Numerical Solutions to Differential Equations

Lecture Notes #5 — Runge-Kutta Methods, Modern Approach

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Outline

Runge-Kutta Methods, continued

Recapping the mission...

- We are trying to solve the ODE

$$y'(t) = f(t, y), \quad y(t_0) = y_0, \quad t < T$$

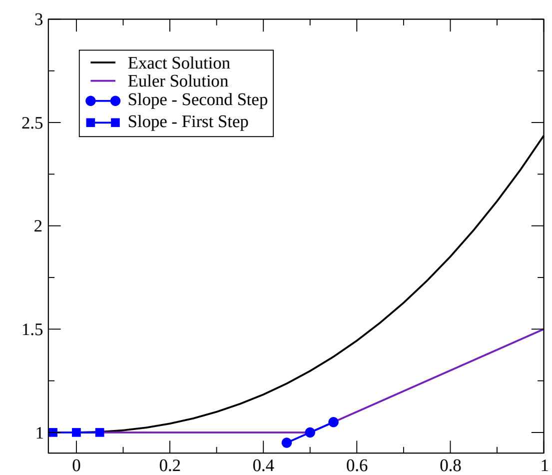
  using a numerical scheme applied to the discretization $t_n = t_0 + n \cdot h$, where h is the step-size (in time).

- In Euler's method we use the slope $f(t, y)$ evaluated at the current (known) time level (t_n, y_n) and use that value as an approximation of the slope throughout the interval $[t_n, t_{n+1}]$.

- RK-methods improve on Euler's method by looking at the slope at **multiple points.**

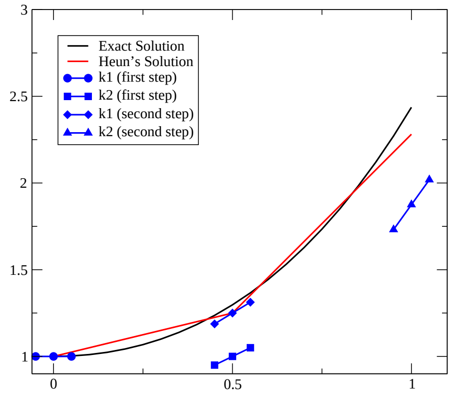
Euler's Method — $y'(t) = y(t) + 2t - 1,\ y(0) = 1\ (h = 1/2)$

Euler's Method samples the slope at the beginning of the step only.



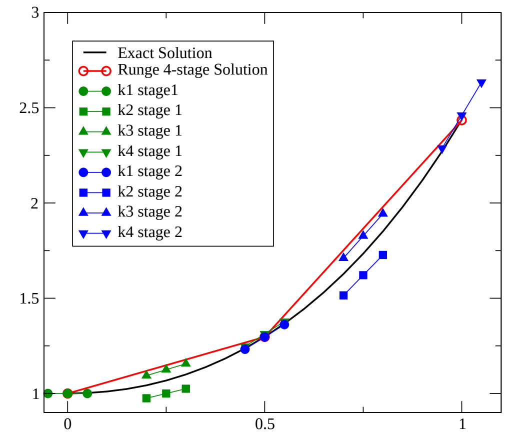
Heun's Method — $y'(t) = y(t) + 2t - 1,\ y(0) = 1\ (h = 1/2)$

Heun's method samples the slope at the beginning and the end, and uses the average as the final approximation of the slope.



Step#1: $k_1 = f(t_0, y_0)$, $k_2 = f(t_0 + h, y_0 + hk_1)$, $y_1 = y_0 + \frac{h}{2}(k_1 + k_2)$. Step#2: $k_1 = f(t_1, y_1)$, $k_2 = f(t_1 + h, y_1 + hk_1)$, $y_2 = y_1 + \frac{h}{2}(k_1 + k_2)$.

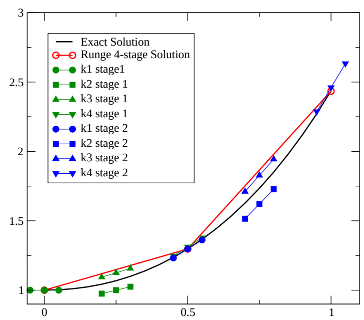
Runge's Method — $y'(t) = y(t) + 2t - 1,\ y(0) = 1\ (h = 1/2)$

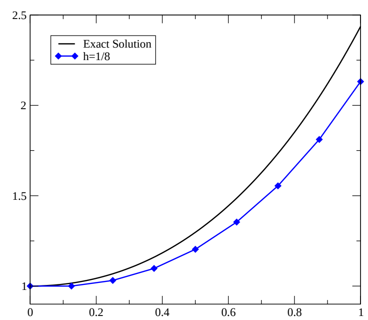


Stage#1: $k_1 = f(t_0, y_0)$, $k_2 = f(t_0 + h/2, y_0 + hk_1/2)$, $k_3 = f(t_0 + h/2, y_0 + hk_2/2)$, $k_4 = f(t_0 + h, y_0 + hk_3)$, $y_1 = y_0 + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$.
Stage#2: $k_1 = f(t_1, y_1)$, $k_2 = f(t_1 + h/2, y_1 + hk_1/2)$, $k_3 = f(t_1 + h/2, y_1 + hk_2/2)$, $k_4 = f(t_1 + h, y_1 + hk_3)$, $y_2 = y_1 + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$.

You may say... *"No Big Surprise There!"*

"Of course we do better with 8 measurements of the derivative (Runge with $h = \frac{1}{2}$), I bet if we used Euler's method with 8 measurements ($h = \frac{1}{8}$) we'd do just as good a job — and we wouldn't have to figure out the coefficients!"





Runge, $h = \frac{1}{2}$; LTE$(h) \sim \mathcal{O}(\mathbf{h^4})$ Euler, $h = \frac{1}{8}$; LTE$(h) \sim \mathcal{O}(h)$

Summary: Runge-Kutta vs. Euler

- By combining multiple "measurements" of the slope $y'(t) = f(t, y)$ in the step-interval, the RK-method builds up a more accurate final step.
  - In the previous example, where LTE$_{RK}(h) \sim \mathcal{O}(h^4)$, cutting the step-size (h) in half ($\Leftrightarrow$ doubling the number of measurements), reduces the error by a factor of $\frac{1}{2^4} = \frac{1}{16}$.
  - Roughly **Work** $\times$ **Error** $\sim \mathcal{O}(h^3)$
- Euler's method with the same number of "measurements" (smaller step-size h) is still a first order method.
  - Doubling the number of measurements reduces the error by $\frac{1}{2}$
  - Roughly **Work** $\times$ **Error** $\sim \mathcal{O}(1)$

The Butcher array for a 2-stage explicit RK method has the form:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ c_2 & a_{2,1} & 0 \\ \hline & b_1 & b_2 \end{array} \sim \begin{array}{c|cc} 0 & 0 & 0 \\ c_2 & c_2 & 0 \\ \hline & b_1 & 1-b_1 \end{array}$$

Hence,

$$\begin{cases} k_1 = f(t_n, y_n) \\ k_2 = f(t_n + c_2 h, y_n + c_2 h k_1) \\ y_{n+1} = y_n + h\left[b_1 k_1 + (1-b_1) k_2\right] \end{cases}$$

Describes all possible explicit 2-stage RK-methods.

We Taylor expand to determine the parameters c_2 and b_1...

With the following Taylor expansions:

$$\begin{array}{rcl} y_{n+1} & = & y_n + hf_n + \frac{h^2}{2} f_n' + \mathcal{O}(h^3) \\ k_1 & = & f_n \\ k_2 & = & f(t_n + c_2 h, y_n + c_2 h k_1) \\ & = & f_n + (c_2 h)\frac{\partial}{\partial t} f(t_n, y_n) + (c_2 h)\frac{\partial}{\partial y} f(t_n, y_n) y'(t) + \mathcal{O}(h^2) \end{array}$$

We can define the Local Truncation Error

$$\begin{array}{rcl} \mathrm{LTE}(h) & = & \dfrac{y_{n+1} - y_n}{h} - b_1 k_1 - (1-b_1) k_2 \\ & = & \left[f_n + \dfrac{h}{2} f_n' + \mathcal{O}(h^2) \right] - \\ & & - \left[b_1 f_n + (1-b_1) \left(f_n + (c_2 h) \left[\dfrac{\partial}{\partial t} f_n + \dfrac{\partial}{\partial y} f_n \cdot f_n \right] \right) \right] \\ & = & \dfrac{h}{2} \left[\dfrac{\partial}{\partial t} f_n + \dfrac{\partial}{\partial y} f_n \cdot f_n \right] - \mathbf{b_2} c_2 h \left[\dfrac{\partial}{\partial t} f_n + \dfrac{\partial}{\partial y} f_n \cdot f_n \right] + \mathcal{O}(h^2) \end{array}$$

We have

$$\mathrm{LTE}(h) = \frac{h}{2} \left[\frac{\partial}{\partial t} f_n + \frac{\partial}{\partial y} f_n \cdot f_n \right] - \mathbf{b_2} c_2 h \left[\frac{\partial}{\partial t} f_n + \frac{\partial}{\partial y} f_n \cdot f_n \right] + \mathcal{O}(h^2)$$

Now, if

$$\frac{h}{2} - b_2 c_2 h = 0 \quad \Leftrightarrow 2 b_2 c_2 = 1$$

we get $\mathrm{LTE}(h) \sim \mathcal{O}(h^2)$, *i.e.* our 2-stage RK-method is **second order**. The corresponding family of Butcher arrays is

$$\begin{array}{c|cc} 0 & 0 & 0 \\ c_2 & c_2 & 0 \\ \hline & 1 - 1/(2c_2) & 1/(2c_2) \end{array}$$

Sanity check: $c_2 = 1/2$ gives Euler's Midpoint Method, and $c_2 = 1$ gives Heun's Method.

Runge-Kutta Methods: Issues to clear up...

- Error Estimation using Richardson's Extrapolation
- Error Analysis
  - $\mathrm{LTE}(h)$
  - consistency
- Stability Analysis

Estimating the Error "on the fly" I/III

In addition to computing the numerical solution, we also need an estimate on the quality of the solution — **an error estimate.**

Suppose we have used a Runge-Kutta method (with step-size $h_1 = h$) of order p to get the numerical solution y^*_{n+1} at t_{n+1}, then the local error in the solution is:

$$e^* = y(t_{n+1}) - y^*_{n+1} = \mathcal{C}h^{p+1} + \mathcal{O}(h^{p+2})$$

If we have another solution y^{**}_{n+1} , computed with $h_2 = h/2$,

$$e^{**} = y(t_{n+1}) - y^{**}_{n+1} = \mathcal{C}\left[\frac{h}{2}\right]^{p+1} + \mathcal{O}(h^{p+2})$$

Estimating the Error "on the fly" II/III

Keeping only the leading order (principal part, h^{p+1}-term) of the error expansion we can write:

$$y^{**}_{n+1} - y^*_{n+1} = -\mathcal{C}h^{p+1}\left[\frac{1}{2^{p+1}} - 1\right]$$

We have

$$y^{**}_{n+1} - y^*_{n+1} = -\mathcal{C}h^{p+1}\left[\frac{1}{2^{p+1}} - 1\right] = -\mathcal{C}\left[\frac{h}{2}\right]^{p+1}\left[1 - 2^{p+1}\right]$$

Estimating the Error "on the fly" III/III

Thus,

$$\underbrace{\mathcal{C}\left[\frac{h}{2}\right]^{p+1}}_{e^{**}} = \frac{\mathbf{y^{**}_{n+1} - y^*_{n+1}}}{\mathbf{2^{p+1} - 1}}$$

is an estimate for principal local truncation error (PLTE).

This works well in practice. The only problem is that it is expensive to implement — 3 times the evaluations of the slope $f(t, y)$ (a total of 12 evaluations for Runge's 4th order scheme) — **200% overhead**.

Finding a More Efficient Error Estimate

It'd be great if we could find an error estimate directly from the computed slopes (the k_i's)...

This idea was introduced by Merson in 1957. The idea is to derive two Runge-Kutta methods of orders p and $p+1$ using the **same** set of k_i's... In terms of the Butcher array:

$$\begin{array}{c|c} \tilde{\mathbf{c}} & A \\ \hline & \tilde{\mathbf{b}}^T \\ & \tilde{\mathbf{b}}_2^T \\ \hline & \tilde{\mathbf{E}}^T \end{array}$$

Where $(A, \tilde{\mathbf{c}}, \tilde{\mathbf{b}})$ defines a method of order p, and $(A, \tilde{\mathbf{c}}, \tilde{\mathbf{b}}_2)$ a method of order $p+1$. The vector $\tilde{\mathbf{E}}^T = \tilde{\mathbf{b}}_2 - \tilde{\mathbf{b}}$, and the error estimate is given by $h\sum_{i=1}^{s} E_i k_i$.

RKF45 — Runge-Kutta-Fehlberg 4th-5th Order Method

The most commonly seen 4th-5th order method is RKF45:

$$\begin{array}{c|c} \tilde{\mathbf{c}} & A \\ \hline & \tilde{\mathbf{b}}^T \\ & \tilde{\mathbf{b}}_2^T \\ \hline & \tilde{\mathbf{E}}^T \end{array} = \begin{array}{c|cccccc} 0 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ \frac{1}{4} & \frac{1}{4} & \ddots & & & & \vdots \\ \frac{3}{8} & \frac{3}{32} & \frac{9}{32} & \ddots & & & \vdots \\ \frac{12}{13} & \frac{1932}{2197} & -\frac{7200}{2197} & \frac{7296}{2197} & \ddots & & \vdots \\ 1 & \frac{439}{216} & -8 & \frac{3680}{513} & -\frac{845}{4104} & \ddots & \vdots \\ \frac{1}{2} & -\frac{8}{27} & 2 & -\frac{3544}{2565} & \frac{1859}{4104} & -\frac{11}{40} & 0 \\ \hline & \frac{25}{216} & 0 & \frac{1408}{2565} & \frac{2197}{4104} & -\frac{1}{5} & 0 \\ & \frac{16}{135} & 0 & \frac{6656}{12825} & \frac{28561}{56430} & -\frac{9}{50} & \frac{2}{55} \\ \hline & \frac{1}{360} & 0 & -\frac{128}{4275} & -\frac{2197}{75240} & \frac{1}{50} & \frac{2}{55} \end{array}$$

RKF45 uses 6 evaluations of $f(t, y)$ to obtain a 4th order method with an error estimate — **50% overhead**.

Stability Analysis of RK-methods

By applying the RK-methods to the scalar test-problem $\mathbf{y}'(\mathbf{t}) = \lambda \mathbf{y}(\mathbf{t}),\ \mathbf{y}(\mathbf{t_0}) = \mathbf{y_0}$ we will find the regions of stability for the methods.

Consider Heun's Method

$$\begin{array}{c|cc} c_1 & a_{1,1} & a_{1,2} \\ c_2 & a_{2,1} & a_{2,2} \\ \hline & b_1 & b_2 \end{array} = \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

Hence

$$\begin{aligned} k_1 &= f(t_n, y_n) = \lambda y_n \\ k_2 &= f(t_n + h, y_n + hk_1) = \lambda(y_n + hk_1) = \lambda y_n + h\lambda^2 y_n \\ y_{n+1} &= y_n \left[1 + \tfrac{h}{2}\left[2\lambda + h\lambda^2\right]\right] = y_n \left[1 + h\lambda + \tfrac{(h\lambda)^2}{2}\right] \end{aligned}$$

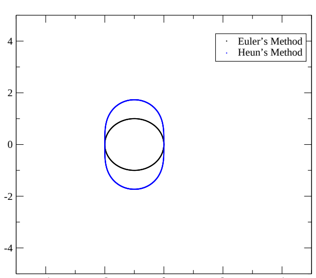
Stability of Heun's Method, continued

The stability region is given by

$$|R(h\lambda)| = \left| 1 + h\lambda + \frac{(h\lambda)^2}{2} \right| \leq 1$$

We find the boundary of the region by find the complex roots of

$$1 - e^{i\theta} + h\lambda + \frac{(h\lambda)^2}{2} = 0, \quad \forall \theta \in [0, 2\pi)$$



Stability Regions for RK-methods

For notational convenience we absorb $h\lambda \to \widehat{h}$.

Using the A from the Butcher array, we can write the k_i's

$$\tilde{\mathbf{k}} = \begin{bmatrix} k_1 \\ k_2 \\ \vdots \\ k_s \end{bmatrix} = y_n \tilde{\mathbf{1}} + \widehat{h} A \tilde{\mathbf{k}}, \quad \text{where } \tilde{\mathbf{1}} = \left.\begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}\right\} s \text{ ones}$$

thus, we can solve for $\tilde{\mathbf{k}}$:

$$\tilde{\mathbf{k}} = (I - \widehat{h}A)^{-1} \tilde{\mathbf{1}} y_n$$

Further,

$$y_{n+1} = y_n + \widehat{h} \tilde{\mathbf{b}}^T \tilde{\mathbf{k}} = y_n + \widehat{h} \tilde{\mathbf{b}}^T (I - \widehat{h}A)^{-1} \tilde{\mathbf{1}} y_n$$

Stability Regions for RK-methods

We have

$$y_{n+1} = y_n + \widehat{h}\tilde{\mathbf{b}}^T\tilde{\mathbf{k}} = y_n + \widehat{h}\tilde{\mathbf{b}}^T(I - \widehat{h}A)^{-1}\tilde{\mathbf{1}}y_n$$

Thus, the stability function is

$$R\left(\widehat{h}\right) = 1 + \widehat{h}\tilde{\mathbf{b}}^T\left(I - \widehat{h}A\right)^{-1}\tilde{\mathbf{1}}$$

As usual, the method is stable for $\widehat{h}$ such that $|R(\widehat{h})| \leq 1$.

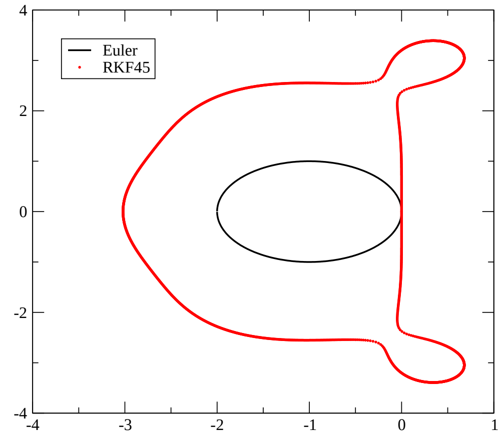
For explicit methods, A strictly lower triangular, the quantity

$$\tilde{\mathbf{d}} = \left(I - \widehat{h}A\right)^{-1}\tilde{\mathbf{1}}$$

is easily computable using forward substitution.

Stability Region for RKF45

$$R(\widehat{h}) = 1 + \widehat{h} + \frac{\widehat{h}^2}{2} + \frac{\widehat{h}^3}{6} + \frac{\widehat{h}^4}{24} + \frac{\widehat{h}^5}{104}$$



Consistency for RK-methods

Theorem

An RK-method

$$\frac{y_{n+1} - y_n}{h} = \sum_{i=1}^{s} b_i k_i$$

where

$$k_i = f\left(t_i + c_i h, y_n + h\sum_{j=1}^{s} a_{ij}k_j\right)$$

is consistent with the ODE, $y'(t) = f(t, y)$, if and only if $\sum b_i = 1$.

Consistency for RK-methods

"Proof" by vigorous hand-waving

We note that each $k_i = f(t_n, y_n) + \mathcal{O}(h)$. Hence we have $LTE(h) = (1 - \sum b_i)f(t, y) + \mathcal{O}(h)$. Since we need $\lim_{h\to 0} LTE(h) = 0$, we must have $1 - \sum b_i = 0$. $\square$

Homework #2, Due 11:00am, 2/20/2015

1. Find the stability function for Runge's 4th-order 4-stage method.
2. Implement RKF45 (don't use matlab's ode45!). Solve

$$\begin{cases} y'(t) = y(t) + 2t - 1 \\ y(0) = 1 \\ t \in [0,1] \end{cases}$$

with step-length $h \in \{1, \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}, \frac{1}{32}\}$.

- Plot the exact, and estimated errors at the terminating point ($t = 1$) vs. the step-length h on a log-log scale (in matlab: `loglog(the_h_values, the_exact_errors, '-o', the_h_values, the_estimated_errors, '-*')`

Chronology

1895 The idea of multiple evaluations of the derivative for each time-step is attributed to Runge.

1900 Heun makes several contributions.

1901 Kutta characterizes the set of Runge-Kutta methods of order 4; proposed the first order 5 method.

1925 Nyström proposes special methods for second order ODEs.

1956 Huta introduces 6th order methods.

Modern analysis of Runge-Kutta methods developed by

1951 Gill

1957 Merson

1963 Butcher

s-stage Runge-Kutta for $\{\ y'(t) = f(t, y), \quad y(t_0) = y_0\ \}$

The Butcher array for a general s-stage RK method is

$$\begin{array}{c|cccc} c_1 & a_{1,1} & a_{1,2} & \cdots & a_{1,s} \\ c_2 & a_{2,1} & a_{2,2} & \cdots & a_{2,s} \\ \vdots & \vdots & & & \vdots \\ c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array} = \begin{array}{c|c} \tilde{\mathbf{c}} & A \\ \hline & \tilde{\mathbf{b}}^T \end{array}$$

is a compact shorthand for the scheme

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i$$

where the k_is are multiple estimates of the right-hand-side $f(t, y)$

$$k_i = f\left(t_n + c_i h,\ y_n + h \sum_{j=1}^{s} a_{i,j} k_j\right), \quad i = 1, 2, \ldots, s$$

Conditions on the Butcher Array

The Butcher array must satisfy the following row-sum condition

$$c_i = \sum_{j=1}^{s} a_{i,j} \quad i = 1, 2, \ldots, s$$

and consistency requires

$$\sum_{j=1}^{s} b_j = 1.$$

Beyond that, we are left with the formidable task of selecting $\tilde{\mathbf{b}}$, $\tilde{\mathbf{c}}$, and the matrix A. Up to this point our only tool is (tedious) Taylor expansions.

Explicit 3-stage RK Methods — The Order Conditions

If we want to build an explicit 3-stage method,

$$
\begin{array}{c|ccc}
0 & & & \\
c_2 & a_{21} & & \\
c_3 & a_{31} & a_{32} & \\
\hline
 & b_1 & b_2 & b_3
\end{array}
$$

it can be shown (Taylor expansion) that in order to achieve a 3rd order scheme, we must satisfy the **Order Conditions**:

$$
\begin{aligned}
b_1 + b_2 + b_3 &= 1 \\
b_2 c_2 + b_3 c_3 &= \tfrac{1}{2} \\
b_2 c_2^2 + b_3 c_3^2 &= \tfrac{1}{3} \\
b_3 a_{32} c_2 &= \tfrac{1}{6}
\end{aligned}
$$

Finding the Order Conditions

Clearly, deriving a Runge-Kutta scheme boils down to a two-stage process:

1. Find the order conditions: — a set of non-linear equations in the parameters sought.
2. Find a solution, or family of solutions, to the order conditions.

As the desired order of the method increases, both deriving and solving these algebraic conditions become increasingly complicated.

We now consider a structured way of deriving the order conditions without explicit Taylor expansions.

Rooted Trees

Definition (Rooted Tree)

A rooted tree is a graph, which is connected, has no cycles, and has one vertex designated as the root.

Definition (Order of a Rooted Tree)

The order of a rooted tree is the number of vertices in the tree.

Definition (Leaves)

A leaf is vertex in a tree (with order greater than one) which has exactly one vertex joined to it.

Examples: Trees

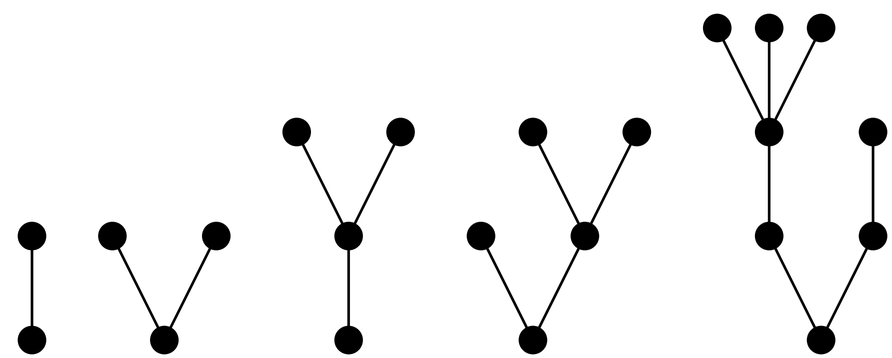


Figure: Trees of order 2, 3, 4, 5, and 8. By convention, we place to root at the bottom of the graph, and let the tree grow "upward."

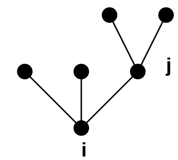
Associated Quantities

For each tree t, we define two quantities

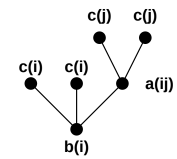
1. $\Phi(t)$: a polynomial in the coefficients which will define a Runge-Kutta method.
2. $\gamma(t)$: an integer

Building $\Phi(t)$

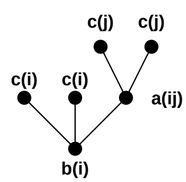
We label each vertex of the tree, except the leaves, *e.g.*



Next, we write down a sequence of factors, starting with b_i (the root factor). For each arc of the tree, write down a factor a_{jk} where j and k are the beginning and end of the arc (in the sense up upward growth). Finally, for the leaves write down a factor c_j, where j is the label attached to the beginning of the arc: *e.g.*



Building $\Phi(t)$



Now, sum the product of these factors, for all possible choices of the labels $\{1, 2, \ldots, s\}$:

$$\Phi(t) = \sum_{ij} b_i c_i^2 a_{ij} c_j^2$$

Building $\gamma(t)$

In order to build $\gamma(t)$, we associate a factor with each vertex in the tree:

- The factor for the leaves is 1.
- For all other vertices, the factor is 1 added to the sum of the factors of the upward growing neighbors

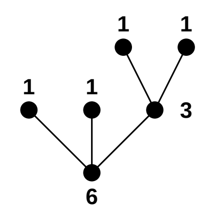
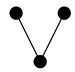
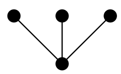
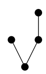
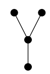


Figure: $\gamma(t)$ is the product of all the factors, here $\gamma(t) = 6 \cdot 3 \cdot 1^4 = 18$.

Rooted Trees Up to Order 4

Tree				
Order	1	2	3	3
$\Phi(t)$	$\sum_i b_i$	$\sum_i b_i c_i$	$\sum_i b_i c_i^2$	$\sum_{ij} b_i a_{ij} c_j$
$\gamma(t)$	1	2	3	6
Tree				
Order	4	4	4	4
$\Phi(t)$	$\sum_i b_i c_i^3$	$\sum_{ij} b_i c_i a_{ij} c_j$	$\sum_{ij} b_i a_{ij} c_j^2$	$\sum_{ijk} b_i a_{ij} a_{jk} c_k$
$\gamma(t)$	4	8	12	24

Runge-Kutta Scheme Based on $\Phi(t)$ and $\gamma(t)$: General condition

In designing an s-stage RK-method, the coefficients must satisfy

$$\Phi(t) = \frac{1}{\gamma(t)}, \quad \forall t \,:\, \textbf{order}(t) \leq s$$

Runge-Kutta Scheme Based on $\Phi(t)$ and $\gamma(t)$: 4-stage Example

A 4-stage **explicit** scheme, where $a_{ij} = 0$ whenever $i \geq j$, thus yields 8 conditions for $\{b_1, b_2, b_3, b_4, c_2, c_3, c_4, a_{32}, a_{42}, a_{43}\}$:

$$\begin{aligned}
b_1 + b_2 + b_3 + b_4 &= 1 && (1)\\
b_2 c_2 + b_3 c_3 + b_4 c_4 &= \tfrac{1}{2} && (2)\\
b_2 c_2^2 + b_3 c_3^2 + b_4 c_4^2 &= \tfrac{1}{3} && (3)\\
b_3 a_{32} c_2 + b_4 a_{42} c_2 + b_4 a_{43} c_3 &= \tfrac{1}{6} && (4)\\
b_2 c_2^3 + b_3 c_3^3 + b_4 c_4^3 &= \tfrac{1}{4} && (5)\\
b_3 c_3 a_{32} c_2 + b_4 c_4 a_{42} c_2 + b_4 c_4 a_{43} c_3 &= \tfrac{1}{8} && (6)\\
b_3 a_{32} c_2^2 + b_4 a_{42} c_2^2 + b_4 a_{43} c_3^2 &= \tfrac{1}{12} && (7)\\
b_4 a_{43} a_{32} c_2 &= \tfrac{1}{24} && (8)
\end{aligned}$$

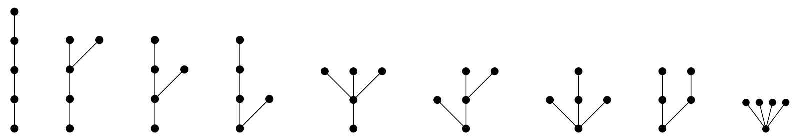
Runge-Kutta Scheme Based on $\Phi(t)$ and $\gamma(t)$: 4-stage Example

Kutta identified five cases where a solution to this non-linear system is guaranteed to exist:

Case 1	$c_2 \notin \{0, \frac{1}{2}, \frac{1}{2} \pm \frac{\sqrt{3}}{6}\}$, $c_3 = 1 - c_2$
Case 2	$b_2 = 0,\ c_2 \neq 0,\ c_3 = \frac{1}{2}$
Case 3	$b_3 \neq 0,\ c_2 = \frac{1}{2},\ c_3 = 0$
Case 4	$b_4 \neq 0,\ c_2 = 1,\ c_3 = \frac{1}{2}$
Case 5	$b_3 \neq 0,\ c_2 = c_3 = \frac{1}{2}$

Beyond 4 Stages...

The number of rooted trees of order s increases rapidly as s goes beyond 4. For $s = 5$ we have the following 9 rooted trees:



Each which leads to a nonlinear condition. (Fun!)

For $s \in \{6, 7, 8, 9, 10\}$ we get $\{20, 48, 115, 286, 719\}$ corresponding rooted trees.

Beyond 4 Stages... More Bad News

Theorem (Butcher, 2008: p.187)

If an explicit s-stage Runge-Kutta method has order p, then $s \geq p$.

Theorem (Butcher, 2008: p.187)

If an explicit s-stage Runge-Kutta method has order $p \geq 5$, then $s > p$.

Theorem (Butcher, 2008: p.188)

For any positive integer p, an explicit Runge-Kutta method exists with order p and s stages, where

$$s = \begin{cases} \frac{3p^2-10p+24}{8}, & p = 2k,\ k \in \mathbb{Z} \\ \frac{3p^2-4p+9}{8}, & p = 2k+1,\ k \in \mathbb{Z} \end{cases}$$

Beyond 4 Stages... Consequences of the 3rd Theorem

Note that the theorem gives an upper bound for the number of required stages (the theorem gives guarantees). The bound grows very quickly.

For certain values of p, s-stage methods with s lower than this bound are known:

Order, $p =$	5	6	7	8	9	10	11	12
Stages, $s =$	8	9	16	17	27	28	41	42
Scheme, $s =$	6	7	9	11		17		

Project, anyone?

Stability Polynomials, Comments

With every explicit Runge-Kutta method, we can find a stability polynomial $R(h\lambda)$ for which the condition $|R(h\lambda)| \leq 1$ defines the region of stability,

We know that for orders $p = 1, 2, 3, 4$ there are explicit s-stage RK-methods with $s = p$, and for higher order methods $s > p$.

Order	Stages	Stability Polynomial
1	1	$R(z) = 1 + z$
2	2	$R(z) = 1 + z + \frac{1}{2}z^2$
3	3	$R(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3$
4	4	$R(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4$
5	6	$R(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 + \frac{1}{120}z^5 + Cz^6$

Where, in the case $p = 5$, $s = 6$, the constant C depends on the particular method.

Stability Polynomials, Comments

Fact

Since the stability function $R(z)$ is a polynomial for all explicit Runge-Kutta methods, it is never possible to build such a method with unbounded region of stability.

Additional Comments

Butcher (2008) develops the theory of rooted trees and their usefulness far beyond what is indicated in the current lecture.

I have deliberately taken a very narrow path through the material and only presented some key ideas that fit into the context of what we have explored so far (Low-order explicit methods).

Some completely ignored topics include

- Two alternative, non-graphical, notations for trees.
- Expression of higher order derivatives in terms of rooted trees.
- Expression of ODEs (linear and non-linear) using rooted trees,

Additional Comments

For the mathematically inclined, the study of Runge-Kutta methods have several interesting connections to ares of mathematics which we sometimes consider "less applied," *e.g.*

- Graph theory
- Group theory

Also, in the context of step-size (h) management, there are some overlap with ideas in

- Control theory

We will revisit some of these topic, as needed, in future lectures.