that of *absolute stability*, which is (roughly) the requirement that if the ODE system has a bounded solution then so does the numerical solution.

Classical treatments of absolute stability use a model problem $\ddot{y} = -\omega^2 y$ and write y_n as a function of ωh and n. The point ωh is stable if y_n is bounded as $n \to \infty$. Goals often pursued for a method with free parameters are to (a) maximize the size of the interval of stable points ωh, (b) get (unconditional) stability for *all* real ωh, or (c) demand periodicity (conditional on ωh) in that y_n is a linear combination of powers of unidomular complex numbers.

A more general treatment is possible,[5] using a model problem

$$\ddot{y} = 2a\dot{y} - (a^2 + b^2)y \quad [\text{solution } y = \exp(at \pm ibt)].$$

Here one demands that y_n be bounded for as much as possible of the left half of the (ah, bh) plane. However, unlike the first-order situation, the behavior of a method on linear second-order systems is *not* generally given by its stability on scalar model problems.

Starting and Stopping

Several issues related to starting, stopping, and restarting an ODE method may be important in the choice of the method itself.

A good initial step size may be known from prior run data. If not, modern codes estimate the constant C in $\|\text{L.T.E.}\| \simeq Ch^p$ and compute h by equating Ch^p to a given tolerance parameter.

Stopping at a given t (e.g., for output) is easily and cheaply done with a linear multistep method, using its underlying interpolatory polynomial, but for almost any other method the step size must be adjusted to hit t exactly.

Stopping at a root of a function $g[\mathbf{y}(t)]$ (e.g., to locate a boundary crossing) is also easier with linear multistep methods.

Restarting at a discontinuity usually requires posing a new initial-value problem, hence discarding all past data. Thus high accuracy and frequent discontinuities may make multistep methods less efficient than suitable high-order one-step (e.g., RK) methods.

IV. SOFTWARE

Many high-quality solvers are available for systems of first-order ODE's. Adams predictor-corrector codes generally perform best for nonstiff systems, especially at high accuracy. Some Adams codes detect when accuracy is limited by roundoff, some have root stopping, and some detect stiffness and switch methods automatically.

For second-order ODE's, much less is available. A trio of codes by F. T. Krogh (Jet Propulsion Lab.), VODQ/SVDQ/DVDQ, is well known and is superseded by his new codes, SIVA and DIVA. These use variable-order variable-step Adams methods for general **f**, do root stopping, and detect limiting tolerance from roundoff. Two codes by P. Deuflhard (Univ. of Heidelberg), KEPLEX and DIFEX2, use extrapolation methods for special **f**. A few other codes, using various fixed-order methods, are mentioned in the literature.

Two sources of test results are of particular interest. In one,[8] two orbit problems were solved by Adams predictor-corrector methods at three tolerances. In all cases, direct treatment of the ODE's required fewer **f** evaluations than reducing to a first-order system, by a factor of about 2. In another comparison,[9] six orbit problems were run with five solvers—DVDQ (Adams method), RADAU (implicit RK), RKF67 (explicit RK), DIFSY2 (extrapolation), and EPISODE (Adams on reduced system). At low to moderate accuracies, the differences were small; at high accuracy the two Adams codes were preferred; at very high accuracy, DVDQ performed best.

RECOMMENDATIONS

As to general numerical methods for $\ddot{\mathbf{y}} = \mathbf{f}$, the main recommendation here is to use generalized Adams methods in a variable-order predictor-corrector form with local error control. For high accuracy, use a high maximum order (12 is typical). As an expendient, a good alternative is to solve the reduced first-order system with a good Adams solver. Depending on the accuracy and nature of $\mathbf{f}$, Runge–Kutta, Taylor-series, or extrapolation methods may be competitive. Analytic solutions should be used where they are trusted, and interfaced with numerical solutions where they are not. Multirevolution methods should be used wherever appropriate.

One final recommendation: Do not reinvent wheels. It pays to consult the experts and the literature and avoid duplicating the efforts of people who have studied the subject.

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