Variable Step Variable Order Methods[1]

This material is adapted from J.D. Lambert, Numerical Methods for Ordinary Differential Systems, Wiley, 1991. That book and its references should be consulted for details.

There are a number of ODE codes in the public domain. One that you may want to try out is in

`/usr/local/math/lsode/lsode.f`

It consists of 3,390 lines of FORTRAN code and is a far cry from e.g., a simple Runge-Kutta code you might find in a simple-minded Numerical Analysis Text.

`lsode` and related codes share the following ingredients:

1. A family of methods
2. A starting strategy
3. A local error estimator
4. A step-size/order policy
5. A technique to change order
6. A technique to change step-size

We discuss these items in turn.

1. Family of Methods.

These are usually one of the following:

— *Adams-Bashforth-Moulton Predictor Corrector Methods*, usually in

$$PECE \quad \text{or} \quad P(EC)^2E$$

mode, with step-numbers ranging as high as 13, for *non-stiff* problems.

The Adams Methods of order k can be written as

$$y_{n+1} = y_n + h\sum_{i=0}^{k-1} \gamma_i \nabla^i f_{n+1} \quad \text{(Adams-Moulton)} \tag{1}$$

and

$$y_{n+1} = y_n + h\sum_{i=0}^{k-1} \gamma_i^* \nabla^i f_n \quad \text{(Adams-Bashforth)} \tag{2}$$

where

$$\nabla^0 f_n = f_n \quad \text{and} \quad \nabla^{i+1} f_n = \nabla^i f_n - \nabla^i f_{n-1} \tag{3}$$

and the γ_i and γ_i^* are constants *independent* of the step-number k. We will use the Adams methods to illustrate details of some of the other ingredients.

[1] by Peter Alfeld. TEX processed July 16, 2014

Note: Thus the Backward Euler Method is considered an Adams-Moulton Method of order 1.

— *Backward Differentiation formulas* of step-number up to 6 for *stiff problems*, combined with Newton's method (and the accompanying linear algebra software) for solving the nonlinear systems.

— *Blended Linear Multistep Methods*, a sophisticated combination of the two types above.

2. A starting strategy.

This is very simple, one starts with the one-step method. As the integration proceeds the step-number typically increases initially.

3. A local Error Estimator.

Virtually all error estimation is based on the comparison of *two* approximations of the same quantity. The *local error* for initial value problems is

$$y_{n+1} - z(x_{n+1}) \tag{4}$$

where z is the exact solution of the differential equation that passes through the point (x_n, y_n). (The estimation of the *global truncation error* is much more difficult and not used in practice.) For predictor corrector methods this takes the form of *Milne's Device*. For the Adams Methods the error estimate is very simple:

$$E_{n+1} = h\gamma_k \tilde{\nabla}^k f_{n+1} \tag{5}$$

where $\tilde{\nabla}^k f_{n+1}$ is just $\nabla^k f_{n+1}$ with f_{n+1} replaced by $f_{n+1}^{[0]}$, i.e., f evaluated at the *predicted* value. Note that this can be evaluated at the PEC stage of the PECE computation, so that the final evaluation can be omitted if the estimated error is too large.

4. A step-size/order policy.

Suppose the last step was taken at step-number k and step-size h. Depending on the particular code, the step is accepted if either

$$\|E_{n+1}\| \leq \tau \tag{6}$$

or

$$\|E_{n+1}\| \leq \tau h. \tag{7}$$

where τ is a user specified quantity that governs the accuracy of the integration. For the sake of this illustration let us consider the requirement (6). The reasoning can be extended easily to the requirement (7). Whether the step is accepted or not the maximum allowable step-sizes h_{k+i}^*, $i \in \{-1, 0, 1\}$ are now estimated for the step number $k+1$, k, and $k-1$. Whichever of these three maximum step-lengths turns out to be the largest will determine the step-number and step-size at the next

step. (The actual step taken will be a little less than the estimated maximum step-size, to reduce the risk of a marginal rejection.) Let E_{n+1}^{k+i}, $i \in \{-1, 0, 1\}$ denote the estimated error for the three contemplated step-numbers. It turns out that the following *computable* asymptotic[2] estimates hold:

$$E_{n+1}^{k+i} = h\gamma_{k+i}\tilde{\nabla}^{k+i} f_{n+1}. \tag{8}$$

By the definition of order, the maximum step-sizes satisfy

$$\tau = K_{k+i}\left(h_{k+i}^{*}\right)^{k+i+1} \tag{9}$$

for some constants K_{k+i}. Similarly,

$$\|E_{n+1}^{k+i}\| = K_{k+i}h^{k+i+1}. \tag{10}$$

We can solve these two equations for h_{k+i}^{*} to give

$$h_{k+i}^{*} = h\left(\frac{\tau}{\|E_{n+1}^{k+i}\|}\right)^{\frac{1}{k+1+i}}. \tag{11}$$

As already stated above, we now pick the order corresponding to the largest h_{k+i}^{*} and a slightly smaller step-size for the next step.

5. A technique to change order.

A change of order is implemented very simply by adding or omitting a term in (1) and (2).

6. Two techniques to change step-size.

For a long time the stumbling block in developing linear multistep methods were the difficulties in changing the step-size. Two techniques evolved as viable:

a. *Interpolation* (in f) to generate missing back values.

b. Computation of the coefficients of a *new Adams-type method* specifically for the current combination of unevenly spaced back values.

[2] Without going into too much detail, the term *asymptotic* in this context means that the approximation becomes exact in the limit as the step-size h tends to zero.