ENGSCI 233 - Iteration

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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
- $t^{(k+1)} = t^{(k)} + h$ (constant 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:

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

estimate of slope across the step taken

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

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

$$y^{(k+1)} = y^{(k)} + hf_0$$

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

$(\alpha_0 = 1)$

$(k_0 = f_0)$

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:

$$y^{(k+1)} = y^{(k)} + h\left(\frac{f_0}{2} + \frac{f_1}{2}\right) \qquad \alpha_0 = \alpha_1 = \frac{1}{2}$$

$$f_0 = f\left(t^{(k)}, y^{(k)}\right) \qquad \text{(same as Euler)}$$

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

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:

$0 \le \beta_i \le 1$

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

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:

weights

nodes

RK matrix

$$
\begin{aligned}
y^{(k+1)} &= y^{(k)} + h\left(\overset{\alpha_0}{\frac{1}{2}} \cdot f_0 + \overset{\alpha_1}{\frac{1}{2}} \cdot f_1\right) \\
f_0 &= f\left(t^{(k)} + \overset{\beta_0}{0} \cdot h, y^{(k)} + h\left(\overset{\gamma_{00}}{0} \cdot f_0 + \overset{\gamma_{01}}{0} \cdot f_1\right)\right) \\
f_1 &= f\left(t^{(k)} + \overset{\beta_1}{1} \cdot h, y^{(k)} + h\left(\underset{\gamma_{10}}{1} \cdot f_0 + \underset{\gamma_{11}}{0} \cdot f_1\right)\right)
\end{aligned}
$$

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:

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

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:

$$\begin{array}{cc|ccc}
 & & \gamma_{00} & \gamma_{01} & \\
\beta_0 & 0 & 0 & 0 & \\
\beta_1 & 1 & 1 & 0 & \gamma_{11} \\
 & & \gamma_{10} & & \\
\hline
 & & \frac{1}{2} & \frac{1}{2} & \\
 & & \alpha_0 & \alpha_1 &
\end{array}$$

The Classic RK4 Method

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

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

$\alpha_0 = \alpha_3 = \frac{1}{6}$

$\alpha_1 = \alpha_2 = \frac{1}{3}$

where:

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

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

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

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

$\beta_0 = 0$

$\beta_1 = \frac{1}{2}$

$\beta_2 = \frac{1}{2}$

$\beta_3 = 1$

$$\gamma = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

The Classic RK4 Method

The Butcher tableau for the classic RK4 method:

$$
\begin{array}{c|c|cccc}
 & & & & & \gamma \\
\beta_0 & 0 & 0 & 0 & 0 & 0 \\
\beta_1 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\
\beta_2 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\
\beta_3 & 1 & 0 & 0 & 1 & 0 \\
\hline
 & & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \\
 & & \alpha_0 & \alpha_1 & \alpha_2 & \alpha_3
\end{array}
$$