Integration Schemes and Their Order Conditions

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February 10, 2015

Oversigt

Introduction

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- How to determine order of convergence?

Collocation Methods

Hammer and Hollingsworth in 1955: Use normal quadratures on the differential equation

Definition

Let $c_1, \dots, c_s$ be distinct real numbers usually ($0 \leq c_i \leq 1$, $\forall i$). The collocation polynomial $u(t)$ is a polynomial of degree s satisfying

$$
\begin{aligned}
u(t_0) &= y_0 && (1)\\
u'(t_0 + c_i h) &= f(t_0 + c_i h, u(t_0 + c_i h)), \quad i = 1, \dots, s && (2)
\end{aligned}
$$

and the numerical solution of the collocation method is defined by $y_1 = u(t_0 + h)$

Collocation Methods

Examples:

- $s = 1$
  - $c_1 = 0$ - Explicit Euler
  - $c_1 = 1$ - Implicit Euler
  - $c_1 = 0.5$ - Midpoint rule

Collocation Methods

Examples:

- $s = 1$
  - $c_1 = 0$ - Explicit Euler
  - $c_1 = 1$ - Implicit Euler
  - $c_1 = 0.5$ - Midpoint rule
- $s = 2$
  - $c_1 = 0$, $c_2 = 1$ - Trapezoidal rule
  - $c_{1,2} = 0.5 \pm \sqrt{3}/6$ - Gauss quadrature (two notes)

Collocation Methods

Theorem (Superconvergence (1969))

The Collocation method has the same order as the underlying quadrature formula.

The above can be extended to a discontinuous version, without breaking the theorem.

Runge-Kutta Methods

Definition

Let b_i, c_i and a_{ij} for $(i, j = 1, \dots, s)$ be real numbers. Then an s-stage Runge-Kutta method is given by:

$$k_i = f(t_0 + c_i h, y_0 + h \sum_{j=1}^{s} a_{ij} k_j), \quad i = 1, \dots, s \tag{3}$$

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i k_i \tag{4}$$

Typically $c_i = \sum_{j=1}^{s} a_{ij}$

Theorem (1970)

All Collocation methods can be rewritten into a Runge-Kutta method

Runge-Kutta Methods

After Butchers work, one typically displays the Runge-Kutta method as below

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \iff \begin{array}{c|c} c & A \\ \hline & b \end{array} \tag{5}$$

Examples:

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \quad \begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \quad \begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array} \quad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \tag{6}$$

Partitioned Runge-Kutta Methods

Now consider the differential equations in the partitioned form:

$$\dot{y} = f(y, z) \quad \dot{z} = g(y, z) \tag{7}$$

where y and z may be vectors of different length.

Definition

Let b_i, c_i, a_{ij} and $\hat{b}_i$, $\hat{c}_i$, $\hat{a}_{ij}$ be the coefficients of two Runge-Kutta methods. A partitioned Runge-Kutta method for the solution of 7 is given by:

$$k_i = f(y_0 + h\sum_{j=1}^{s} a_{ij}k_j, z_0 + h\sum_{j=1}^{s} \hat{a}_{ij}l_j), \tag{8}$$

$$l_i = g(y_0 + h\sum_{j=1}^{s} a_{ij}k_j, z_0 + h\sum_{j=1}^{s} \hat{a}_{ij}l_j), \tag{9}$$

$$y_1 = y_0 + h\sum_{i=1}^{s} b_i k_i \quad z_1 = z_0 + h\sum_{i=1}^{s} \hat{b}_i l_i \tag{10}$$

Partitioned Runge-Kutta Methods

Examples:

- Symplectic Euler

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \qquad \begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \tag{11}$$

- Störmer Verlet

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array} \tag{12}$$

Composition Methods

Definition

A one step method to recursively obtain approximation values y_i to the solution of the IVP at x_i is given by:

$$y_i = \Phi(t, y; h), \tag{13}$$

we will use the shorthand notation $\Phi_h = \Phi(t, y; h)$

Definition (Composition Method)

Let Φ_h be as above and $\gamma_1, \ldots, \gamma_s$ real numbers. Then we call its composition with step-sizes $\gamma_1 h, \ldots, \gamma_s h$:

$$\Psi_h = \Phi_{\gamma_s h} \circ \ldots \circ \Phi_{\gamma_1 h} \tag{14}$$

the corresponding composition method.

Composition Methods

Theorem

Let Φ_h be as above and of order p. Then if

$$\begin{aligned} \gamma_1 + \ldots + \gamma_s &= 1 \\ \gamma_1^{p+1} + \ldots + \gamma_s^{p+1} &= 0, \end{aligned} \tag{15}$$

then the composition method is at least of order $p+1$ (if Ψ_h is symmetric then p have to be even)

Note: The above equations do only have solutions for even p

Composition Methods

Definition (Adjoint method)

The adjoint method Φ_h^* *of a method* Φ_h *is the inverse map of the original method with reversed time-step:*

$$\Phi_h^* := \Phi_{-h}^{-1} \tag{16}$$

Note: A symmetric method fulfils that $\Phi_h^* = \Phi_h$

Definition (Composition with the Adjoint Method)

Let Φ_h *and* Φ_h^* *be as before, further let* $\alpha_1, \ldots, \alpha_s$ *and* $\beta_1, \ldots, \beta_s$ *be real numbers. Then we call its composition with step-sizes* $\alpha_1 h, \ldots, \alpha_s h$ *and* $\beta_1 h, \ldots, \beta_s h$*:*

$$\Psi_h = \Phi_{\alpha_s h} \circ \Phi_{\beta_s h}^* \circ \ldots \circ \Phi_{\alpha_1 h} \circ \Phi_{\beta_1 h}^* \tag{17}$$

the corresponding composition method.

Composition Methods

Theorem

Let Φ_h be as above and of order p. Then if

$$\begin{aligned} \beta_1 + \alpha_1 + \ldots + \beta_s + \alpha_s &= 1 \\ (-1)^p \beta_1^{p+1} + \alpha_1^{p+1} + \ldots + (-1)^p \beta_s^{p+1} + \alpha_s^{p+1} &= 0, \end{aligned}$$

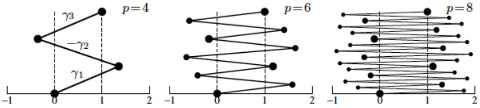
then the composition method is at least of order $p+1$ (if Ψ_h is symmetric then p have to be even)

Note: This have solutions for all ps

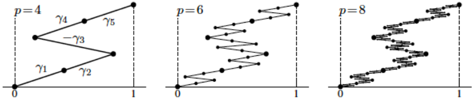
Composition Methods

Examples:

- Implicit Euler → Trapezoidal
- Triple jump

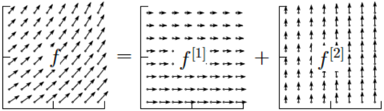


- Suzuki's Fractals



Splitting Methods

Decomposition of vectorfield:



$$\dot{y} = f^{[1]}(y) + f^{[2]}(y)$$

Eksamples:

- Lie-Trotter splitting (first order)
  - $\Phi_h^* = \phi_h^{[2]} \circ \phi_h^{[1]}$
  - $\Phi_h = \phi_h^{[1]} \circ \phi_h^{[2]}$
- Strang splitting 1968 (symmetric, second order)
  - $\Phi_h^{[S]} = \phi_{h/2}^{[1]} \circ \phi_h^{[2]} \circ \phi_{h/2}^{[1]}$

Runge-Kutta Methods

Consider the autonomous IVP:

$$\dot{y} = f(y), \quad y(t_0) = y_0 \tag{18}$$

assume here that f is sufficiently differentiable and that is fulfils the necessary Lipschitz conditions.

Runge-Kutta Methods

Step 1: We compute the higher order derivatives
Let $f'(y)$ denote the derivative as a linear map, $f''(y)$ the second derivative as a bilinear map etc..

$$\begin{aligned}
\dot{y} &= f(y) \\
\ddot{y} &= f'(y)\dot{y} \\
y^{(3)} &= f''(y)(\dot{y},\dot{y}) + f'(y)\ddot{y} \qquad (19) \\
y^{(4)} &= f'''(y)(\dot{y},\dot{y},\dot{y}) + 3f''(y)(\ddot{y},\dot{y}) + f'(y)y^{(3)} \\
&\vdots
\end{aligned}$$

Runge-Kutta Methods

Step 2: Recursively substitute

$$\begin{aligned}
\dot{y} &= f \\
\ddot{y} &= f'f \\
y^{(3)} &= f''(f,f) + f'f'f \\
y^{(4)} &= f'''(f,f,f) + 3f''(f'f,f) \\
&\quad + f'f''(f,f) + f'f'f'f \\
&\vdots
\end{aligned} \tag{20}$$

Runge-Kutta Methods

Step 2: Recursively substitute

Definition (Trees)

The set of rooted trees T is recursively defined as follows:

1. *the graph $\bullet$ belongs to T*
2. *if $\tau_1, \ldots, \tau_m \in T$ then the graph obtained by grafting the roots of $\tau_1, \ldots, \tau_m$ to a new root belongs to T. it is denoted by $\tau = [\tau_1, \ldots, \tau_m]$*

further let $|\tau|$ be the order (number of vertices) and $\alpha(\tau)$ be the coefficients.

Definition (Elementary Differentials)

For a tree $\tau \in T$. The elementary differential is a mapping $F(\tau) : \mathbb{R}^n \to \mathbb{R}^n$, defined recursively by $F(\bullet)(y) = f(y)$ and:

$$F(\tau)(y) = f^{(m)}(y)\left(F(\tau_1)(y), \ldots, F(\tau_m)(y)\right) \qquad (21)$$

where $\tau = [\tau_1, \ldots, \tau_m]$

Runge-Kutta Methods

Step 2: Recursively substitute

Theorem

The qth derivative of the exact solution is given by:

$$y^{(q)}(t_0) = \sum_{|\tau|=q} \alpha(\tau) F(\tau)(y_0)$$

Runge-Kutta Methods

Step 3: Consider the numerical solution of the Runge-Kutta method
By setting $hk_i = g_i$ we obtain:

$$g_i = hf(u_i)$$

and

$$u_i = y_0 + \sum_j a_{ij} g_j, \quad y_1 = y_0 + \sum_i b_i g_i$$

Using Leibniz' rule, we obtain:

$$g_i^{(q)} = h(f(u_i))^{(q)} + q(f(u_i))^{(q-1)}$$

for $h = 0$ we get:

$$g_i^{(q)} = q(f(u_i))^{(q-1)}$$

Runge-Kutta Method

Step 3: Consider the numerical solution of the Runge-Kutta method
Consequently we obtain for $h = 0$:

$$\begin{aligned} \dot{g}_i &= 1 \cdot f \\ \ddot{g}_i &= 2 \cdot f' \dot{u}_i \\ g_i^{(3)} &= 3 \cdot \left(f''(\dot{u}_i, \dot{u}_i) + f' \ddot{u}_i \right) \\ g_i^{(4)} &= 4 \cdot \left(f'''(\dot{u}_i, \dot{u}_i, \dot{u}_i) + 3f''(\ddot{u}_i, \dot{u}_i) + f' u_i^{(3)} \right) \\ &\vdots \end{aligned} \tag{22}$$

Runge-Kutta Method

Step 4: Substitute back
Recall that:

$$u_i^{(q)} = \sum_j a_{ij} g_j^{(q)} \tag{23}$$

we now start the process:

$$\begin{aligned} \dot{g}_i &= 1 \cdot f & \dot{u}_i &= 1 \cdot (\textstyle\sum_j a_{ij}) f \\ \ddot{g}_i &= (1 \cdot 2)(\textstyle\sum_j a_{ij}) f' f & \ddot{u}_i &= (1 \cdot 2)(\textstyle\sum_j a_{ij} a_{jk}) f' f \end{aligned} \tag{24}$$

By induction we obtain:

$$g_i^{(q)}|_{h=0} = \sum_{|\tau|=q} \gamma(\tau) \cdot \mathbf{g}_i(\tau) \cdot \alpha(\tau) F(\tau)(y_0) \tag{25}$$

$$u_i^{(q)}|_{h=0} = \sum_{|\tau|=q} \gamma(\tau) \cdot \mathbf{u}_i(\tau) \cdot \alpha(\tau) F(\tau)(y_0) \tag{26}$$

Runge-Kutta Method

Step 4: Substitute back

We see that this for a general tree $\tau = [\tau_1, \ldots, \tau_m]$, implies that:

$$\mathbf{g}_i(\tau) = \mathbf{u}_i(\tau_1) \cdot \ldots \cdot \mathbf{u}_i(\tau_m)$$

$$\gamma(\tau) = |\tau| \gamma(\tau_1) \cdot \ldots \cdot \gamma(\tau_m)$$

then by the previous:

$$\mathbf{u}_i(\tau) = \sum_j a_{ij} \mathbf{g}_j(\tau)$$

we set

$$\phi(\tau) = \sum_i b_i \mathbf{g}_i(\tau)$$

Now summarizing we get:

$$y_1^{(q)}|_{h=0} = \sum_{|\tau|=q} \gamma(\tau)\phi(\tau)\alpha(\tau)F(\tau)(y_0) \qquad (27)$$

Runge-Kutta Method

Step 5: Compare

Now comparing the derivatives of the exact solution:

$$y^{(q)}(t_0) = \sum_{|\tau|=q} \alpha(\tau)F(\tau)(y_0)$$

and the derivatives of the approximation:

$$y_1^{(q)}|_{h=0} = \sum_{|\tau|=q} \gamma(\tau)\phi(\tau)\alpha(\tau)F(\tau)(y_0).$$

Then from Taylor expansion we get:

Theorem

(Order Condition) The Runge-Kutta Method has order p if and only if:

$$\phi(\tau) = \frac{1}{\gamma(\tau)}, \quad \forall |\tau| \leq p \tag{28}$$

Examples:

Now with B-series

B-Series

Definition (Symmetry coefficient)

The symmetry coefficient $\sigma(\tau)$ are defined by $\sigma(\bullet) = 1$ and for $\tau = [\tau_1, \dots, \tau_m]$.

$$\sigma(\tau) = \sigma(\tau_1) \cdot \ldots \cdot \sigma(\tau_m) \cdot \mu_1! \mu_2! \cdot \ldots,$$

where the integers u_1, $u_2, \dots$ count equal trees among $\tau_1, \dots, \tau_m$.

Definition (B-series)

For a mapping $a : T \cup \{\emptyset\} \to \mathbb{R}$ a formal series of the form.

$$B(a, y) = a(\emptyset) y + \sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)} a(\tau) F(\tau)(y)$$

is called a B-series.

B-Series

Lemma

Let $a : T \cup \{\emptyset\} \to \mathbb{R}$ be a mapping satisfying $a(\emptyset) = 1$ then the corresponding B-series inserted into $hf((\cdot)$ is again a B-series. That is:

$$hf\left(B(a,y)\right) = B(a',y) \tag{29}$$

where $a'(\emptyset) = 0$, $a'(\bullet) = 1$, and

$$a'(\tau) = a(\tau_1) \cdot \ldots \cdot a(\tau_m), \quad \tau = [\tau_1, \ldots, \tau_m] \tag{30}$$

Assuming the exact solution to be a B-series $B(e, y_0)$ we obtain:

$$e(\tau) = \frac{1}{|\tau|} e(\tau_1) \cdot \ldots \cdot e(\tau_m) = \frac{1}{\gamma(\tau)}, \tag{31}$$

now assuming the numerical solution to be a B-series $B(\phi, y_0)$ we reprove the order conditions

Partitioned Runge-Kutta Methods

Recall that this problem is being approximated by two Runge-Kutta methods

Bicolored trees

Theorem

A partitioned Runge-Kutta Method has order p if and only if:

$$\phi(\tau) = \frac{1}{\gamma(\tau)}, \quad \forall |\tau| < p \tag{32}$$

$\lvert\tau\rvert$	τ	graph	$\alpha(\tau)$	$F(\tau)$	$\gamma(\tau)$	$\phi(\tau)$	$\sigma(\tau)$
1	$\bullet$	$\bullet$	1	f	1	$\sum_i b_i$	1
2	$[\bullet]_y$		1	$f_y f$	2	$\sum_{ij} b_i a_{ij}$	1
2	$[\circ]_y$		1	$f_z g$	2	$\sum_{ij} b_i \widehat{a}_{ij}$	1
3	$[\bullet, \bullet]_y$		1	$f_{yy}(f, f)$	3	$\sum_{ijk} b_i a_{ij} a_{ik}$	2
3	$[\bullet, \circ]_y$		2	$f_{yz}(f, g)$	3	$\sum_{ijk} b_i a_{ij} \widehat{a}_{ik}$	1
3	$[\circ, \circ]_y$		1	$f_{zz}(g, g)$	3	$\sum_{ijk} b_i \widehat{a}_{ij} \widehat{a}_{ik}$	2
3	$[[\bullet]_y]_y$		1	$f_y f_y f$	6	$\sum_{ijk} b_i a_{ij} a_{jk}$	1
3	$[[\circ]_y]_y$		1	$f_y f_z g$	6	$\sum_{ijk} b_i a_{ij} \widehat{a}_{jk}$	1
3	$[[\bullet]_z]_y$		1	$f_z g_y f$	6	$\sum_{ijk} b_i \widehat{a}_{ij} a_{jk}$	1
3	$[[\circ]_z]_y$		1	$f_z g_z g$	6	$\sum_{ijk} b_i \widehat{a}_{ij} \widehat{a}_{jk}$	1
1	$\circ$	$\circ$	1	g	1	$\sum_i \widehat{b}_i$	1
2	$[\bullet]_z$		1	$g_y f$	2	$\sum_{ij} \widehat{b}_i a_{ij}$	1
	etc	etc		etc		etc	

Integration Schemes and Their Order Conditions

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Introduction

Different Schemes for Solving ODEs

Trees and B-series

Nyström Methods

Apply the previous theory to:

$$\dot{y} = z, \qquad \dot{z} = g(y, z)$$

Black vertices have at most one son and this son must be white

Without drag:

$$\ddot{y} = g(y)$$

White vertices have only black sons

Composition Methods

Let the Taylor series expansion of the method be:

$$\Phi_h(y) = y + hd_1(y) + h^2 d_2(y) + h^3 d_3(y) + \dots \tag{33}$$

The only thing we require here is first order consistency i.e.

$$d_1(y) = f(y) \tag{34}$$

all other functions are arbitrary

Composition Methods

Recall that:

$$\Psi_h = \Phi_{\alpha_s h} \circ \Phi^*_{\beta_s h} \circ \ldots \circ \Phi_{\alpha_s 1} \circ \Phi^*_{\beta_1 h} \qquad (35)$$

Definition (∞-trees and B_∞-series)

We extend the previous definitions to T_∞, the set of all rooted trees where each vertex bears a positive integer without any further restriction, an use the notation:

$$\begin{aligned}
\textcircled{1}, \textcircled{2}, \textcircled{3}, \ldots &= \text{the trees with one vertex} \\
[\tau_1, \ldots, \tau_m]_i &= \textcircled{i} \text{ connected to } \tau_1, \ldots, \tau_m \\
F(\textcircled{i})(y) &= d_i(y) \\
F(\tau)(y) &= d_i^{(m)}(y)(F(\tau_1)(y), \ldots, F(\tau_m)(y)) \\
|\tau| &= \text{number of vertices} \\
\|\tau\| &= \text{sum of the labels} \\
\sigma(\tau) &= \text{symmetry coefficient respecting the labels} \\
i(\tau) &= \text{label of the root}
\end{aligned}$$

Example

Composition Method

Lemma (Recurrence Relation)

The following compositions are B_∞-series:

$$\begin{aligned}(\Phi^*_{\beta_k h} \circ \ldots \circ \Phi_{\alpha_1 h} \circ \Phi^*_{\beta_1 h})(y) &= B_\infty(b_k, y) \\ (\Phi_{\alpha_k h} \circ \Phi^*_{\beta_k h} \circ \ldots \circ \Phi_{\alpha_1 h} \circ \Phi^*_{\beta_1 h})(y) &= B_\infty(a_k, y)\end{aligned} \tag{36}$$

Their coefficients are recursively given by $a_k(\emptyset) = 1$, $b_k(\emptyset) = 1$, $b'_k(\textcircled{i}) = 1$, $a_0(\tau) = 0$ *for all* $\tau \in T_\infty$, *and:*

$$\begin{aligned}b_k(\tau) &= a_{k-1}(\tau) - (-\beta_k)^{i(\tau)} b'_k(\tau) \\ a_k(\tau) &= b_k(\tau) + a_k^{i(\tau)} b'_k(\tau) \\ b'_k(\tau) &= b_k(\tau_1) \cdot \ldots \cdot b_k(\tau_m)\end{aligned} \tag{37}$$

Adding them we obtain:

$$a_k(\tau) = a_{k-1}(\tau) + \left(\alpha_k^{i(\tau)} - (-\beta_k)^{i(\tau)}\right) b'_k(\tau) \tag{38}$$

Composition Method

We now obtain:

$$a_k(\text{ⓘ}) = \sum_{l=1}^{k}(\alpha_l^i - (-\beta_l)^i)$$
$$b_k(\text{ⓘ}) = \sum_{l=1}^{k-1}\alpha_l^i - \sum_{l=1}^{k}(-\beta_l)^i) = \sum_{l=1}^{\prime k}(\alpha_l^i - (-\beta_l)^i)$$

Example (continued)

Composition Methods

Theorem (Order condition)

Let $e(\tau)$ be as follows for $\tau = [\tau_1, \ldots, \tau_m]$:

$$e(\tau) = \frac{1}{|\tau|} e(\tau_1) \cdot \ldots \cdot e(\tau_m) \quad \text{if } \tau = [\tau_1, \ldots, \tau_m]_1. \tag{39}$$

The composition method has order p if and only if:

$$a_s(\tau) = e(\tau), \quad \forall \|\tau\| \leq p \tag{40}$$

Beautiful, but e.g. for $P = 6$ we have 166 trees, a lot of them are luckily **not** independent $\implies$ reduce to 22 independent trees.

Hall set

Definition

The Hall set corresponding to an order relation is a subset $\mathcal{H} \subset T_\infty$ defined by:

$$\begin{array}{lcr} \textcircled{i} \in \mathcal{H} & \textit{for} & i = 1, 2, \ldots \\ \tau \in \mathcal{H} & \iff & \exists u, v \in \mathcal{H}, u > v : \tau = u \circ v \end{array} \tag{41}$$

Theorem

For the composition method we do only have to consider the trees in the Hall set

Splitting Methods

Recall that:

$$\dot{y} = f_1(y) + f_2(y) \tag{42}$$

Assuming we know the respective flows exactly, we have a first order method:

$$\Phi_h = \phi_h^{[1]} \circ \phi_h^{[2]} \tag{43}$$

together with its adjoint $\Phi_h^* = \phi_h^{[2]} \circ \phi_h^{[1]}$ we can make a composition method:

Theorem

The splitting method in Equation (42) is of order p if and only if the corresponding composition method is of order p