Runge-Kutta and Collocation Methods

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Overview

• Define Runge-Kutta methods.

• Introduce collocation methods.

• Identify collocation methods as Runge-Kutta methods.

• Find conditions to determine, of what order collocation methods are.
General Goal: Find approximation to the solutions of

\[ \dot{y}(t) = f(t, y), \quad y(t_0) = y_0 \]

using one step methods.

3 Examples of one step methods (step size \( h = 1 \)) for the Riccati equation \( \partial_t y = y^2 + t^2 \):

- Explicit Euler Rule
- Explicit Trapezoidal Rule
- Explicit 3-stage Runge–Kutta method
**Runga-Kutta Method**

**Definition 1 (Runge-Kutta)** Let $b_i, a_{ij} \ (i, j = 1, \ldots, s)$ be real numbers and let $c_i = \sum_{j=1}^{s} a_{ij}$. An $s$-stage Runge-Kutta method is given by

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

$$ y_1 = y_0 + h \sum_{j=1}^{s} b_i k_i. $$

Distinguish:

**explicit Runge-Kutta** $a_{ij} = 0$ for $j \geq i$

**implicit Runge-Kutta** full matrix $(a_{ij})$ of non-zero coefficients allowed

*Implicit function theorem:* for $h$ small enough, (1) has a locally unique solution close to $k_i \approx f(t_0, y_0)$. 

Geometrical Numeric Integration
The coefficients of the Runge-Kutta method are usually displayed in a Butcher diagram:

\[
\begin{array}{c|ccc}
 c_1 & a_{11} & \ldots & a_{1s} \\
\vdots & \vdots & & \vdots \\
 c_s & a_{s1} & \ldots & a_{ss} \\
\hline
 b_1 & \ldots & b_s
\end{array}
\]

Example for explicit Runge-Kutta:

\[
\begin{array}{c|ccc}
 0 & 0.5 & 0.5 & 0.5 \\
 0.5 & 0.5 & 0.3 & 0.4 \\
 0.7 & 0.3 & 0.4 & \text{\rightarrow}
\end{array}
\]

\[\frac{dy}{dt} = y^2 + t^2\]
A general one-step method has order $p$, if

$$y_1 - y(t_0 + h) = \mathcal{O}(h^{p+1}) \quad \text{as } h \to 0.$$ 

By the Taylor expansions

$$y(t_0 + h) = y(t_0) + h \cdot f(t_0, y(t_0)) + \frac{1}{2} h^2 \cdot \left. \frac{d}{dt} f(t, y(t)) \right|_{t=t_0} + \ldots$$

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i \left[ f(t_0, y_0) + h \cdot \left. \frac{d}{dh} f \left( t_0 + c_i h, y_0 + h \sum_{j=1}^{s} a_{ij} k_j \right) \right|_{h=0} + \ldots \right]$$

of $y$ and $y_1$ of the Runge-Kutta method, one obtains the following conditions for the coefficients:

$$\sum_{i=1}^{s} b_i = 1 \quad \text{for order 1},$$
$$\sum_{i=1}^{s} b_i c_i = 1/2 \quad \text{for order 2},$$
$$\sum_{i=1}^{s} b_i c_i^2 = 1/3$$

and

$$\sum_{i,j} b_i a_{ij} c_j = 1/6 \quad \text{for order 3}.$$
Definition 2 (Collocation Method) Let $c_1, \ldots, c_s$ be distinct real numbers (usually $0 \leq c_i \leq 1$). The collocation polynomial $u(t)$ is a polynomial of degree $s$ satisfying

\[
\begin{align*}
  u(t_0) &= y_0, \\
  \dot{u}(t_0 + c_i h) &= f(t_0 + c_i h, u(t_0 + c_i h)), \quad i = 1, \ldots, s,
\end{align*}
\]

and the numerical solution of the collocation method is defined by

\[y_1 = u(t_0 + h).\]
**The Collocation Method**

**Theorem 1 (Guillou & Soulé 1969, Wright 1970)** The collocation method for $c_1, \ldots, c_s$ is equivalent to the $s$-stage Runge-Kutta method with coefficients

$$a_{ij} = \int_0^{c_i} \ell_j(\tau) \, d\tau, \quad b_i = \int_0^1 \ell_i(\tau) \, d\tau,$$

where $\ell_i(\tau)$ is the Lagrange polynomial $\ell_i(\tau) = \prod_{l \neq i} (\tau - c_l)/(c_i - c_l)$.

Moreover:

$$u(t_0 + \tau h) = y_0 + h \sum_{j=1}^s k_j \int_0^\tau \ell_j(\sigma) \, d\sigma.$$ 

Thus, the existence of the collocation polynomial depends on the existence of the $k_i$ (given for $h \to 0$).
Proof. Let $u(t)$ be the collocation polynomial and define $k_i := \dot{u}(t_0 + c_i h)$. By the Lagrange interpolation formula we have

$$\dot{u}(t_0 + \tau h) = \sum_{j=1}^{s} k_j \cdot \ell_j(\tau),$$

and by integration we get

$$u(t_0 + c_i h) = y_0 + h \sum_{j=1}^{s} k_j \int_{0}^{c_i} \ell_j(\tau) \, d\tau.$$  

Inserted into the definition of the collocation polynomial

$$\dot{u}(t_0 + c_i h) = f(t_0 + c_i h, u(t_0 + c_i h)),$$

this gives the first formula of the Runge-Kutta equation

$$k_i = f\left(t_0 + c_i h, y_0 + h \sum_{j=1}^{s} a_{ij} k_j\right).$$

Integration from 0 to 1 yields $y_1 = y_0 + h \sum_{j=1}^{s} b_i k_i$. □
If a Runge-Kutta methods corresponds to a collocation method of order $s$, 

$$a_{ij} = \int_0^{c_i} \ell_j(\tau) \, d\tau, \quad b_i = \int_0^1 \ell_i(\tau) \, d\tau,$$

leads to:

$$C(q = s) : \quad \sum_{j=1}^s a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, \quad \forall i, \ k = 1, \ldots, q$$

$$B(p = s) : \quad \sum_{j=1}^s b_i c_i^{k-1} = \frac{1}{k}, \quad k = 1, \ldots, p$$

since $\tau^{k-1} = \sum_{j=1}^s c_j^{k-1} \ell_j(\tau)$ for $k = 1, \ldots, s$.

Note: $B(p) \Rightarrow y_0 + \sum_{i=1}^s b_i f(t_0 + hc_i)$ approximates the solution to 

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

with order $p$. 

Geometrical Numeric Integration
**Lemma 2** The collocation polynomial $u(t)$ is an approximation of order $s$ to the exact solution of $\dot{y} = f(t, y)$, $y(t_0) = y_0$ on the whole interval, i.e.,

$$\|u(t) - y(t)\| \leq C \cdot h^{s+1} \quad \text{for} \ t \in [t_0, t_0 + h]$$

and for sufficiently small $h$.

Moreover, the derivatives of $u(t)$ satisfy for $t \in [t_0, t_0 + h]$

$$\|u^{(k)}(t) - y^{(k)}(t)\| \leq C \cdot h^{s+1-k} \quad \text{for} \ k = 0, \ldots, s.$$
Proof of Lemma 2

\[
\dot{u}(t_0 + \tau h) = \sum_{j=1}^{s} f(t_0 + c_i h, u(t_0 + c_i h)) \ell_j(\tau),
\]

\[
\dot{y}(t_0 + \tau h) = \sum_{j=1}^{s} f(t_0 + c_i h, y(t_0 + c_i h)) \ell_j(\tau) + h^s E(\tau, h)
\]

\[
\|E(\tau, h)\| \leq 2 \max_{t \in [t_0, t_0 + h]} \|y^{(s+1)}(t)\| / s!
\]

Integrating the difference of the above two equations gives

\[
y(t_0 + \tau h) - u(t_0 + \tau h) = h \sum_{i=1}^{s} \Delta f_i \int_{0}^{\tau} \ell_i(\sigma) \, d\sigma + h^{s+1} \int_{0}^{\tau} E(\sigma, h) \, d\sigma
\]

with \(\Delta f_i = f(t_0 + c_i h, y(t_0 + c_i h)) - f(t_0 + c_i h, u(t_0 + c_i h))\).
**Proof of Lemma 2**

Using a Lipschitz condition for $f(t, y)$ on the Integral

$$y(t_0 + \tau h) - u(t_0 + \tau h) = h \sum_{i=1}^{s} \Delta f_i \int_0^{\tau} \ell_i(\sigma) \, d\tau + h^{s+1} \int_0^{\tau} E(\sigma, h) \, d\sigma$$

yields

$$\max_{t \in [t_0, t_0+h]} ||y(t) - u(t)|| \leq h C L \max_{t \in [t_0, t_0+h]} ||y(t) - u(t)|| + \text{Const.} \cdot h^{s+1},$$

implying $||u(t) - y(t)|| \leq C \cdot h^{s+1}$ for sufficiently small $h > 0$. 
Theorem 3 (Superconvergence) If the condition \( B(p) \) holds for some \( p \geq s \), then the collocation method has order \( p \). This means that the collocation method has the same order as the underlying quadrature formula.

\[
B(p) : \sum_{j=1}^{s} b_i c_i^{k-1} = \frac{1}{k}, \quad k = 1, \ldots, p
\]

Note: \( B(p) \) cannot be met for \( p > 2s \).
Proof of Superconvergence

**Proof.** We consider the collocation polynomial \( u(t) \) as the solution of a perturbed differential equation

\[
\dot{u} = f(t, u) + \delta(t)
\]

with defect \( \delta(t) := \dot{u}(t) - f(t, u(t)) \). Subtracting \( \dot{y}(t) = f(t, y) \) from the above we get after linearization that

\[
\dot{u}(t) - \dot{y}(t) = \frac{\partial f}{\partial y}(t, y(t)) (u(t) - y(t)) + \delta(t) + r(t),
\]

where, for \( t_0 \leq t \leq t_0 + h \), the remainder \( r(t) \) is of size \( O\left(\|u(t) - y(t)\|^2\right) = O(h^{2s+2}) \) by lemma 2.
Collocation methods with polynomials of degree \( s \) are equivalent to \( s \)-stage Runge-Kutta methods:

\[
a_{ij} = \int_0^{c_i} \ell_j(\tau) \, d\tau, \quad b_i = \int_0^1 \ell_i(\tau) \, d\tau,
\]

Collocation polynomials of degrees \( s \) lead to collocation methods of order \( s \) or better:

If \( B(p) \) is met for \( p > s \), the corresponding collocation method is of order \( p \).

\[
B(p) : \quad \sum_{j=1}^{s} b_i c_i^{k-1} = \frac{1}{k}, \quad k = 1, \ldots, p.
\]
Proof of Lemma 2

The second statement follows from the first one: Taking the $k$th derivative of

$$y(t_0 + \tau h) - u(t_0 + \tau h) = h \sum_{i=1}^{s} \Delta f_i \int_{0}^{\tau} \ell_i(\sigma) \, d\tau + h^{s+1} \int_{0}^{\tau} E(\sigma, h) \, d\sigma$$

gives

$$h^k (y^{(k)}(t_0 + \tau h) - u^{(k)}(t_0 + \tau h)) = h \sum_{i=1}^{s} \Delta f_i \ell_i^{(k-1)}(\tau) + h^{s+1} E^{(k-1)}(\tau, h).$$

With

$$||E^{(k-1)}(\tau, h)|| \leq \max_{t \in [t_0, t_0 + h]} \frac{||y^{(s+1)}(t)||}{(s - k + 1)!}$$

and a Lipschitz condition for $f(t, y), \ ||u^{(k)} - y^{(k)}|| \leq C \cdot h^{s+1-k}$ follows.
Variation of Constants Formula

For homogeneous systems of linear equations

$$\dot{y}(t) = A(t)y(t)$$

with initial condition $y(t_0) = y_0$, the solution can be written as

$$y(t) = R(t, t_0)y_0 \Leftrightarrow \dot{R}(t, s) = A(t)R(t, s).$$

Using this resolvent of the homogeneous differential system, the solution to inhomogeneous problems

$$\dot{y}(t) = A(t)y(t) + f(t)$$

can be found with the variation of constants formula:

$$y(t) = R(t, t_0)y_0 + \int_{t_0}^{t} R(t, s)f(s)\,ds.$$
Proof of Superconvergence

With

\[ \dot{R}(t, s) = \frac{\partial}{\partial y} f(t, y(t)) R(t, s) \]

The variation of constants formula then yields

\[ y_1 - y(t_0 + h) = \mathcal{E}(t_0 + h) = \int_{t_0}^{t_0+h} R(t_0 + h, s) \left( \delta(s) + r(s) \right) \, ds \]

as the solution of

\[ \dot{\mathcal{E}}(t_0 + h) = \frac{\partial f}{\partial y} \left( t, y(t) \right) \mathcal{E}(t) + \delta(t) + r(t). \]

The contribution of \( r(t) \):

\[ r(t) \sim O(h^{2s+2}) \Rightarrow \int_{t_0}^{t_0+h} R(t_0 + h, s) r(s) \, ds \sim O(h^{2s+3}) \]
Proof of Superconvergence

The main idea now is to apply the quadrature formula \((b_i, c_i)_{i=1}^s\) to the integral of \(g(s) = R(t_0 + h, s)\delta(s)\):

\[
\int_{t_0}^{t_0+h} g(s) \, ds = \sum_{i=1}^{s} b_i g(t_0 + hc_i) + \text{quadrature Error}.
\]

From \(\delta(s)|_{t_0+c_ih} = 0\) follows \(\sum_{i=1}^{s} b_i g(t_0 + hc_i) = 0\). Thus,

\[
\int_{t_0}^{t_0+h} g(s) \, ds = \text{quadrature Error} \leq h^{p+1} \frac{\partial^p}{\partial s^p} g(s).
\]

\(\frac{\partial^p}{\partial s^p} g(s)\) is bounded independently of \(h\) by Lemma 2. Therefore

\[
\mathcal{E}(t_0 + h) = \int_{t_0}^{t_0+h} R(t_0 + h, s) \left(\delta(s) + r(s)\right) \, ds \sim \mathcal{O}(h^{p+1}).
\]