Foundations for Runge-Kutta Methods

MATH 375 *Numerical Analysis*

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Objectives

In this lesson we will learn to:

- write an IVP as an equivalent integral equation,
- approximate the solution to an IVP using various quadrature methods.

Equivalence of IVPs and Integral Equations

Consider the first-order IVP:

$$\begin{aligned} y' &= f(t, y) \\ y(t_0) &= y_0 \end{aligned}$$

If we wish to know $y(t_1)$ then integrate the ODE.

$$\begin{aligned} \int_{t_0}^{t_1} y' \, dt &= \int_{t_0}^{t_1} f(t, y) \, dt \\ [y(t)]_{t=t_0}^{t=t_1} &= \int_{t_0}^{t_1} f(t, y) \, dt \\ y(t_1) - y(t_0) &= \int_{t_0}^{t_1} f(t, y) \, dt \\ y(t_1) &= y_0 + \int_{t_0}^{t_1} f(t, y) \, dt \end{aligned}$$

Any of the available quadrature formulas can be used to approximate the remaining integral.

Solving Iteratively

If $y' = f(t, y)$ and $y(t_i)$ is known, then

$$y(t_{i+1}) = y(t_i + h) = y(t_i) + \int_{t_i}^{t_i+h} f(t, y)\, dt.$$

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Suppose the Trapezoidal Rule is used to approximate the integral.

$$y(t_{i+1}) = y(t_i) + \frac{h}{2}\left[f(t_i, y(t_i)) + f(t_{i+1}, y(t_{i+1}))\right] + O(h^3)$$

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Remarks:

- The RHS depends on $y(t_{i+1})$ which is what we are trying to approximate.
- We could solve this equation numerically for $y(t_{i+1})$.
- If $h = t_{i+1} - t_i$ is small then Euler's method may be accurate enough.

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Suppose the Trapezoidal Rule is used to approximate the integral.

$$\begin{aligned} y(t_{i+1}) &= y(t_i) + \frac{h}{2}\left[f(t_i, y(t_i)) + f(t_{i+1}, y(t_{i+1}))\right] + O(h^3) \\ &= y(t_i) + \frac{h}{2}\left[f(t_i, y(t_i)) + f(t_{i+1}, y(t_i) + h\, f(t_i, y(t_i)))\right] + O(h^3) \end{aligned}$$

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Simplification

The solution to the IVP:

$$\begin{aligned} y' &= f(t, y) \\ y(t_0) &= y_0 \end{aligned}$$

is approximated by

$$y(t_{i+1}) = y(t_i) + \frac{h}{2}(k_1 + k_2)$$

where

$$\begin{aligned} k_1 &= f(t_i, y(t_i)) \\ k_2 &= f(t_{i+1}, y(t_i) + h\,k_1). \end{aligned}$$

Pseudocode

Given an initial-value problem:

$$\begin{aligned} y' &= f(t, y) \\ y(t_0) &= y_0 \end{aligned}$$

the stopping time t_1 and the number of time steps N,

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Step 1: Set $t = t_0$; $y = y_0$; $h = (t_1 - t_0)/N$.
Step 2: For $j = 1, 2, \ldots, N$ do Steps 3–6:
    Step 3: Set $k_1 = f(t, y)$.
    Step 4: Set $k_2 = f(t + h, y + h\, k_1)$.
    Step 5: Set $y = y + \frac{h}{2}(k_1 + k_2)$.
    Step 6: Set $t = t + h$.
Step 7: OUTPUT $y$.
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Example

Consider the initial-value problem:

$$\frac{dy}{dt} = y - t^2 + 1$$
$$y(0) = \frac{1}{2}.$$

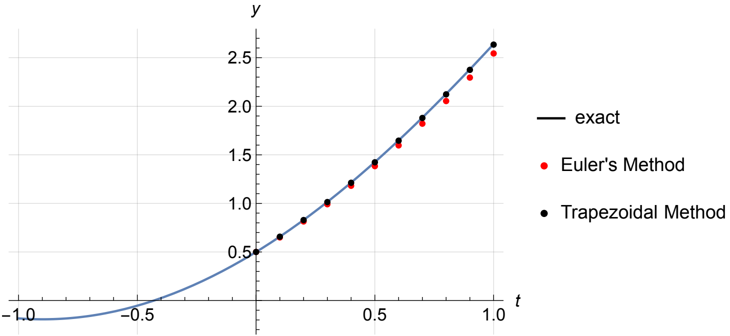
The exact solution is $y(t) = (1 + t)^2 - \frac{1}{2}e^t$.

Approximate the solution to this IVP for $0 \leq t \leq 1$ using Euler's method and the new method based on the Trapezoidal rule.

Results

t	**Euler**	**Trapezoidal**	**Exact**	**Euler error**	**Trapezoidal error**
0.0	0.5	0.5	0.5	0.0	0.0
0.1	0.65	0.657	0.657415	0.00741454	0.000414541
0.2	0.814	0.828435	0.829299	0.0152986	0.000863621
0.3	0.9914	1.01372	1.01507	0.0236706	0.00134992
0.4	1.18154	1.21221	1.21409	0.0325477	0.00187631
0.5	1.38369	1.42319	1.42564	0.0419454	0.00244583
0.6	1.59706	1.64588	1.64894	0.0518772	0.00306174
0.7	1.82077	1.8794	1.88312	0.0623539	0.00372751
0.8	2.05385	2.12278	2.12723	0.0733828	0.0044468
0.9	2.29523	2.37497	2.3802	0.0849671	0.00522352
1.0	2.54375	2.6348	2.64086	0.0971046	0.0060618

Illustration



The ODE-solver based on the Trapezoidal rule appears to give a more accurate result than the ODE-solver based on Euler’s method.

Using Simpson's Rule

If $y' = f(t, y)$ and $y(t_i)$ is known, then

$$y(t_{i+1}) = y(t_i + h) = y(t_i) + \int_{t_i}^{t_i+h} f(t, y)\, dt.$$

Suppose the Simpson's Rule is used to approximate the integral.

$$y(t_{i+1}) = y(t_i) + \frac{h}{6}\left[f(t_i, y(t_i)) + 4f(t_{i+\frac{1}{2}}, y(t_{i+\frac{1}{2}}) + f(t_{i+1}, y(t_{i+1}))\right] + O(h^5)$$

We must approximate the values of $f(t_{i+\frac{1}{2}}, y(t_{i+\frac{1}{2}}))$ and $f(t_{i+1}, y(t_{i+1}))$ using Euler's method as before.

Approximation

The solution to the IVP:

$$\begin{aligned} y' &= f(t, y) \\ y(t_0) &= y_0 \end{aligned}$$

is approximated by

$$y(t_{i+1}) = y(t_i) + \frac{h}{6}(k_1 + 4k_2 + k_3)$$

where

$$\begin{aligned} k_1 &= f(t_i, y(t_i)) \\ k_2 &= f(t_i + \frac{h}{2}, y(t_i) + \frac{h}{2}\,k_1) \\ k_3 &= f(t_i + h, y(t_i) + h\,k_2). \end{aligned}$$

Open Newton-Cotes: $n = 1$

Recall that

$$\int_{x_0}^{x_0+3h} f(x)\,dx = \frac{3h}{2}\left(f(x_0+h) + f(x_0+2h)\right) + O(h^3).$$

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Recall that

$$\int_{x_0}^{x_0+3h} f(x)\,dx = \frac{3h}{2}(f(x_0+h) + f(x_0+2h)) + O(h^3).$$

The solution to the IVP is approximated by

$$y(t_{i+1}) = y(t_i) + \frac{h}{2}(k_2 + k_3)$$

where

$$\begin{aligned} k_1 &= f(t_i, y(t_i)) \\ k_2 &= f(t_i + \frac{h}{3}, y(t_i) + \frac{h}{3}k_1) \\ k_3 &= f(t_i + \frac{2h}{3}, y(t_i) + \frac{2h}{3}k_2), \end{aligned}$$

Using Other Quadrature Formulas (1 of 2)

Suppose we develop a novel quadrature formula like

$$\int_{x_0}^{x_0+3h} f(x)\,dx = Af(x_0) + Bf(x_0+h) + Cf(x_0+2h) + E(f).$$

It can be engineered to have a precision of 2.

$$\int_{x_0}^{x_0+3h} 1\,dx = 3h = A + B + C$$

$$\int_{x_0}^{x_0+3h} (x-x_0)\,dx = \left[\frac{1}{2}(x-x_0)^2\right]_{x=x_0}^{x=x_0+3h} \frac{9h^2}{2} = A(0) + B\,h + C(2h)$$

$$\int_{x_0}^{x_0+3h} (x-x_0)^2\,dx = \left[\frac{1}{3}(x-x_0)^3\right]_{x=x_0}^{x=x_0+3h} 9h^3 = A(0) + B\,h^2 + C(4h^2)$$

Using Other Quadrature Formulas (2 of 2)

Solving the linear system:

$$\begin{aligned} A + B + C &= 3h \\ h\,B + (2h)C &= \frac{9h^2}{2} \\ (2h)\,B + (4h^2)C &= 9h^3 \end{aligned}$$

yields $A = \frac{3h}{4}$, $B = 0$, and $C = \frac{9h}{4}$.

Using Other Quadrature Formulas (2 of 2)

Solving the linear system:

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yields $A = \frac{3h}{4}$, $B = 0$, and $C = \frac{9h}{4}$.

Therefore

$$\int_{x_0}^{x_0+3h} f(x)\,dx \approx \frac{3h}{4}\left[f(x_0) + 3f(x_0+2h)\right].$$

We wil refer to this as a half-open (half-closed) Newton-Cotes quadrature formula.

Error Term (1 of 3)

The difference between the exact value of the definite integral and the quadrature formula is the error term $E(f)$.

$$\int_{x_0}^{x_0+3h} f(x)\,dx - \frac{3h}{4}\left[f(x_0) + 3f(x_0+2h)\right] = E(f)$$

Replace each occurence of f with its Taylor polynomial of degree 3 and the Taylor remainder.

$$\begin{aligned} E(f) = & \int_{x_0}^{x_0+3h} \left(f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2}(x-x_0)^2 + \frac{f'''(z(x))}{6}(x-x_0)^3 \right) dx \\ & - \frac{3h}{4} f(x_0) - \frac{9h}{4} \left(f(x_0) + f'(x_0)(2h) + \frac{f''(x_0)}{2}(2h)^2 + \frac{f'''(\xi)}{6}(2h)^3 \right) \end{aligned}$$

Carry out the integration step.

Error Term (2 of 3)

$$
\begin{aligned}
E(f) = & \int_{x_0}^{x_0+3h} \left(f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2}(x-x_0)^2 + \frac{f'''(z(x))}{6}(x-x_0)^3 \right) dx \\
& - \frac{3h}{4} f(x_0) - \frac{9h}{4} \left(f(x_0) + f'(x_0)(2h) + \frac{f''(x_0)}{2}(2h)^2 + \frac{f'''(\xi)}{6}(2h)^3 \right) \\
= & \, 3hf(x_0) + \frac{9h^2}{2} f'(x_0) + \frac{27h^3}{6} f''(x_0) + \int_{x_0}^{x_0+3h} \frac{f'''(z(x))}{6}(x-x_0)^3 \, dx \\
& - 3hf(x_0) - \frac{9h^2}{2} f'(x_0) - \frac{9h^3}{2} f''(x_0) - 3h^4 f'''(\xi) \\
= & \int_{x_0}^{x_0+3h} \frac{f'''(z(x))}{6}(x-x_0)^3 \, dx - 3h^4 f'''(\xi)
\end{aligned}
$$

Since $(x - x_0)^3 \geq 0$ for $x_0 \leq x \leq x_0 + 3h$ we may apply the weighted mean value theorem for integrals.

Error Term (3 of 3)

$$\begin{aligned} E(f) &= \int_{x_0}^{x_0+3h} \frac{f'''(z(x))}{6}(x-x_0)^3\,dx - 3h^4 f'''(\xi) \\ &= f'''(c)\int_{x_0}^{x_0+3h} \frac{1}{6}(x-x_0)^3\,dx \\ &= \frac{27h^4}{8} f'''(c) \end{aligned}$$

where $x_0 < c < x_0 + 3h$.

Thus the quadrature formula has error $O(h^4)$.

Half-Open Newton-Cotes

Recall that

$$\int_{x_0}^{x_0+3h} f(x)\,dx = \frac{3h}{4}(f(x_0) + 3f(x_0 + 2h)) + O(h^4).$$

Half-Open Newton-Cotes

Recall that

$$\int_{x_0}^{x_0+3h} f(x)\,dx = \frac{3h}{4}(f(x_0) + 3f(x_0 + 2h)) + O(h^4).$$

The solution to the IVP is approximated by

$$y(t_{i+1}) = y(t_i) + \frac{h}{4}(k_1 + 3k_3)$$

where

$$\begin{aligned} k_1 &= f(t_i, y(t_i)) \\ k_2 &= f(t_i + \frac{h}{3}, y(t_i) + \frac{h}{3}\,k_1) \\ k_3 &= f(t_i + \frac{2h}{3}, y(t_i) + \frac{2h}{3}\,k_2), \end{aligned}$$

Performance Comparison

Consider the IVP:

$$\frac{dy}{dt} = y - t^2 + 1$$
$$y(0) = \frac{1}{2}.$$

The exact solution is $y(t) = (1+t)^2 - \frac{1}{2}e^t$.

t	Simpson's	Open NC	Half-Open NC	Simpson's Error	Open NC Error	Half-Open NC Error
0.0	0.5	0.5	0.5	0.0	0.0	0.0
0.1	0.657454	0.657385	0.657411	1.270×10^{-4}	2.936×10^{-5}	3.430×10^{-6}
0.2	0.829885	0.829240	0.829292	2.628×10^{-4}	5.865×10^{-5}	6.997×10^{-6}
0.3	1.01709	1.01498	1.01506	4.078×10^{-4}	8.755×10^{-5}	1.069×10^{-5}
0.4	1.21886	1.21397	1.21407	5.624×10^{-4}	1.156×10^{-5}	1.450×10^{-5}
0.5	1.43495	1.4255	1.42562	7.270×10^{-4}	1.425×10^{-4}	1.841×10^{-5}
0.6	1.66509	1.64877	1.64892	9.020×10^{-4}	1.674×10^{-4}	2.240×10^{-5}
0.7	1.90899	1.88293	1.8831	1.088×10^{-3}	1.897×10^{-4}	2.644×10^{-5}
0.8	2.16631	2.12702	2.1272	1.285×10^{-3}	2.087×10^{-4}	3.049×10^{-5}
0.9	2.43671	2.37998	2.38016	1.493×10^{-3}	2.234×10^{-4}	3.452×10^{-5}
1.0	2.71978	2.64063	2.64082	1.713×10^{-3}	2.326×10^{-4}	3.848×10^{-5}

Remarks

In terms of absolute error, from largest to smallest the methods rank as

- Simpson's method
- Open Newton-Cotes $n = 1$
- Half-open Newton-Cotes.

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Since Simpson's method is $O(h^5)$ it seems odd that Simpson's method is performing so poorly. We will do an extended error analysis in the next section.

Order of Convergence (1 of 2)

Consider the absolute error in the calculation of $y(1)$ for the various ODE solving methods.

h	Euler	Trap	Open	1/2-Open	Simpson
$1/2$	3.909×10^{-1}	1.252×10^{-1}	8.272×10^{-3}	4.430×10^{-3}	3.992×10^{-2}
$1/4$	2.219×10^{-1}	3.537×10^{-2}	1.723×10^{-3}	5.876×10^{-4}	1.048×10^{-2}
$1/8$	1.195×10^{-1}	9.367×10^{-3}	3.755×10^{-4}	7.493×10^{-5}	2.668×10^{-3}
$1/16$	6.219×10^{-2}	2.407×10^{-3}	8.617×10^{-5}	9.433×10^{-6}	6.721×10^{-4}
$1/32$	3.176×10^{-2}	6.098×10^{-4}	2.053×10^{-5}	1.182×10^{-6}	1.686×10^{-4}
$1/64$	1.605×10^{-2}	1.534×10^{-4}	5.003×10^{-6}	1.480×10^{-7}	4.221×10^{-5}
$1/128$	8.070×10^{-3}	3.849×10^{-5}	1.234×10^{-6}	1.851×10^{-8}	1.056×10^{-5}

Divide the absolute error reported in each row by the absolute error in the row above.

Order of Convergence (2 of 2)

Each entry in the table below is nearly an integer power of $\frac{1}{2}$.

Euler	Trap	Open	1/2-Open	Simpson
0.567759	0.282401	0.20827	0.132658	0.262451
0.538382	0.264851	0.217939	0.12751	0.254687
0.520562	0.256969	0.229501	0.125887	0.251879
0.510663	0.253352	0.238256	0.125346	0.250812
0.505432	0.251641	0.243687	0.125148	0.250372
0.502742	0.250811	0.246723	0.125067	0.250178

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0.510663	0.253352	0.238256	0.125346	0.250812
0.505432	0.251641	0.243687	0.125148	0.250372
0.502742	0.250811	0.246723	0.125067	0.250178

	Euler	Trap	Open	1/2-Open	Simpson
Integration method	$O(h^2)$	$O(h^3)$	$O(h^3)$	$O(h^4)$	$O(h^5)$
ODE solver	$O(h^1)$	$O(h^2)$	$O(h^2)$	$O(h^3)$	$O(h^2)$

Homework

- Read Section 6.3.
- Exercises: