ENGSCI 233 - Iteration

Colin Simpson

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Department of Engineering Science
University of Auckland
(Beamer Theme: Metropolis)

Introduction

This module focuses on numerical solution methods for Ordinary Differential Equations (ODEs).

As well as algorithmic implementation, we will consider:

- Accuracy
- Stability
- Convergence

1. Iterative Methods for ODEs

First-Order ODE

Consider a first-order linear ODE of the generalised form:

$$\frac{dy}{dt} = f\left(t, y\right)$$

where the derivative of y with respect to t can be represented as a function of both these variables, $f\left(t, y\right)$.

The aim is to iteratively solve this ODE numerically for $y\left(t\right)$, starting from some initial condition $y^{(0)} = y\left(t^{(0)}\right)$.

Notation in ENGSCI 233/331

The notation I will try to use consistently throughout this topic:

- t is the independent variable
- y is the dependent variable
- h is the step size along t
- k is the iteration or step number
- $k = 0$ represents an initial state
- $t^{(k+1)} = t^{(k)} + h$
- $y^{(k)} = y\left(t^{(k)}\right)$

Euler as a Runge-Kutta Method

Runge-Kutta (RK) methods use a sum of n weighted derivative evaluations to iterate the solution. Expressed in a general form:

$$y^{(k+1)} = y^{(k)} + h \sum_{i=0}^{n-1} \alpha_i f_i$$

where α_i are weights assigned to each derivative evaluation, f_i.

Expressing the Euler method ($n = 1$) as an RK method:

$$y^{(k+1)} = y^{(k)} + h f_0$$
$$f_0 = f\left(t^{(k)}, y^{(k)}\right)$$

This derivative is evaluated at the start of the step.

Improved Euler as a Runge-Kutta Method

The Improved Euler method ($n = 2$) expressed as an RK method:

$$y^{(k+1)} = y^{(k)} + h\left(\frac{f_0}{2} + \frac{f_1}{2}\right)$$
$$f_0 = f\left(t^{(k)}, y^{(k)}\right)$$
$$f_1 = f\left(t^{(k)} + h, y^{(k)} + hf_0\right)$$

Where we evaluate the f_1 derivative is dependent on the f_0 derivative evaluation. This is an explicit method i.e. derivative evaluations depend only on previously evaluated ones.

Derivative Evaluations in Explicit Runge-Kutta Methods

The derivative evaluations in an explicit Runge-Kutta method depend on previous ones. This can be generalised to:

$$f_i = f\left(t^{(k)} + \beta_i h, y^{(k)} + h\sum_{j=0}^{n-1} \gamma_{ij} f_j\right)$$

where:

- β are nodes i.e. how far along the independent variable we evaluate the derivative.
- γ form the RK matrix i.e. how our derivative evaluation depends on the other derivative evaluations.

Improved Euler (Again)

Expressing the derivative evaluations of the Improved Euler method $(n = 2)$ in our most generalised form:

$$
\begin{aligned}
y^{(k+1)} &= y^{(k)} + h\left(\frac{1}{2} \cdot f_0 + \frac{1}{2} \cdot f_1\right) \\
f_0 &= f\left(t^{(k)} + 0 \cdot h, y^{(k)} + h\left(0 \cdot f_0 + 0 \cdot f_1\right)\right) \\
f_1 &= f\left(t^{(k)} + 1 \cdot h, y^{(k)} + h\left(1 \cdot f_0 + 0 \cdot f_1\right)\right)
\end{aligned}
$$

Allowing us to write out the nodes and RK matrix as:

Butcher Tableau

A convenient tool for displaying α, β and γ is known as the Butcher Tableau (developed by a staff member at UoA):

$$\begin{array}{c|c} \beta^T & \gamma \\ \hline & \alpha \end{array}$$

RK methods are commonly presented in this format. It is easy to re-construct the governing equations from the tableau.

Explicit RK Methods

For an explicit RK method, γ must be a lower triangular matrix, as well as zero along the diagonal. This is because each derivative calculated only depends on the *prior* derivatives.

Euler Method

The Euler method ($n = 1$) governing equation:

$$y^{(k+1)} = y^{(k)} + hf_0$$
$$f_0 = f\left(t^{(k)}, y^{(k)}\right)$$

The Butcher tableau for the Euler method:

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$

Improved Euler Method

The Improved Euler method ($n = 2$) expressed as an RK method:

$$y^{(k+1)} = y^{(k)} + h\left(\frac{f_0}{2} + \frac{f_1}{2}\right)$$

$$f_0 = f\left(t^{(k)}, y^{(k)}\right)$$

$$f_1 = f\left(t^{(k)} + h, y^{(k)} + hf_0\right)$$

The Butcher tableau for the Improved Euler method:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

The Classic RK4 Method

The classic RK4 method uses $n = 4$ derivative evaluations and is fourth-order accurate:

$$y^{(k+1)} = y^{(k)} + h\left(\frac{f_0 + 2f_1 + 2f_2 + f_3}{6}\right)$$

where:

$$f_0 = f\left(t^{(k)}, y^{(k)}\right)$$

$$f_1 = f\left(t^{(k)} + \frac{h}{2}, y^{(k)} + \frac{hf_0}{2}\right)$$

$$f_2 = f\left(t^{(k)} + \frac{h}{2}, y^{(k)} + \frac{hf_1}{2}\right)$$

$$f_3 = f\left(t^{(k)} + h, y^{(k)} + hf_2\right)$$

The Classic RK4 Method

The Butcher tableau for the classic RK4 method:

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$