Stability Analysis of Multi-step Methods

Adrian Down

April 27, 2006

1 Multistep method

1.1 Review

Last time, we investigated the fourth-order Runge-Kutta method. We saw that the computations involved in performing this approximation were less than ideal.

To create more computationally viable methods, we introduced multi-step methods, in which the approximation at a given point is obtained using only the values of the differential equation to be approximated and the approximation itself at previous points. Although these methods involve fewer computations, they can become unstable.

1.2 Initial conditions

The multi-step method also has the disadvantage that it requires multiple points for initialization. Usually we know only the value of the approximation $y(t)$ at $t = 0$, where $y(0)$ is equal to the exact solution $x(t = 0)$.

To obtain the other necessary initial points, we can use a Runge-Kutta or other single-step method. This Runge-Kutta approximation introduces some truncation error in the approximation $y(h)$ to the exact solution $x(h)$. Choose a Runge-Kutta method that gives the same order of truncation error as does the multi-step method being used. A Runge-Kutta method with lower order error will limit the accuracy of the subsequent multi-step approximation, and a Runge-Kutta method with higher order error require extra calculations without providing any additional benefit.
1.3 Stability analysis

As a minimal check, examine the multi-step method in the case that \( f \equiv 0 \). In this case, \( \dot{x} = 0 \), from which we expect \( x(t) \) to be constant. The exact solutions that we obtain for the multistep methods will contain perturbations due to the initial conditions, and will not always be constant. However, we require that these perturbations die out far from \( t = 0 \). Hence, a stable method is one for which the solution becomes constant as \( n \to \infty \), where \( n \) is the number of steps away from \( t = 0 \) to which the approximation is computed.

2 Example of stability analysis: two step method

2.1 Review

Recall the two-step method developed in the previous lecture,

\[
y(t + h) + 2y(t) - 5y(t - h) = h \{4F(t) + 2F(t - h)\}
\]

where \( F(t) = f(t, y(t)) \). This method was designed to have fourth order local truncation error, from which we expect to achieve third order global truncation error.

2.2 Set \( f = 0 \)

Examining the case that \( f = 0 \),

\[
y(t + h) + 4y(t) - 5y(t - h) = 0
\]

Writing \( y_n \equiv y(t = nh) \), the previous equation becomes,

\[
y_{n+1} + 4y_n - 5y_{n-1} = 0
\]

2.3 Homogeneous recursion relation

2.3.1 Analogy with the ODE

The recursion relation above is analogous to an ordinary linear homogenous differential equation with constant coefficients. An example of such an ODE
is,

\[ y'' + y' + y = 0 \]

To solve this type of equation, we assumed an elementary solution of the form \( y = e^{\lambda t} \). Substituting this assumed form of the solution into the differential equation,

\[ \lambda^2 \left( e^{\lambda t} \right) + \lambda \left( e^{\lambda t} \right) + e^{\lambda t} = 0 \]

\[ \Rightarrow \lambda^2 + \lambda + 1 = 0 \]

This quadratic equation determines the possible values of \( \lambda \). Using the quadratic formula,

\[ \lambda = \frac{-1 \pm \sqrt{1 - 4}}{2} = \frac{-1 \pm i\sqrt{3}}{2} \]

Substituting these values of \( \lambda \) into the assumed form of the solution, the homogeneous solutions are,

\[ y = e^{-\frac{1}{2}t} e^{\frac{i\sqrt{3}}{2}t} \quad y = e^{-\frac{1}{2}t} e^{-\frac{i\sqrt{3}}{2}t} \]

The general solution would be a linear combination of these two solutions.

### 2.3.2 Difference equation

In the case of the difference equation above, we can use the same strategy. Assume the same form of the general solution, in this case taking \( n \) in place of \( t \),

\[ y = e^{\lambda t} = \left( e^{\lambda} \right)^t \mapsto y_n = r^n \]

As before, substitute this assumed form of the solution into the recursion relation to determine the value of \( r \),

\[ r^{n+1} + 4r^n - 5r^{n-1} = 0 \]

\[ \Rightarrow r^2 + 4r - 5 = 0 \]

The solutions for \( r \) are obtained using the quadratic formula,

\[ r = \frac{-4 \pm \sqrt{16 - 4(1)(-5)}}{2} = \frac{-4 \pm 6}{2} = 1, -5 \]
The general solution to the difference equation is a linear combination of these two solutions,

$$y_n = a(1)^n + b(-5)^n$$

The $a(1)^n = a$ term is constant as $n \to \infty$, as we require of a stable solution in the case that $\dot{x}(t) = 0$. However, $(-5)^n$ is oscillatory without bound as $n$ increases. Hence, this term is a spurious solution that does not yield an approximate solution to the ODE.

2.4 Initial conditions

The constants $a$ and $b$ are determined by the initial conditions. Suppose as an example that we have the initial condition $y(0) = 0$. Since $\dot{x} = 0$, we expect that $y_n$ should be equal to 0 for all $n$.

As a practical example, consider the case in which the value of $y(h)$ is computed numerically using some computer algorithm, which introduces an error of $10^{-N}$. In the case of MatLab or similar computational tools, $N$ could be about 16. We would have then, as a second initial condition, $y(h) = 10^{-N}$.

To determine $a$ and $b$, substitute $n = 0$ and $n = 1$ into the solution.

- $n = 0$: $0 = a + b \Rightarrow a = -b$
- $n = 1$: $10^{-N} = a - 5b \Rightarrow a = 10^{-N} + 5b$

The solution to this system of equations is $a = \frac{1}{6}10^{-N}$. Hence the solution to $y_n$ takes the form,

$$y_n = \frac{1}{6}10^{-N}(1 - (-5)^n)$$

As $n$ becomes large, the 1 in the parentheses becomes negligible, and so,

$$|y_n| \to \frac{1}{6}10^{-N}5^n$$

It can be shown that $|y_n| > 1$ for $n > 25$. We expected that $y_n$ should approach 0, and here we see that it is growing. Hence this two-step method is not stable.
3 Improving the multi-step method

3.1 Motivation

We just saw that our previous attempt at a multi-step method was not stable. We obtained this method by canceling all terms of $O(h^3)$ and lower in the local truncation error. Our method was not stable because by canceling the third order error term, the conditions we placed on the method were too stringent. To obtain a stable solution, we relax our conditions and not attempt to cancel the third order term in the local truncation error.

3.2 Calculation

Recall the previous general form of the two-step method,

$$y(t + h) + a_2 y(t) + a_1 y(t - h) = h \{ A_2 F(t) + A_1 F(t - h) \}$$

By taking Taylor expansions and matching powers of $h$ on both sides, we previously obtained four equations. In this case, since we have relaxed the constraints on the $O(h^3)$ term, we obtain only three equations,

$$1 + a_1 + a_2 = 0$$
$$1 - a_1 = A_1 + D_2$$
$$1 + a_1 = -2A_1$$

Since this is a system of three equations with four unknowns, the system is under-determined. Hence there is a one-parameter family of such two-step methods. Taking $a_1$ to be the independent variable,

$$a_2 = -(1 + a_1)$$
$$A_1 = -\frac{1}{2} - \frac{a_1}{2}$$
$$A_2 = \frac{3}{2} - \frac{a_1}{2}$$

Substituting these forms of the coefficients into the general form of the two-step method,

$$y(t + h) - (1 + a_1)y(t) + a_1 y(t - h) = \frac{h}{2} \{ (3 - a_1)F(t) - (1 + a_1)F(t - h) \}$$
3.3 Stability

We have obtained a family of two-step approximation methods in the variable $a_1$. However, not all values of $a_1$ produce useful methods. Using stability analysis, we can determine the values of $a_1$ that produce stable schemes.

Taking $f \equiv 0$ as before, a stable scheme will produce solutions that are constant after many iterations. We assume an elementary solution of the form $y_n = r^n$. Substituting into the general two-step method, taking $F = 0$,

$$r^{n+1} - (1 + a_1)r + a_1 = 0$$
$$\Rightarrow r^2 - (1 + a_1) + a_1 = 0$$

We could solve for $r$ using the quadratic formula. However, we can avoid this calculation by noting that $r = 1$ should be a solution to any approximation scheme in the case that $\dot{x} = 0$. Assuming this root facilitates the factorization,

$$(r - 1)(r - a_1) = 0$$

Thus the solutions are $r = 1$ and $a_1$. The general solution is a linear combination of the two,

$$y_n = a + ba_1^n$$

For stability, we would like $y_n$ to approach a constant as $n$ becomes large. If $|a_1| < 1$, then $y_n \to a$ as $n \to \infty$. This $a$ is constant, as desired to ensure stability. Hence the two-step method is stable if $|a_1| < 1$.

4 Diffusion equation

4.1 Motivation

We have just seen the importance of stability in computing approximations to solutions to ordinary differential equations. Up to this point, the analysis has been routine. However, we will see in our study of the diffusion equation that stability becomes more interesting in the case of partial differential equations.
4.2 Review of the diffusion partial differential equation

Let \( c(x, t) \) represent the concentration of the substance under study that is diffusing. The total amount of substance in the interval \( x \in (x_1, x_2) \) is,

\[
\text{total amount of substance} \in (x_1, x_2) = \int_{x_1}^{x_2} c(x, t)dx
\]

Fick’s Law relates the rate of transmission across the endpoints of the interval to the concentration gradient of the substance in the interval. The concentration gradient is given by the spatial partial derivative of \( c \),

\[
\frac{d}{dt} \int_{x_1}^{x_2} c(x, t)dx = D c_x(x_2, t) - D c_x(x_1, t)
\]

where \( c_x \equiv \frac{\partial c}{\partial x} \)

\( D \) is a constant.

4.3 Diffusion PDE

Note. The calculation is similar to that performed in our previous study of splines.

Notice that the right hand side of Fick’s Law can be rewritten using the Fundamental Theorem of Calculus,

\[
D c_x(x_2, t) - D c_x(x_1, t) = \int_{x_1}^{x_2} Dc_{xx}(x, t)dx
\]

On the left side of Fick’s Law, the time derivative and the integral can be interchanged,

\[
\frac{d}{dt} \int_{x_1}^{x_2} c(x, t)dx = \int_{x_1}^{x_2} c_t(x, t)dx
\]

Using these two substitutions,

\[
\int_{x_1}^{x_2} c_t(x, t)dx = \int_{x_1}^{x_2} Dc_{xx}(x, t)dx
\]

\[
\Rightarrow \int_{x_1}^{x_2} (c_t - Dc_{xx}) (x, t)dx = 0
\]

Since this equation must hold for any values of \( x_1 \) and \( x_2 \), it must be that the integrand is identically 0.
This is the diffusion PDE.

4.4 Dimensional analysis

4.4.1 Units of the constant $D$

We would like to know the units of the constant $D$. The three fundamental types of units in nature are mass ($M$), length ($L$), and time ($T$). We would like to form the units of $D$ in terms of these three types of units. We will also see how the dimensional analysis approach developed here will be useful in other numerical analysis problems.

Let brackets denote units, so that $[D] = \text{units of } D$. With this notation,

$$[c] = \frac{[c]}{[T]} \quad [c_{xx}] = \frac{[c]}{[L]^2}$$

Since the units of the quantities in the diffusion PDE must be the same,

$$\frac{[\mathcal{C}]}{[T]} = \frac{[D][\mathcal{C}]}{[T]^2}$$

$$\Rightarrow [D] = \frac{[L]^2}{[T]}$$

Note. The units of $c$ canceled in this calculation. This is a general occurrence in linear PDEs: if the PDE is linear, the units of the dependent variable will are not important for dimensional analysis.

4.4.2 Speed of diffusion

This dimensional analysis can be useful as follows. Imagine a concentrated spot of one liquid within a larger body of another liquid. This small spot will spread over time. Let $d(t)$ be the size of the spot at the time $t$.

Note. We treat the case in which the larger body of liquid is still, otherwise the concentration would spread by advection, which is a different transport process that is not governed by the diffusion equation.

We would like to estimate $d$ using only dimensional analysis knowing that this is a diffusion process. The simplest possibility is given by the Buckingham-$\pi$ theorem. Since $d$ has units of length, and $D$ has units of
length squared divided by time, we expect that \( d \) should be proportional to some power of \( D \) times some power of \( T \),

\[
d \propto D^\alpha t^\beta
\]

where \( \alpha \) and \( \beta \) are constants to be determined. Using our previous numerical analysis, we can compare the units of these quantities,

\[
L^2 = \left( \frac{L^2}{T} \right)^\alpha T^\beta = L^{2\alpha}T^{\beta-\alpha}
\]

Matching powers of \( L \) and \( T \) on both sides of the equation,

\[
1 = 2\alpha \Rightarrow \alpha = \frac{1}{2} \quad \beta - \alpha = 0 \Rightarrow \beta = \alpha = \frac{1}{2}
\]

Using this simple calculation, we can now make an estimate of the size of the concentration,

\[
d(t) \propto \sqrt{Dt}
\]

This example relates to numerical solutions of the diffusion equation as follows. In this and other similar numerical ODE problems, we consider two variables: space and time. We create a two-dimensional mesh on which to calculate an approximation to the solution to the ODE. Let the spacings of the mesh be \( \Delta x \) and \( \Delta t \).

We would like to know what parameter determines the stability of the method that we will examine shortly. There is only one way to create a dimensionless combination of the variables \( D \), \( \Delta x \), and \( \Delta t \), and so we presume that this quantity will relate to the stability of the method. Performing the dimensional analysis,

\[
[D \cdot \Delta t] = \frac{L^2}{T} \cdot T = L^2
\]

\[
\Rightarrow \left[ D \cdot \frac{\Delta t}{(\Delta x)^2} \right] = [0]
\]

We will see that in order to achieve stability with the numerical method that we will use to solve the diffusion equation, we must have,

\[
D \cdot \frac{\Delta t}{(\Delta x)^2} < \frac{1}{2}
\]
4.4.3 Megatonnage of an atomic bomb explosion

We now take a digression to consider an example that illustrates the full power of this method of dimensional analysis.

Numerical analysis can be used to determine the megatonnage of an atomic blast. When an atomic bomb is detonated, the initial shape of the cloud is approximately spherical before it begins to rise and form a mushroom cloud. It is possible to measure the radius of the blast cloud as a function of time, call it \( r(t) \).

A famous British fluid mechanist named G.I. Taylor used a measurement of \( r(t) \) and dimensional analysis to determine the megatonnage of an atomic bomb blast. He determined \( r(t) \) by measuring a time-series of photos in a newspaper report about an atomic bomb test. He then plotted \( \log r \) as a function of \( \log t \) from his measurements. He obtained a straight line with slope \( \frac{2}{5} \). He was able to compute the megatonnage of the blast using the intercept of this line with the horizontal axis, which corresponds to the point \( \log t = 0 \).

He began with \( r(t) \), which has units of length. This quantity should depend on the megatonnage of the explosion, \( E \), the density of the air in which the cloud is forming, \( \rho \), and the time elapsed, \( t \). Since \( r \) is a length, mass cannot appear in the final answer. Hence \( E \) and \( \rho \) must be combined to cancel the factor of mass. The proper combination is \( \frac{E}{\rho} \),

\[
\left[ \frac{E}{\rho} \right] = \frac{ML^2}{MT^3} = \frac{L^5}{T^2}
\]

Now use the same general form of the combination of the two quantities in the dimensional analysis,

\[
r(t) = \left( \frac{E}{\rho} \right)^\alpha t^\beta \Rightarrow L^1 = \left( \frac{L^5}{T^2} \right)^\alpha T^\beta = L^{5\alpha}T^{\beta-2\alpha}
\]

Matching powers of \( L \) and \( T \) as before,

\[
1 = 5\alpha \Rightarrow \alpha = \frac{1}{5} \quad \beta - 2\alpha = 0 \Rightarrow \beta = \frac{2}{5}
\]
Hence \( r(t) \propto \left( \frac{E}{\rho} \right)^{\frac{1}{5}} t^{\frac{2}{5}} \). Taking the logarithm with respect to time gives the slope of \( \frac{2}{5} \) as claimed. The point \( \log t = 0 \) corresponds to \( t = 1 \), at which point \( r(t) \propto \left( \frac{E}{\rho} \right)^{\frac{1}{5}} \). Since the density of air is known, this value can be used to find \( E \), the megatonnage of the blast.

**Note.** It turns out that the constant of proportionality between \( r \) and \( \left( \frac{E}{\rho} \right)^{\frac{1}{5}} t^{\frac{2}{5}} \) is 1.03, so our results are very nearly exact.

### 4.5 Initial value problem

The usual initial condition for the diffusion equation is to specify the concentration at all points at \( t = 0 \), meaning \( c(x, 0) \) is given \( \forall x \). We will see that the solutions take the form,

\[
c(x, t) = \frac{1}{2\sqrt{\pi Dt}} \int_{-\infty}^{\infty} c(x', 0) e^{-\frac{(x-x')^2}{4Dt}} \, dx'
\]