Introduction

• In this topic, we will
  – Derive the 4th-order Runge-Kutta method by estimating and averaging slopes
  – Look at the technique visually
  – See the error is $O(h^5)$ for a single step
  – Look at two examples of a single step
  – See how to apply this method under multiple steps
    • We will implement this in C++
  – Look at two examples of multiple steps
  – Compare the algorithm with Euler’s and Heun’s methods
Simpson’s rule

- A simple Reimann sum approximates an integral with one value:
  \[ \int_{a}^{b} f(x) \, dx \approx f(a)(b-a) \]

- The value of the function, however, changes across \([a, b]\), so Simpson’s rule integrates an interpolating quadratic:
  \[ \int_{a}^{b} f(x) \, dx \approx \frac{f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)}{6}(b-a) \]

4th-order Runge-Kutta method

- Heun’s method uses two slopes
  - We’d like to take more samples of the slope...

\[ y(t) = -0.2y(t) - \sin(t) - 0.1 \quad y(0) = 1 \]
4th-order Runge-Kutta method

• Without justification, 4th-order Runge-Kutta says to proceed as follows:

\[
\begin{align*}
    s_0 & \leftarrow f(t_k, y_k) \\
    s_1 & \leftarrow f\left(t_k + \frac{1}{2} h, y_k + \frac{1}{2} hs_0\right) \\
    s_2 & \leftarrow f\left(t_k + \frac{1}{2} h, y_k + \frac{1}{2} hs_1\right) \\
    s_3 & \leftarrow f\left(t_k + h, y_k + hs_2\right) \\
    y_{k+1} & \leftarrow y_k + h \frac{s_0 + 2s_1 + 2s_2 + s_3}{6}
\end{align*}
\]

• Visually, we proceed as follows

\[
y^{(i)}(t) = -0.2y(t) - \sin(t) - 0.1 \\
y(0) = 1
\]
One step of the 4th-order Runge-Kutta method

- What is the error? $O(h^4)$ or $O(h^5)$ or better?
  - We will look at two initial-value problems and approximate $y(t_0 + h)$ for successively smaller values of $h$
  - For example, approximate $y(0.4)$ with:

\[
y^{(1)}(t) = -y(t)
\]

\[
s_0 \leftarrow f(0, 1) = -1 \quad y(0) = 1
\]

\[
s_1 \leftarrow f(0.2, 1 + 0.2s_0) = -0.8
\]

\[
s_2 \leftarrow f(0.2, 1 + 0.2s_1) = -0.84
\]

\[
s_3 \leftarrow f(0.4, 1 + 0.4s_2) = -0.664
\]

\[
y_1 \leftarrow 1 + 0.4 \left( -1 + 2 \left( -0.8 + 2 \left( -0.84 + (-0.664) \right) \right) \right) = 0.6704
\]

\[e^{-0.4} = 0.6703200460356393\]

One step of the 4th-order Runge-Kutta method

- Let's approximate the solution at $y(0 + h)$ to

\[
y^{(1)}(t) = -y(t)
\]

\[
y(0) = 1
\]

\[
\begin{array}{|c|c|c|c|c|}
\hline
n & h = 2^{-n} & \text{Exact} & \text{Approximation} & \text{Error} & \text{Ratio} \\
\hline
1 & 0.5 & 0.606530659712633 & 0.606770833333333 & -0.0002402 & 0.03252 \\
2 & 0.25 & 0.7788007830714049 & 0.778808593750000 & -0.000007811 & 0.03189 \\
3 & 0.125 & 0.8824969025845955 & 0.882497151692708 & -0.000002491 & 0.03157 \\
4 & 0.0625 & 0.9394130628134758 & 0.939413070678109 & -0.0000007865 & 0.03141 \\
5 & 0.03125 & 0.9692332344763441 & 0.969233234723409 & -0.00000002471 & 0.03133 \\
6 & 0.015625 & 0.9844964370054085 & 0.984496437013149 & -0.000000007741 & 0.03130 \\
7 & 0.0078125 & 0.9922179382604858 & 0.992217938260485 & -0.0000000002423 & 0.03120 \\
8 & 0.00390625 & 0.9961013694701175 & 0.9961013694701251 & -0.00000000007550 & 0.03116 \\
9 & 0.001953125 & 0.9980487811074755 & 0.9980487811074757 & -0.000000000002220 & 0.02941 \\
10 & 0.0009765625 & 0.9990239141819757 & 0.9990239141819757 & 0 & 0 \\
\hline
\end{array}
\]
One step of the 4th-order Runge-Kutta method

- Let's approximate the solution at $y(0 + h)$ to
  
  $y^{(1)}(t) = -0.2y(t) - \sin(t) - 0.1$
  
  $y(x) = \frac{-13 + 25\cos(t) - 5\sin(t) + 14e^{-\frac{t}{5}}}{26}$

$$
\begin{array}{|c|c|c|c|c|}
\hline
n & h = 2^{-n} & \text{Exact} & \text{Approximation} & \text{Error} & \text{Ratio} \\
\hline
1 & 0.5 & 0.738852315643913 & 0.738856449702695 & -0.000004134 & 0.04123 \\
2 & 0.25 & 0.8962693342116731 & 0.8962695046719316 & -0.0000001705 & 0.03493 \\
3 & 0.125 & 0.9552271839309132 & 0.9552271898849072 & -0.00000005954 & 0.03286 \\
4 & 0.0625 & 0.997942225078814 & 0.997942227035564 & -0.00000000937 & 0.03201 \\
5 & 0.03125 & 0.99901670100357426 & 0.99901670100420059 & -0.0000000006263 & 0.03162 \\
6 & 0.015625 & 0.99951978758220640 & 0.99951978758222620 & -0.00000000001981 & 0.03195 \\
7 & 0.0078125 & 0.999976275785667972 & 0.999976275785668035 & -0.000000000006328 & 0.05263 \\
8 & 0.00390625 & 0.99999999999999999 & 0.99999999999999999 & -0.00000000000000000 & 0 \\
9 & 0.001953125 & 0.99999999999999999 & 0.99999999999999999 & -0.00000000000000000 & 0 \\
\hline
\end{array}
$$

Multiple steps of Heun’s method

- Can we see that the error is indeed $O(h^2)$
- As with Euler’s method:
  - First, we will implement a function to find the $n$ approximations by dividing a range $[t_0, t_f]$ into $n$ sub-intervals
  - For two IVPs with the initial condition $y(0) = 1$, we will approximate $y(5)$ by using $2^n$ intervals
Implementation

```cpp
std::tuple<double *, double *, double *> rk4(
    double f( double t, double y ), std::pair<double, double> t_rng, double y0,
    unsigned int n )
{
    double h{ (t_rng.second - t_rng.first)/n };
    double *ts{ new double[n + 1] };
    double *ys{ new double[n + 1] };
    double *dys{ new double[n + 1] };
    ts[0] = t_rng.first;
    ys[0] = y0;
    dys[0] = f( ts[0], ys[0] );
    for ( unsigned int k{0}; k < n; ++k )
    {
        ts[k + 1] = t_rng.first + h*(k + 1); // ts[k + 1] = ts[k] + h;
        double s0{ f( ts[k] + h/2.0, ys[k] + h*dys[k]/2.0 ) };
        double s1{ f( ts[k] + h/2.0, ys[k] + h*s0/2.0 ) };
        double s2{ f( ts[k] + h, ys[k] + h*s1/2.0 ) };
        double s3{ f( ts[k] + h, ys[k] + h*s2 ) };
        ys[k + 1] = ys[k] + h*(s0 + 2.0*s1 + 2.0*s2 + s3)/6.0;
        dys[k + 1] = f( ts[k + 1], ys[k + 1] );
    }
    return std::make_tuple( ts, ys, dys );
}
```

Multiple steps of 4th-order RK method

- Let's approximate the solution at $y(5)$ to

\[
y'(t) = -y(t) \\
y(0) = 1
\]

<table>
<thead>
<tr>
<th>$n$</th>
<th>Approximation</th>
<th>Error</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.42047119140625</td>
<td>-0.4137</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.00893558527119917</td>
<td>-0.002198</td>
<td>0.005312</td>
</tr>
<tr>
<td>8</td>
<td>0.006810674597968526</td>
<td>-0.00007273</td>
<td>0.03309</td>
</tr>
<tr>
<td>16</td>
<td>0.006741425022840268</td>
<td>-0.000003478</td>
<td>0.04782</td>
</tr>
<tr>
<td>32</td>
<td>0.006738137657266484</td>
<td>-0.00000001907</td>
<td>0.05482</td>
</tr>
<tr>
<td>64</td>
<td>0.00673798161994555</td>
<td>-0.0000001116</td>
<td>0.05855</td>
</tr>
<tr>
<td>128</td>
<td>0.006737947674390917</td>
<td>-0.000000006753</td>
<td>0.06050</td>
</tr>
<tr>
<td>256</td>
<td>0.006737947040610186</td>
<td>-0.0000000034152</td>
<td>0.06149</td>
</tr>
<tr>
<td>512</td>
<td>0.006737947001659729</td>
<td>-0.0000000002574</td>
<td>0.06199</td>
</tr>
<tr>
<td>1024</td>
<td>0.006737946999245688</td>
<td>-0.0000000001602</td>
<td>0.06224</td>
</tr>
</tbody>
</table>
Multiple steps of 4th-order RK method

- Let’s approximate the solution at \( y(5) \) to 4th-order Runge-Kutta method

\[
y(t) = \frac{-13 + 25 \cos(t) - 5 \sin(t) + 14e^{-t}}{26}
\]

\[
y(0) = 1
\]

<table>
<thead>
<tr>
<th>( n )</th>
<th>Approximation</th>
<th>Error</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.1469019038207984</td>
<td>0.008348</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.1548307896015398</td>
<td>0.0004188</td>
<td>0.05016</td>
</tr>
<tr>
<td>8</td>
<td>0.1552239200410955</td>
<td>0.00002570</td>
<td>0.06119</td>
</tr>
<tr>
<td>16</td>
<td>0.1552479334528051</td>
<td>0.000001612</td>
<td>0.06291</td>
</tr>
<tr>
<td>32</td>
<td>0.1552494441496338</td>
<td>0.0000001015</td>
<td>0.06294</td>
</tr>
<tr>
<td>64</td>
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<tr>
<td>256</td>
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<td>1024</td>
<td>0.1552495456266942</td>
<td>0.00000009581</td>
<td>0.06131</td>
</tr>
</tbody>
</table>

Comparison

- We could compare Euler, Heun and 4th-order Runge-Kutta for 1024 intervals
  - Issue: This isn’t really fair, as
    - Euler’s method uses one function evaluation per interval
    - Heun’s uses two
    - 4th-order Runge-Kutta uses four
  - For 1024 function evaluations, how accurate is each?

<table>
<thead>
<tr>
<th>Method</th>
<th>( n )</th>
<th>Approximation</th>
<th>Error</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Euler</td>
<td>1024</td>
<td>0.006655931188587414</td>
<td>0.00008202</td>
<td></td>
</tr>
<tr>
<td>Heun</td>
<td>512</td>
<td>0.006738486441915978</td>
<td>0.000005394</td>
<td></td>
</tr>
<tr>
<td>RK4</td>
<td>256</td>
<td>0.006737947040610186</td>
<td>0.00000004152</td>
<td></td>
</tr>
<tr>
<td>Euler</td>
<td>1024</td>
<td>0.152997481619969</td>
<td>0.002252</td>
<td></td>
</tr>
<tr>
<td>Heun</td>
<td>512</td>
<td>0.1552516585204115</td>
<td>0.000002113</td>
<td></td>
</tr>
<tr>
<td>RK4</td>
<td>256</td>
<td>0.1552495456018131</td>
<td>0.00000002498</td>
<td></td>
</tr>
</tbody>
</table>
Comparison

• Another question is:
  – How many function evaluations are required to get the same accuracy as Euler’s method with 1024 intervals?

<table>
<thead>
<tr>
<th>Method</th>
<th>Function Evaluations</th>
<th>Accuracy Difference</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Euler</td>
<td>1024</td>
<td>-0.00008202</td>
<td>1024</td>
</tr>
<tr>
<td>Heun</td>
<td>43</td>
<td>-0.00008336</td>
<td>86</td>
</tr>
<tr>
<td>RK4</td>
<td>8</td>
<td>-0.00007273</td>
<td>32</td>
</tr>
</tbody>
</table>

\[ y(5) = 0.00682130435141457 \]

<table>
<thead>
<tr>
<th>Method</th>
<th>Function Evaluations</th>
<th>Accuracy Difference</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Euler</td>
<td>1024</td>
<td>-0.002252</td>
<td>1024</td>
</tr>
<tr>
<td>Heun</td>
<td>16</td>
<td>-0.002317</td>
<td>32</td>
</tr>
<tr>
<td>RK4</td>
<td>3</td>
<td>0.0013827</td>
<td>12</td>
</tr>
</tbody>
</table>

\[ y(5) = 0.1552495456267901 \]

Summary

• Following this topic, you now
  – Understand the 4\textsuperscript{th}-order Runge-Kutta method for approximating a solution to a 1\textsuperscript{st}-order initial-value problem
  – Are aware of a visual interpretation with respect to slopes
  – Understand the error is \( O(h^5) \) for a single step
  – Are aware that we must apply this technique multiple times to estimate the solution on a larger interval
  – Know that the error drops in this case to \( O(h^4) \)
  – Have seen a number of examples and an implementation
  – Understand how much better the algorithm is, even when we consider the number of function evaluations
References


Acknowledgments

None so far.
Colophon

These slides were prepared using the Cambria typeface. Mathematical equations use Times New Roman, and source code is presented using Consolas. Mathematical equations are prepared in MathType by Design Science, Inc. Examples may be formulated and checked using Maple by Maplesoft, Inc.

The photographs of flowers and a monarch butter appearing on the title slide and accenting the top of each other slide were taken at the Royal Botanical Gardens in October of 2017 by Douglas Wilhelm Harder. Please see https://www.rbg.ca/ for more information.

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