Second Order ODEs

- Often physical or biological systems are best described by second or higher-order ODEs. That is, second or higher order derivatives appear in the mathematical model of the system.

  For example, from physics we know that Newtons laws of motion describe trajectory or gravitational problems in terms of relationships between velocities, accelerations and positions. These can often be described as IVPs, where the ODE has the form,

  $$y''(x) = f(x, y)$$

  or

  $$y''(x) = f(x, y, y').$$

Second Order ODEs (cont)

A Second-order scalar ODE can be reduced to an equivalent system of first-order ODEs as follows: With $y^{''} = f(x, y, y')$ we let $Z(x)$ be defined by,

$$Z(x) = [z_1(x), z_2(x)]^T,$$

where $z_1(x) \equiv y(x)$ and $z_2(x) \equiv y'(x)$. It is then clear that $Z(x)$ is the solution of the first order system of IVPs:

$$\begin{aligned} Z' &= \begin{bmatrix} z_1'(x) \\ z_2'(x) \end{bmatrix} = \begin{bmatrix} y'(x) \\ y''(x) \end{bmatrix} \\ &= \begin{bmatrix} z_2(x) \\ f(x, y, y') \end{bmatrix} = \begin{bmatrix} z_2(x) \\ f(x, z_1, z_2) \end{bmatrix} \\ &\equiv F(x, Z). \end{aligned}$$

Observations re 2^{nd}-order ODEs

- Note that in solving this ‘equivalent’ system for $Z(x)$, we determine an approximation to $y'(x)$ as well as to $y(x)$. This has implications for numerical methods as, when working with this equivalent system, we will also be trying to accurately approximate $y'(x)$ and this may be more difficult than just approximating $y(x)$.
- Note also that to determine a unique solution to our problem we must prescribe initial conditions for $Z(a)$, that is for both $y(a)$ and $y'(a)$.
- Second order systems of ODEs can be reduced to first order systems similarly (doubling the number of equations).
- Higher order equations can be reduced to first order systems in a similar way.

Numerical Methods for IVPs

Taylor Series Methods:

If $f(x,y)$ is sufficiently differentiable wrt x and y then we can determine the Taylor series expansion of the unique solution $y(x)$ to

$$y' = f(x,y), \;\; y(a) = y_0,$$

by differentiating the ODE at the point $x_0 = a$. That is, for x near $x_0 = a$ we have,

$$y(x) = y(x_0) + (x - x_0)y'(x_0) + \frac{(x-x_0)^2}{2} y''(x_0) + \cdots,$$

Taylor Series Methods (cont)

To generate the TS coefficients, $y^{(n)}(x_0)/n!$, we differentiate the ODE and evaluate at $x = x_0 = a$. The first few terms are computed from the expressions,

$$\begin{aligned} y'(x) = f(x,y) &= f, \\ y''(x) = \frac{d}{dx} f(x,y) &= f_x + f_y y' \;\; = f_x + f_y f, \\ y'''(x) = \frac{d}{dx}[y''(x)] &= (f_{xx} + f_{xy} f) + (f_{yx} + f_{yy} f) f + f_y (f_x + f_y f) \\ &= f_{xx} + 2 f_{xy} f + f_{yy} f^2 + f_y f_x + f_y^2 f. \end{aligned}$$

Key Observation for TS Methods

- In general, if $f(x, y)$ is sufficiently differentiable, we can use the first $(k+1)$ terms of the Taylor series as an approximation to $y(x)$ for $|(x-x_0)|$ 'small'. That is, we can approximate $y(x)$ by $\hat{z}_{k,0}(x)$,

$$\hat{z}_{k,0}(x) \equiv y_0 + (x-x_0)y_0' + \cdots + \frac{(x-x_0)^k}{k!}y_0^k.$$

Note that the derivatives of y become quite complicated so one usually chooses a small value of k ($k \leq 6$ or 7).

Key Observation for TS (cont)

- One can use $\hat{z}_{k,0}(x_1)$ as an approximation, y_1, to $y(x_1)$. We can then evaluate the derivatives of $y(x)$ at $x = x_1$ to define a new polynomial $\hat{z}_{k,1}(x)$ as an approximation to $y(x)$ for $|(x - x_1)|$ 'small' and repeat the procedure.

  Note:
  - The resulting $\hat{z}_{k,j}(x)$ for $j = 0, 1, \cdots$ define a piecewise polynomial approximation to $y(x)$ that is continuous on $[a, b]$.
  - How do we choose $h_j = (x_j - x_{j-1})$ and k?

TS Method – Summary

Let $T_k(x, y_{j-1})$ denote the first $k+1$ terms of the Taylor series expanded about the discrete approximation, (x_{j-1}, y_{j-1}), and $\hat{z}_{k,j}(x)$ be the polynomial approximation (to $y(x)$) associated with this truncated Taylor series,

$$\begin{aligned} \hat{z}_{k,j}(x) &= y_{j-1} + \Delta\, T_k(x, y_{j-1}), \\ T_k(x, y_{j-1}) &\equiv f(x_{j-1}, y_{j-1}) + \frac{\Delta}{2} f^{'}(x_{j-1}, y_{j-1}) \cdots + \frac{\Delta^{k-1}}{k!} f^{(k-1)}(x_{j-1}, y_{j-1}), \end{aligned}$$

where $\Delta = (x - x_{j-1})$.

A simple, constant stepsize (fixed h) TS method is then given by:

-Set $h = (b-a)/N$;

-for $j = 1, 2, \cdots N$

$x_j = x_{j-1} + h$;

$y_j = y_{j-1} + h\, T_k(x_j, y_{j-1})$;

-end

Local/Global Errors

Note that, strictly speaking, $z_{k,j}(x)$ is not a direct approximation to $y(x)$ but to the solution of the 'local' IVP:

$$z_j' = f(x, z_j), \quad z_j(x_{j-1}) = y_{j-1}.$$

Since y_{j-1} will not be equal to $y(x_{j-1})$ in general, the solution to this local problem, $z_j(x)$, will not then be the same as $y(x)$.
To understand and appreciate the implications of this observation we distinguish between the 'local' and 'global' errors.
Definitions:

- The local error associated with step j is $z_j(x_j) - y_j$.
- The global error at x_j is $y(x_j) - y_j$.

A Classical Approach

A Classical (pre 1965) numerical method approximates $y(x)$ by dividing $[a, b]$ into equally spaced subintervals, $x_j = a + j\ h$ (where $h = (b - a)/N$) and, proceeding in a step-by-step fashion, generates y_j after $y_1, y_2, \cdots y_{j-1}$ have been determined.

- If the Taylor series method is used in this way, then the TS theorem with remainder shows that the local error on step j (for the TS method of order k) is:

$$E_j = \frac{h^{k+1} f^{(k)}(\eta_j, z_j(\eta_j))}{(k+1))!} = \frac{h^{k+1} z_j^{(k+1)}(\eta_j)}{(k+1)!}.$$

- If $k = 1$ we have Eulers Method where $y_j = y_{j-1} + h\ f(x_{j-1}, y_{j-1})$, and the associated local error satisfies,

$$LE_j = \frac{h^2}{2} y''(\eta_j).$$

Error Bounds for IVP Methods

Definition: A method is said to converge iff,

$$\lim_{h\to 0,(N\to\infty)} \left\{ \max_{j=1,2,\cdots N} |y(x_j) - y_j| \right\} \to 0.$$

- **Theorem:** (typical of classical convergence results) Let $[x_j, y_j]_{j=0}^{N}$ be the approximate solution of the IVP, $y^{'} = f(x,y),\ y(a) = y_0$ over $[a,b]$ generated by Euler's method with constant stepsize $h = (b-a)/N$. If the exact solution, $y(x), \in C^2[a,b]$ and $|f_y| < L,\ |y^{''}(x)| < Y$ then the associated GE, $e_j = y(x_j) - y_j$, $x_j = a + j\ h$ satisfies (for all $j > 0$),

$$\begin{aligned} |e_j| &\leq \frac{hY}{2L}(e^{(x_j - x_0)L} - 1) + e^{(x_j - x_0)L}|e_0|, \\ &\leq \frac{hY}{2L}(e^{(b-a)L} - 1) + e^{(b-a)L}|e_0|. \end{aligned}$$

Observations re Convergence

1. e_0 will usually be equal to zero.
2. This bound is generally pessimistic as it is exponential in $(b-a)$ where linear error growth is often observed on practical or realistic problems.
3. In the general case one can show that when local error is $O(h^{p+1})$ the global error is $O(h^p)$.

Proof of Conv Th (outline)

Eulers Method satisfies,

$$y_j = y_{j-1} + hf(x_{j-1}, y_{j-1}).$$

A Taylor series expansion of $y(x)$ about $x = x_{j-1}$ implies

$$y(x_j) = y(x_{j-1}) + hf(x_{j-1}, y(x_{j-1})) + \frac{h^2}{2} y^{''}(\eta_j).$$

Subtracting the first equation from the second we obtain,

$$y(x_j) - y_j \;\; = \;\; y(x_{j-1}) - y_{j-1} + h[f(x_{j-1}, y(x_{j-1})) - f(x_{j-1}, y_{j-1})] + \frac{h^2}{2} y^{''}(\eta_j).$$

If $Y = \max_{x \in [a,b]} |y^{''}(x)|$ and $|f_y| \leq L$, then, from the definition of e_j and the observation that $f(x, y)$ satisfies a Lipschitz condition with respect to y, we have ...

Proof (cont)

$$\begin{aligned}|e_j| &\leq |e_{j-1}| + hL|y(x_{j-1}) - y_{j-1}| + |\frac{h^2}{2}y^{''}(\eta_j)|, \\ &\leq |e_{j-1}| + hL|e_{j-1}| + \frac{h^2}{2}Y, \\ &= |e_{j-1}|(1 + hL) + \frac{h^2}{2}Y.\end{aligned}$$

This is a linear recurrence relation (or inequality) which after some work (straightforward) can be shown to imply our desired result,

$$|e_j| \leq \frac{hY}{2L}(e^{(b-a)L} - 1) + e^{(b-a)L}|e_0|.$$

Note that this is only an upper bound on the global error and it may not be sharp.

An Example

Consider the following equation,

$$y^{'} = y, \;\; y(0) = 1, \;\; \text{on } [0, 1].$$

Now since $\frac{\partial f}{\partial y} = 1$, $L = 1$ and since $y(x) = e^x$, we have $Y = e$ and $e_0 = 0$. Applying our error bound with $h = 1/N$ and $y_N \approx y(1) = e$ we obtain,

$$|GE_N| = |y_N - e| \leq \frac{he}{2}(e - 1) < 2.4h.$$

But for $h = .1$ we observe that $y_{10} = 2.5937..$ with an associated true error of $.1246..$ ($\equiv e - y_{10}$). This error bound is $.24$. This is an overestimate by a factor of 2.

Exercise: Compare the bound to the true error for $h = .01, \;\; h = .001$.

Limitations of Classical Approach

- Analysis is valid only in the limit as $h \to 0$.
- Bounds are usually very pessimistic (can overestimate the error by several orders of magnitude).
- Analysis does not consider the affect of f.p. arithmetic.