Runge-Kutta Methods with Rooted Trees

The Motivation of the Project

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Outline

A brief review of numerical methods for ODEs

Given an Ordinary Differential Equation of form

$$y'(x) = f(x, y), \forall x \in [a, b]$$

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with initial condition $y(a) = y_0$, we can obtain a numerical approximation for $y(b)$ by first dividing the interval $[a, b]$ into N equally spaced subintervals $[x_0, x_1], [x_1, x_2], \dots, [x_{N-1}, x_N]$ where

$$h = \frac{(b-a)}{N}$$

$$x_{n+1} = x_n + h$$

Looking at individual steps

We then compute a sequence of approximations for $y(x)$

$$y_0 = y(x_0), y_1 \approx y(x_1) = y(x_0 + h), \ldots, y_N \approx y(x_N) = y(b)$$

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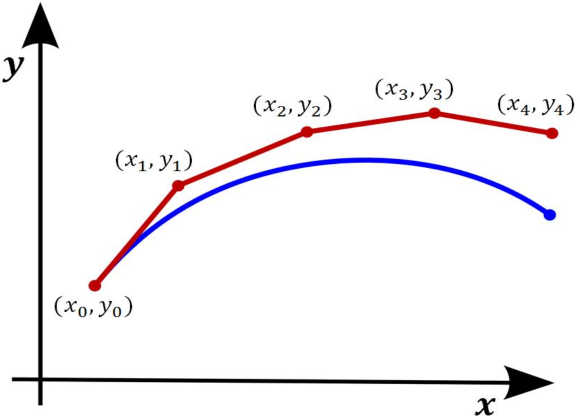
$$y(a) = y_0 \to y_1 \to \cdots \to y_N \approx y(b)$$

Example: Euler's method

$$x_{n+1} - x_n = h$$
$$y_{n+1} = y_n + hf(x_n, y_n)$$



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The order of a method tells us how fast it converges to the true value of what it is approximating.

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Taylor methods work using the Taylor Series expansion

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$$x_{n+1} - x_n = h$$

$$y_{n+1} = y_n + f(x_n, y_n)h + \frac{f'(x_n, y_n)h^2}{2!} + \ldots + \frac{f^{(p-1)}(x_n, y_n)h^p}{p!}$$

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What's nice about this is that if we want our numerical algorithm to be of a given order, then there exists a Taylor method with that order.

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$$f'''(x, y) = f_{xxx} + 3f_{xxy}f + 3f_{xyy}f^2 + f_{yyy}f^3 +$$
$$f_y(f_{xx} + 2f_{xy}f + f_{yy}f^2) + 3(f_x + f_y f)(f_{xy} + f_{yy}f) + f_y^2(f_x + f_y f)$$

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As before, we will split the interval into subintervals of equal width h and compute approximations y_n.

How to do Runge-Kutta

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So when going from y_n to y_{n+1} we will have $\mathbf{Y_1}, \mathbf{Y_2}, ..., \mathbf{Y_s}$ as our stages and $\mathbf{f}(\mathbf{X_1}, \mathbf{Y_1}), \mathbf{f}(\mathbf{X_2}, \mathbf{Y_2}), ..., \mathbf{f}(\mathbf{X_s}, \mathbf{Y_s})$ as our stage derivatives.

Computing stages

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$$Y_2 = y_n + a_{21} h f(x_n, y_n)$$

$$Y_3 = y_n + a_{31} h f(X_1, Y_1) + a_{32} h f(X_2, Y_2)$$

$$\vdots$$

$$Y_s = y_n + \sum_{j=1}^{s-1} a_{sj} h f(X_j, Y_j)$$

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The b_i terms are known as the **weights**.

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Since $X_1 = x_n$, we have $c_1 = 0$

Putting it all together

A convenient way to represent a Runge-Kutta method is by using a tableau of form

$$
\begin{array}{c|ccccc}
0 & & & & & \\
c_2 & a_{21} & & & & \\
c_3 & a_{31} & a_{32} & & & \\
\vdots & \vdots & \vdots & \ddots & & \\
c_s & a_{s1} & a_{s2} & \dots & a_{s(s-1)} & \\
\hline
 & b_1 & b_2 & \dots & b_s &
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\end{array}
$$

Where

- a_{ij} represents how stage i depends on the jth stage derivative,
- b_i represents the weight of $hf(X_i, Y_i)$ in computing y_{n+1},
- c_i represents the location of X_i in the interval $[x_n, x_{n+1}]$

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Deriving Runge-Kutta methods

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First we choose the number of stages to use in the algorithm. At least $s = p$ stages are necessary and there are advantages to using $s = p + 1$.

Then we compute the Taylor series expansions for the Taylor method of order p and the Runge-Kutta method with s stages. Equating coefficients leads us to a system of equations which when solved, tells us the values we can use for the Runge-Kutta method's parameters.

A necessary tool for deriving Runge-Kutta methods

In order to compare the Taylor series expansions we need the following general result:

Theorem

Bivariate Taylor Expansion: *Let $f(x, y)$ be an infinitely differentiable function in some open neighbourhood around (x_0, y_0), then*

$$f(x, y) = f(x_0, y_0) + f_x(x - x_0) + f_y(y - y_0)$$

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$$f(x,y) = f(x_0,y_0) + f_x(x-x_0) + f_y(y-y_0)$$

$$+\frac{1}{2!}(f_{xx}(x-x_0)^2 + f_{xy}(x-x_0)(y-y_0)$$

$$+f_{yx}(y-y_0)(x-x_0) + f_{yy}(y-y_0)^2)$$

$$+\ldots$$

2nd order Runge-Kutta methods with 2 stages

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and stage derivatives

$$f(X_1, Y_1) = f(x_n, y_n),$$

$$f(X_2, Y_2) = f(x_n + c_2 h, y_n + a_{21} h f(x_n, y_n)).$$

Obtaining the Taylor expansions

We thus have

$$y_{n+1} = y_n + hb_1 f(x_n, y_n) + hb_2 f(x_n + c_2 h, y_n + a_{21} hf(x_n, y_n))$$

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with expansion

$$y(x_{n+1}) = y_n + b_1 hf + b_2 hf + b_2 c_2 h^2 f_x + b_2 a_{21} h^2 f_y f + O(h^3)$$

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Equating coefficients gives us the system of equations

$$b_1 + b_2 = 1$$

$$b_2c_2 = \frac{1}{2}$$

$$b_2a_{21} = \frac{1}{2}$$

Obtaining the parameter values

Allowing b_2 to be a free parameter gives us the solution

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So all 2nd order Runge-Kutta methods with two stages are of form

$$\begin{array}{c|cc} 0 & & \\ \frac{1}{2b_2} & \frac{1}{2b_2} & \\ \hline & 1 - b_2 & b_2 \end{array}$$

Special cases of 2nd order Runge-Kutta methods

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Setting $b_2 = 1$ gives us the **midpoint method**

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and setting $b_2 = \frac{1}{2}$ gives us **Heun's method**.

$$y_{n+1} = y_n + \frac{h}{2}f(x_n, y_n) + \frac{h}{2}f(x_n + h, y_n + hf(x_n, y_n))$$

The RK4

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The RK4 is as follows

$$f(X_1, Y_1) = f(x_n, y_n)$$

$$f(X_2, Y_2) = f(x_n + \frac{h}{2}, y_n + \frac{h}{2} f(X_1, Y_1))$$
$$f(X_3, Y_3) = f(x_n + \frac{h}{2}, y_n + \frac{h}{2} f(X_2, Y_2))$$
$$f(X_4, Y_4) = f(x_n + h, y_n + hf(X_3, Y_3))$$

The RK4 (continued)

with weights

$$y_{n+1} = y_n + \frac{h}{6} f(X_1, Y_1) + \frac{h}{3} f(X_2, Y_2) + \frac{h}{3} f(X_3, Y_3) + \frac{h}{6} f(X_4, Y_4)$$

The RK4 (continued)

with weights

$$y_{n+1} = y_n + \frac{h}{6} f(X_1, Y_1) + \frac{h}{3} f(X_2, Y_2) + \frac{h}{3} f(X_3, Y_3) + \frac{h}{6} f(X_4, Y_4)$$

and tableau

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

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- we need higher derivatives of $f(x, y)$ for the coefficients of the Taylor method,
- we will need more terms from the bivariate Taylor expansion,
- more stage derivatives are popping up in the computation of Y_i.

System of equations for 4th order methods with four stages

$$a_{21} = c_2$$

$$a_{31} + a_{32} = c_3$$

$$a_{41} + a_{42} + a_{43} = c_4$$

$$b_1 + b_2 + b_3 + b_4 = 1$$

$$b_2 c_2 + b_3 c_3 + b_4 c_4 = \frac{1}{2}$$

$$b_2 c_2^2 + b_3 c_3^2 + b_4 c_4^2 = \frac{1}{3}$$

$$b_2 c_2^3 + b_3 c_3^3 + b_4 c_4^3 = \frac{1}{4}$$

System of equations for 4th order methods with four stages (continued)

$$b_3 a_{32} c_2 + b_4 a_{42} c_2 + b_4 a_{43} c_3 = \frac{1}{6}$$

$$b_3 c_3 c_2 a_{32} + b_4 c_4 c_2 a_{42} + b_4 c_4 c_3 a_{43} = \frac{1}{8}$$

$$b_3 c_2^2 a_{32} + b_4 c_2^2 a_{42} + b_4 c_3^2 a_{43} = \frac{1}{12}$$

$$b_4 c_2 a_{32} a_{43} = \frac{1}{24}$$

System of equations for 4th order methods with four stages (continued)

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From the way these equations are written, we can see some patterns.

Outline

The goal of the project

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What is the pattern?

The pattern

The first 3 equations

$$a_{21} = c_2$$

$$a_{31} + a_{32} = c_3$$

$$a_{41} + a_{42} + a_{43} = c_4$$

Correspond to summing the rows of a's in order to get the c values

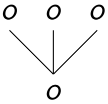
$$\begin{array}{c|cccc} 0 & & & & \\ c_2 & a_{21} & & & \\ c_3 & a_{31} & a_{32} & & \\ c_4 & a_{41} & a_{42} & a_{43} & \\ \hline & b_1 & b_2 & b_3 & b_4 \end{array}$$

Equations with trees

$$b_1 + b_2 + b_3 + b_4 = 1$$

$$b_1 c_1 + b_2 c_2 + b_3 c_3 + b_4 c_4 = \frac{1}{2}$$

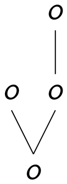
$$b_1 c_1^2 + b_2 c_2^2 + b_3 c_3^2 + b_4 c_4^2 = \frac{1}{3}$$



$$b_1 c_1^3 + b_2 c_2^3 + b_3 c_3^3 + b_4 c_4^3 = \frac{1}{4}$$

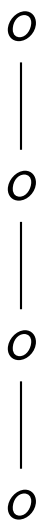
Equations with trees (continued)

$$\sum_{i,j=1}^{s} b_i a_{ij} c_j = \frac{1}{6}$$

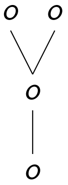


$$\sum_{i,j=1}^{s} b_i c_i a_{ij} c_j = \frac{1}{8}$$

Equations with trees (continued)



$$\sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk} c_k = \frac{1}{24}$$



$$\sum_{i,j=1}^{s} b_i a_{ij} c_j^2 = \frac{1}{12}$$

Obtaining the trees

Obtaining the trees

First order

o

Obtaining the trees

First order

o

Second order

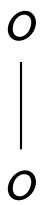
$$\begin{array}{c} o \\ | \\ o \end{array}$$

Obtaining the trees

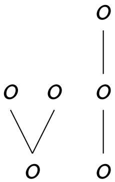
First order

o

Second order

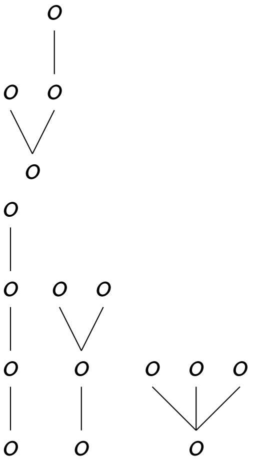


Third order



Fourth order trees

Fourth order



Conclusion

The goal of the project is to understand (with proof) how to use rooted trees to derive the system of equations for Runge-Kutta methods of a given order.

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Thank you for viewing my presentation ☺.

References

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