Title: Lobatto methods

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Lobatto methods

Introduction

Lobatto methods for the numerical integration of differential equations are named after Rehuel Lobatto[1]. They are characterized by the use of approximations to the solution at the two end points t_n and t_{n+1} of each subinterval of integration $[t_n, t_{n+1}]$. Two well-known Lobatto methods based on the trapezoidal quadrature rule which are often used in practice are the *(implicit) trapezoidal rule* and the *Störmer-Verlet-leapfrog method*.

The (implicit) trapezoidal rule

Consider a system of ordinary differential equations (ODEs)

$$\frac{d}{dt}y = f(t, y) \tag{1}$$

[1] Rehuel Lobatto (1796-1866) was a Dutch mathematician working most of his life as an advisor for the government in the fields of life insurance and of weights and measures. In 1842 he was appointed professor of mathematics at the Royal Academy in Delft (known nowadays as Delft University of Technology).

where $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$. Starting from y_0 at t_0 one step $(t_n, y_n) \mapsto (t_{n+1}, y_{n+1})$ of the (implicit) trapezoidal rule applied to (1) is given by the implicit relation

$$y_{n+1} = y_n + \frac{h_n}{2}\left(f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right)$$

where $h_n = t_{n+1} - t_n$ is the step size. The (implicit) trapezoidal rule is oftentimes called the *Crank-Nicholson method* when considered in the context of time-dependent partial differential equations (PDEs). This implicit method requires the solution of a system of d equations for $y_{n+1} \in \mathbb{R}^d$ that can be expressed as

$$F(y_{n+1}) := y_{n+1} - y_n - \frac{h_n}{2}\left(f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right) = 0$$

and which is nonlinear when $f(t, y)$ is nonlinear in y. Starting from an initial guess $y_{n+1}^{(0)} \approx y_{n+1}$, the solution y_{n+1} can be approximated iteratively by modified Newton iterations as follows

$$y_{n+1}^{(k+1)} = y_{n+1}^{(k)} + p_{n+1}^{(k)}, \qquad J_n p_{n+1}^{(k)} = -F(y_{n+1}^{(k)})$$

using for example an approximate Jacobian

$$J_n = I_d - \frac{h_n}{2} D_y f(t_n, y_n) \approx D_y F(y_{n+1}^{(k)}).$$

Taking $J_n = I_d$ leads to fixed-point iterations

$$y_{n+1}^{(k+1)} = y_n + \frac{h_n}{2}\left(f(t_n, y_n) + f(t_{n+1}, y_{n+1}^{(k)})\right).$$

The generalized Newton-Störmer-Verlet-leapfrog method

Consider now a partitioned system of ODEs

$$\frac{d}{dt} q = v(t, p, q), \quad \frac{d}{dt} p = f(t, q, p) \tag{2}$$

where $v : \mathbb{R} \times \mathbb{R}^{d_q} \times \mathbb{R}^{d_p} \to \mathbb{R}^{d_q}$ and $f : \mathbb{R} \times \mathbb{R}^{d_q} \times \mathbb{R}^{d_p} \to \mathbb{R}^{d_p}$. Starting from (q_0, p_0) at t_0 one step $(t_n, q_n, p_n) \mapsto (t_{n+1}, q_{n+1}, p_{n+1})$ of the *generalized Newton-Störmer-Verlet-leapfrog method* applied to (2) reads

$$
\begin{aligned}
p_{n+1/2} &= p_n + \frac{h_n}{2} f(t_n, q_n, p_{n+1/2}), \\
q_{n+1} &= q_n + \frac{h_n}{2} \left(v(t_n, q_n, p_{n+1/2}) + v(t_{n+1}, q_{n+1}, p_{n+1/2}) \right), \\
p_{n+1} &= p_{n+1/2} + \frac{h_n}{2} f(t_{n+1}, q_{n+1}, p_{n+1/2})
\end{aligned} \tag{3}
$$

where $h_n = t_{n+1} - t_n$ is the step size. The first equation is implicit for $p_{n+1/2}$, the second equation is implicit for q_{n+1}, and the last equation is explicit for p_{n+1}. When $v(t, q, p) = v(t, p)$ is independent of q and $f(t, q, p) = f(t, q)$ is independent of p the method is fully explicit. If in addition $v(t, q, p) = v(p)$ is independent of t and q the method can be simply expressed as

$$
\begin{aligned}
p_{n+1/2} &= p_n + \frac{h_n}{2} f(t_n, q_n), \\
q_{n+1} &= q_n + h_n v(p_{n+1/2}), \\
p_{n+1} &= p_{n+1/2} + \frac{h_n}{2} f\left(t_{n+1}, q_{n+1}\right).
\end{aligned}
$$

This explicit method is often applied as follows

$$
\begin{aligned}
p_{n+1/2} &= p_{n-1/2} + \frac{1}{2}(h_{n-1} + h_n) f\left(t_n, q_n\right), \\
q_{n+1} &= q_n + h_n v(p_{n+1/2}).
\end{aligned}
$$

Depending on the field of applications this method is known under different names: the *Störmer method* in astronomy; the *Verlet method* in molecular dynamics; the *leapfrog method* in the context of time-dependent PDEs, in particular for wave equations. This method can be traced back to Newton's Principia (1687), see (Hairer et al, 2003).

Lobatto methods

In this article we consider families of Runge-Kutta (RK) methods based on Lobatto quadrature formulas whose simplest member is the trapezoidal quadrature rule. When applied to (1) Lobatto RK methods can be expressed as follows

$$
Y_{ni} = y_n + h_n \sum_{j=1}^{s} a_{ij} f(t_n + c_j h, Y_{nj}) \qquad \text{for } i = 1, \ldots, s, \tag{4}
$$

$$y_{n+1}=y_n + h_n \sum_{j=1}^{s} b_j f(t_n + c_j h, Y_{nj}) \tag{5}$$

where the stage value s satisfies $s \geq 2$ and the coefficients a_{ij}, b_j, c_j characterize the Lobatto RK method. The s intermediate values Y_{nj} for $j = 1, \ldots, s$ are called the *internal stages* and can be considered as approximations to the solution at $t_n + c_j h_n$, the main numerical RK approximation at $t_{n+1} = t_n + h_n$ is given by y_{n+1}. Lobatto RK methods are characterized by $c_1 = 0$ and $c_s = 1$. They can also be considered in combination with other families of RK methods, e.g., with Gauss methods in the context of certain systems of differential-algebraic equations (DAEs), see the section *Lobatto methods for DAEs* below. The symbol III is usually found in the literature associated to Lobatto methods, the symbols I and II being reserved for the two types of Radau methods. The (implicit) trapezoidal rule is the simplest member ($s = 2$) in the Lobatto IIIA family. The generalized Newton-Störmer-Verlet-leapfrog method seen above can be interpreted as a partitioned Runge-Kutta (PRK) resulting from the combination of the (implicit) trapezoidal rule and of the Lobatto IIIB method for $s = 2$, see the section *additive Lobatto methods for split and partitioned ODEs* below.

Families of Lobatto methods

For a fixed value of s the various families of Lobatto methods described below all share the same coefficients b_j, c_j of the corresponding Lobatto quadrature formula.

Lobatto quadrature formulas

The problem of approximating a Riemannn integral

$$\int_{t_n}^{t_n+h_n} f(t)dt \tag{6}$$

with f assumed to be continuous is equivalent to the problem of solving the initial value problem at $t = t_n + h_n$

$$\frac{d}{dt}y = f(t), \quad y(t_n) = 0$$

since $y(t_n + h_n) = \int_{t_n}^{t_n+h_n} f(t)dt$. The integral (6) can be approximated by using a standard quadrature formula

$$\int_{t_n}^{t_n+h_n} f(t)dt \approx h_n \left(\sum_{i=1}^{s} b_i f(t_n + c_i h_n) \right)$$

with s *node* coefficients $c_1, \ldots, c_s$, and s *weight* coefficients $b_1, \ldots, b_s$. Lobatto quadrature formulas, also known as Gauss-Lobatto quadrature formulas in the literature, are given for $s \geq 2$ by a set of nodes and weights satisfying conditions described hereafter. The s nodes c_j are the roots of the polynomial of degree s

$$\frac{d^{s-2}}{dt^{s-2}}(t^{s-1}(1-t)^{s-1}).$$

These nodes satisfy $c_1 = 0 < c_2 < \ldots < c_s = 1$. The weights b_j and nodes c_j satisfy the condition $B(2s-2)$ where

$$B(p) \ : \ \sum_{j=1}^{s} b_j c_j^{k-1} = \frac{1}{k} \qquad \text{for } k = 1, \ldots, p,$$

implying that the quadrature formula is of order $2s-2$. There exists an explicit formula for the weights

$$b_j = \frac{1}{s(s-1)P_{s-1}(2c_j-1)^2} > 0 \qquad \text{for } j = 1, \ldots, s \quad \left(b_1 = b_s = \frac{1}{s(s-1)} \right)$$

where

$$P_k(x) = \frac{1}{k!2^k} \frac{d^k}{dx^k} \left((x^2-1)^k \right)$$

is the kth Legendre polynomial. Lobatto quadrature formulas are symmetric, i.e., their nodes and weights satisfy

$$b_{s+1-j} = b_j, \quad c_{s+1-j} = 1 - c_j \qquad \text{for } j = 1, \ldots, s.$$

For $s = 3$ we obtain the famous Simpson's rule

$$(b_1, b_2, b_3) = (1/6, 2/3, 1/6), \quad (c_1, c_2, c_3) = (0, 1/2, 1).$$

Procedures to compute numerically accurately the nodes and weights of high order Lobatto quadrature formulas can be found in (Gautschi, 2000) and (von Matt, 2004). The subroutine `GQRUL` from the `IMSL/MATH-LIBRARY` can compute numerically these nodes and weights.

Lobatto families

The families of Lobatto RK methods differ only in the values of their coefficients a_{ij}. Various equivalent definitions can be found in the literature. The coefficients a_{ij} of these families can be linearly implicitly defined with the help of so-called *simplifying assumptions*

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

$$D(r): \quad \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} = \frac{b_j}{k}(1 - c_j^k) \quad \text{for } j = 1, \ldots, s \text{ and } k = 1, \ldots, r.$$

The importance of these simplifying assumptions comes from a fundamental result due to Butcher, see (Butcher, 2008; Hairer et al, 1993), saying that a RK method satisfying the simplifying assumptions $B(p)$, $C(q)$, and $D(r)$ is of order at least $\min(p, 2q+2, q+r+1)$. The coefficients a_{ij}, b_j, c_j characterizing the Lobatto RK method (4)-(5) will be displayed below in the form of a table called a *Butcher-tableau*

$$\begin{array}{r|ccccc}
c_1 = 0 & a_{11} & a_{12} & \cdots & a_{1,s-1} & a_{1s} \\
c_2 & a_{21} & a_{22} & \cdots & a_{2,s-1} & a_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
c_{s-1} & a_{s-1,1} & a_{s-1,2} & \cdots & a_{s-1,s-1} & a_{s-1,s} \\
c_s = 1 & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & a_{ss} \\
\hline
 & b_1 & b_2 & \cdots & b_{s-1} & b_s
\end{array}$$

In the four main families of Lobatto methods described below, namely Lobatto IIIA, Lobatto IIIB, Lobatto IIIC, and Lobatto IIIC*, only one method does not satisfy the relation $C(1)$, i.e.,

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

this is the Lobatto IIIB method for $s = 2$, see below. The Lobatto IIIA, IIIB, IIIC, and IIIC* methods can all be interpreted as perturbed collocation methods (Nørsett and Wanner, 1981) and discontinuous collocation methods (Hairer et al, 2006).

Lobatto IIIA

The coefficients a_{ij}^A of Lobatto IIIA methods can be defined by $C(s)$. They satisfy $D(s-2)$, $a_{sj}^A = b_j$ for $j = 1, \ldots, s$, and $a_{1j}^A = 0$ for $j = 1, \ldots, s$. Lobatto IIIA methods are symmetric and of nonstiff order $2s-2$. Their stability function $R(z)$ is given by the $(s-1, s-1)$-Padé approximation to e^z. They are A-stable, but not L-stable since $R(\infty) = (-1)^{s+1}$. They are not B-stable and thus not algebraically stable.. They can be interpreted as collocation methods. Since the first internal stage Y_{n1} of Lobatto IIIA methods is explicit ($Y_{n1} = y_n$ and $f(t_n + c_1 h_n, Y_{n1}) = f(t_n, y_n)$) and the last internal stage satisfies $Y_{ns} = y_{n+1}$ (and thus $f(t_{n+1}, y_{n+1}) = f(t_n + c_s h_n, Y_{ns})$) these methods are comparable in term of computational work to Gauss methods with $s-1$ internal stages since they also have the same nonstiff order $2s-2$. For $s = 2$ we obtain the (implicit) trapezoidal rule which is often expressed without its two internals stages Y_{n1}, Y_{n2} since they are respectively equal to y_n and y_{n+1}. The method for $s = 3$ is sometimes called the *Hermite-Simpson (or Clippinger-Dimsdale) method* and it has been used for example in trajectory optimization problems (Betts, 2008). This method can be equivalently expressed in a compact form as

$$\begin{aligned} Y_{n2} &= \frac{1}{2}(y_n + y_{n+1}) + \frac{h_n}{8}(f(t_n, y_n) - f(t_{n+1}, y_{n+1})), \\ y_{n+1} &= y_n + \frac{h_n}{6}\left(f(t_n, y_n) + 4f(t_{n+1/2}, Y_{n2}) + f(t_{n+1}, y_{n+1})\right) \end{aligned}$$

where $t_{n+1/2} = t_n + h_n/2$. It can be even further reduced by rewriting

$$y_{n+1} = y_n + \frac{h_n}{6}\left(f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right)$$

$$+\frac{2h_n}{3}f\left(t_{n+1/2},\frac{1}{2}(y_n+y_{n+1})+\frac{h_n}{8}(f(t_n,y_n)-f(t_{n+1},y_{n+1}))\right).$$

Table 1. Coefficients of Lobatto IIIA for $s=2,3,4,5$.

0	0	0
1	$\frac{1}{2}$	$\frac{1}{2}$
$A_{s=2}$	$\frac{1}{2}$	$\frac{1}{2}$

0	0	0	0
$\frac{1}{2}$	$\frac{5}{24}$	$\frac{1}{3}$	$-\frac{1}{24}$
1	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$
$A_{s=3}$	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$

0	0	0	0	0
$\frac{1}{2}-\frac{\sqrt{5}}{10}$	$\frac{11+\sqrt{5}}{120}$	$\frac{25-\sqrt{5}}{120}$	$\frac{25-13\sqrt{5}}{120}$	$\frac{-1+\sqrt{5}}{120}$
$\frac{1}{2}+\frac{\sqrt{5}}{10}$	$\frac{11-\sqrt{5}}{120}$	$\frac{25+13\sqrt{5}}{120}$	$\frac{25+\sqrt{5}}{120}$	$\frac{-1-\sqrt{5}}{120}$
1	$\frac{1}{12}$	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{12}$
$A_{s=4}$	$\frac{1}{12}$	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{12}$

0	0	0	0	0	0
$\frac{1}{2}-\frac{\sqrt{21}}{14}$	$\frac{119+3\sqrt{21}}{1960}$	$\frac{343-9\sqrt{21}}{2520}$	$\frac{392-96\sqrt{21}}{2205}$	$\frac{343-69\sqrt{21}}{2520}$	$\frac{-21+3\sqrt{21}}{1960}$
$\frac{1}{2}$	$\frac{13}{320}$	$\frac{392+105\sqrt{21}}{2880}$	$\frac{8}{45}$	$\frac{392-105\sqrt{21}}{2880}$	$\frac{3}{320}$
$\frac{1}{2}+\frac{\sqrt{21}}{14}$	$\frac{119-3\sqrt{21}}{1960}$	$\frac{343+69\sqrt{21}}{2520}$	$\frac{392+96\sqrt{21}}{2205}$	$\frac{343+9\sqrt{21}}{2520}$	$\frac{-21-3\sqrt{21}}{1960}$
1	$\frac{1}{20}$	$\frac{49}{180}$	$\frac{16}{45}$	$\frac{49}{180}$	$\frac{1}{20}$
$A_{s=5}$	$\frac{1}{20}$	$\frac{49}{180}$	$\frac{16}{45}$	$\frac{49}{180}$	$\frac{1}{20}$

Lobatto IIIB

The coefficients a^B_{ij} of Lobatto IIIB methods can be defined by $D(s)$. They satisfy $C(s-2)$, $a^B_{i1}=b_1$ for $i=1,\ldots,s$ and $a^B_{is}=0$ for $i=1,\ldots,s$. Lobatto IIIB methods are symmetric and of nonstiff order $2s-2$. Their stability function $R(z)$ is given by the $(s-1,s-1)$-Padé approximation to e^z. They are A-stable, but not L-stable since $R(\infty)=(-1)^{s+1}$. They are not B-stable and thus not algebraically stable.. The coefficients a^B_{ij} can also be obtained from the coefficients a^A_{ij} of Lobatto IIIA through the relations

$$b_i a^B_{ij}+b_j a^A_{ji}-b_i b_j=0 \quad \text{for } i,j=1,\ldots,s,$$

or

$$a^B_{ij}=b_j-a^A_{s+1-i,s+1-j} \quad \text{for } i,j=1,\ldots,s.$$

Table 2. Coefficients of Lobatto IIIB for $s = 2, 3, 4, 5$.

0	$\frac{1}{2}$	0
1	$\frac{1}{2}$	0
$B_{s=2}$	$\frac{1}{2}$	$\frac{1}{2}$

0	$\frac{1}{6}$	$-\frac{1}{6}$	0
$\frac{1}{2}$	$\frac{1}{6}$	$\frac{1}{3}$	0
1	$\frac{1}{6}$	$\frac{5}{6}$	0
$B_{s=3}$	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$

0	$\frac{1}{12}$	$\frac{-1-\sqrt{5}}{24}$	$\frac{-1+\sqrt{5}}{24}$	0
$\frac{1}{2}-\frac{\sqrt{5}}{10}$	$\frac{1}{12}$	$\frac{25+\sqrt{5}}{120}$	$\frac{25-13\sqrt{5}}{120}$	0
$\frac{1}{2}+\frac{\sqrt{5}}{10}$	$\frac{1}{12}$	$\frac{25+13\sqrt{5}}{120}$	$\frac{25-\sqrt{5}}{120}$	0
1	$\frac{1}{12}$	$\frac{11-\sqrt{5}}{24}$	$\frac{11+\sqrt{5}}{24}$	0
$B_{s=4}$	$\frac{1}{12}$	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{12}$

0	$\frac{1}{20}$	$\frac{-7-\sqrt{21}}{120}$	$\frac{1}{15}$	$\frac{-7+\sqrt{21}}{120}$	0
$\frac{1}{2}-\frac{\sqrt{21}}{14}$	$\frac{1}{20}$	$\frac{343+9\sqrt{21}}{2520}$	$\frac{56-15\sqrt{21}}{315}$	$\frac{343-69\sqrt{21}}{2520}$	0
$\frac{1}{2}$	$\frac{1}{20}$	$\frac{49+12\sqrt{21}}{360}$	$\frac{8}{45}$	$\frac{49-12\sqrt{21}}{360}$	0
$\frac{1}{2}+\frac{\sqrt{21}}{14}$	$\frac{1}{20}$	$\frac{343+69\sqrt{21}}{2520}$	$\frac{56+15\sqrt{21}}{315}$	$\frac{343-9\sqrt{21}}{2520}$	0
1	$\frac{1}{20}$	$\frac{119-3\sqrt{21}}{360}$	$\frac{13}{45}$	$\frac{119+3\sqrt{21}}{360}$	0
$B_{s=5}$	$\frac{1}{20}$	$\frac{49}{180}$	$\frac{16}{45}$	$\frac{49}{180}$	$\frac{1}{20}$

Lobatto IIIC

The coefficients a_{ij}^C of Lobatto IIIC methods can be defined by $a_{i1}^C = b_1$ for $i = 1, \ldots, s$ and $C(s-1)$. They satisfy $D(s-1)$ and $a_{sj}^C = b_j$ for $j = 1, \ldots, s$. Lobatto IIIC methods are of nonstiff order $2s-2$. They are not symmetric. Their stability function $R(z)$ is given by the $(s-2, s)$-Padé approximation to e^z. They are L-stable. They are algebraically stable and thus B-stable. They are excellent methods for stiff problems.

Lobatto IIIC*

Lobatto IIIC*[2] are also known as Lobatto III methods (Butcher, 2008), Butcher's Lobatto methods (Hairer et al, 1993), and Lobatto III$\overline{C}$ methods (Sun, 2000) in the literature. The coefficients $a_{ij}^{C^*}$ of Lobatto IIIC* methods can be defined by $a_{is}^{C^*} = 0$ for $i = 1, \ldots, s$ and $C(s-1)$. They satisfy $D(s-1)$ and $a_{1j}^{C^*} = 0$ for $j = 1, \ldots, s$. Lobatto IIIC* methods are of nonstiff order $2s-2$. They are not symmetric. Their

[2] The name Lobatto IIIC* was suggested by Robert P.K. Chan in an e-mail correspondence with the author on June 13, 1995.

Table 3. Coefficients of Lobatto IIIC for $s = 2, 3, 4, 5$.

0	$\frac{1}{2}$	$-\frac{1}{2}$
1	$\frac{1}{2}$	$\frac{1}{2}$
$C_{s=2}$	$\frac{1}{2}$	$\frac{1}{2}$

0	$\frac{1}{6}$	$-\frac{1}{3}$	$\frac{1}{6}$
$\frac{1}{2}$	$\frac{1}{6}$	$\frac{5}{12}$	$-\frac{1}{12}$
1	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$
$C_{s=3}$	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$

0	$\frac{1}{12}$	$-\frac{\sqrt{5}}{12}$	$\frac{\sqrt{5}}{12}$	$-\frac{1}{12}$
$\frac{1}{2}-\frac{\sqrt{5}}{10}$	$\frac{1}{12}$	$\frac{1}{4}$	$\frac{10-7\sqrt{5}}{60}$	$\frac{\sqrt{5}}{60}$
$\frac{1}{2}+\frac{\sqrt{5}}{10}$	$\frac{1}{12}$	$\frac{10+7\sqrt{5}}{60}$	$\frac{1}{4}$	$-\frac{\sqrt{5}}{60}$
1	$\frac{1}{12}$	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{12}$
$C_{s=4}$	$\frac{1}{12}$	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{12}$

0	$\frac{1}{20}$	$-\frac{7}{60}$	$\frac{2}{15}$	$-\frac{7}{60}$	$\frac{1}{20}$
$\frac{1}{2}-\frac{\sqrt{21}}{14}$	$\frac{1}{20}$	$\frac{29}{180}$	$\frac{47-15\sqrt{21}}{315}$	$\frac{203-30\sqrt{21}}{1260}$	$-\frac{3}{140}$
$\frac{1}{2}$	$\frac{1}{20}$	$\frac{329+105\sqrt{21}}{2880}$	$\frac{73}{360}$	$\frac{329-105\sqrt{21}}{2880}$	$\frac{3}{160}$
$\frac{1}{2}+\frac{\sqrt{21}}{14}$	$\frac{1}{20}$	$\frac{203+30\sqrt{21}}{1260}$	$\frac{47+15\sqrt{21}}{315}$	$\frac{29}{180}$	$-\frac{3}{140}$
1	$\frac{1}{20}$	$\frac{49}{180}$	$\frac{16}{45}$	$\frac{49}{180}$	$\frac{1}{20}$
$C_{s=5}$	$\frac{1}{20}$	$\frac{49}{180}$	$\frac{16}{45}$	$\frac{49}{180}$	$\frac{1}{20}$

stability function $R(z)$ is given by the $(s, s-2)$-Padé approximation to e^z. They are not A-stable. They are not B-stable and thus not algebraically stable.. The Lobatto IIIC* method for $s = 2$ is sometimes called the *explicit trapezoidal rule*. The coefficients $a_{ij}^{C^*}$ can also be obtained from the coefficients a_{ij}^{C} of Lobatto IIIC through the relations

$$b_i a_{ij}^{C^*} + b_j a_{ji}^{C} - b_i b_j = 0 \quad \text{for } i, j = 1, \ldots, s,$$

or

$$a_{ij}^{C^*} = b_j - a_{s+1-i,s+1-j}^{C} \quad \text{for } i, j = 1, \ldots, s.$$

Other families of Lobatto methods

Most Lobatto methods of interest found in the literature can be expressed as linear combinations of the four fundamental Lobatto IIIA, IIIB, IIIC, and IIIC* methods. In fact one can consider a very general family of methods with three real parameters $(\alpha_A, \alpha_B, \alpha_C)$ by considering Lobatto coefficients of the form

$$a_{ij}(\alpha_A, \alpha_B, \alpha_C) = \alpha_A a_{ij}^{A} + \alpha_B a_{ij}^{B} + \alpha_C a_{ij}^{C} + \alpha_{C^*} a_{ij}^{C^*} \tag{7}$$

Table 4. Coefficients of Lobatto IIIC* for $s = 2, 3, 4, 5$.

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline C^*_{s=2} & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 \\ 1 & 0 & 1 & 0 \\ \hline C^*_{s=3} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{5+\sqrt{5}}{60} & \frac{1}{6} & \frac{15-7\sqrt{5}}{60} & 0 \\ \frac{1}{2}+\frac{\sqrt{5}}{10} & \frac{5-\sqrt{5}}{60} & \frac{15+7\sqrt{5}}{60} & \frac{1}{6} & 0 \\ 1 & \frac{1}{6} & \frac{5-\sqrt{5}}{12} & \frac{5+\sqrt{5}}{12} & 0 \\ \hline C^*_{s=4} & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \end{array}$$

$$\begin{array}{c|ccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2}-\frac{\sqrt{21}}{14} & \frac{1}{14} & \frac{1}{9} & \frac{13-3\sqrt{21}}{63} & \frac{14-3\sqrt{21}}{126} & 0 \\ \frac{1}{2} & \frac{1}{32} & \frac{91+21\sqrt{21}}{576} & \frac{11}{72} & \frac{91-21\sqrt{21}}{576} & 0 \\ \frac{1}{2}+\frac{\sqrt{21}}{14} & \frac{1}{14} & \frac{14+3\sqrt{21}}{126} & \frac{13+3\sqrt{21}}{63} & \frac{1}{9} & 0 \\ 1 & 0 & \frac{7}{18} & \frac{2}{9} & \frac{7}{18} & 0 \\ \hline C^*_{s=5} & \frac{1}{20} & \frac{49}{180} & \frac{16}{45} & \frac{49}{180} & \frac{1}{20} \end{array}$$

where $\alpha_{C^*} = 1 - \alpha_A - \alpha_B - \alpha_C$. For any choice of $(\alpha_A, \alpha_B, \alpha_C)$ the corresponding Lobatto RK method is of nonstiff order $2s-2$ (Jay, 1998). The Lobatto IIIS methods presented in (Chan, 1990) depend on a real parameter σ. They can be expressed as

$$a^S_{ij}(\sigma) = (1-\sigma)\left(a^A_{ij} + a^B_{ij}\right) + \left(\sigma - \frac{1}{2}\right)\left(a^C_{ij} + a^{C^*}_{ij}\right) \qquad \text{for } i,j = 1,\ldots,s,$$

corresponding to $\alpha_A = \alpha_B = 1-\sigma$ and $\alpha_C = \alpha_{C^*} = \sigma - \frac{1}{2}$ in (7). These methods satisfy $C(s-2)$ and $D(s-2)$. They are symmetric and symplectic. Their stability function $R(z)$ is given by the $(s-1,s-1)$-Padé approximation to e^z. They are A-stable, but not L-stable. They are algebraically stable and thus B-stable. The Lobatto IIIS coefficients for $\sigma = 1/2$ are given by

$$a^S_{ij}\,(1/2) = \frac{1}{2}\left(a^A_{ij} + a^B_{ij}\right) \qquad \text{for } i,j = 1,\ldots,s.$$

For $\sigma = 1$ we obtain the Lobatto IIID methods (Chan, 1990; Jay, 1998)

$$a^D_{ij} = a^S_{ij}(1) = \frac{1}{2}\left(a^C_{ij} + a^{C^*}_{ij}\right) \qquad \text{for } i,j = 1,\ldots,s.$$

These methods are called Lobatto III$_E$ in (Nørsett and Wanner, 1981) and Lobatto IIIE in (Sun, 2000). They satisfy $C(s-1)$ and $D(s-1)$ and they can be interpreted as

perturbed collocation methods (Nørsett and Wanner, 1981). Another family of Lobatto RK methods is given by the Lobatto III_D family of (Nørsett and Wanner, 1981)[3] called here Lobatto IIINW where the coefficients for $s = 2, 3$ are given in Table 5. These

Table 5. Coefficients of Lobatto IIINW for $s = 2, 3$ (Nørsett and Wanner, 1981)

$$\begin{array}{c|cc} 0 & \frac{1}{2} & \frac{1}{2} \\ 1 & -\frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{c|ccc} 0 & \frac{1}{6} & 0 & -\frac{1}{6} \\ \frac{1}{2} & \frac{1}{12} & \frac{5}{12} & 0 \\ 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

methods correspond to $\alpha_A = 2$, $\alpha_B = 2$, $\alpha_C = -1$, and $\alpha_{C^*} = -2$ in (7). Their stability function $R(z)$ is given by the $(s-2, s)$-Padé approximation to e^z. These methods are L-stable. They are algebraically stable and thus B-stable. They are of nonstiff order $2s - 2$. They are not symmetric. They can be interpreted as perturbed collocation methods (Nørsett and Wanner, 1981).

Additive Lobatto methods for split and partitioned ODEs

Consider a split system of ODEs

$$\frac{d}{dt}y = f_1(t, y) + f_2(t, y) \tag{8}$$

where $f_1, f_2 : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$. Starting from y_0 at t_0 one step $(t_n, y_n) \mapsto (t_{n+1}, y_{n+1})$ of an *additive Lobatto RK method* applied to (8) reads

$$\begin{aligned} Y_{ni} &= y_n + h_n \sum_{j=1}^{s} (a_{1,ij} f_1(t_n + c_j h, Y_{nj}) + a_{2,ij} f_2(t_n + c_j h, Y_{nj})) \qquad \text{for } i = 1, \ldots, s, \\ y_{n+1} &= y_n + h_n \sum_{j=1}^{s} b_j (f_1(t_n + c_j h, Y_{nj}) + f_2(t_n + c_j h, Y_{nj})) \end{aligned}$$

[3] notice on p. 205 of (Nørsett and Wanner, 1981) that $\gamma_1 = -4(2m - 1)$.

where $s \geq 2$ and the coefficients $a_{1,ij}, a_{2,ij}, b_j, c_j$ characterize the additive Lobatto RK method. Consider for example any coefficients $a_{1,ij}$ and $a_{2,ij}$ from the family (7), the additive method is of nonstiff order $2s-2$ (Jay, 1998). The partitioned system of ODEs (2) can be expressed in the form (8) by having $d = d_q + d_p$, $y = (q, p) \in \mathbb{R}^{d_q} \times \mathbb{R}^{d_p}$, and

$$f_1(t,q,p) = \begin{pmatrix} v(t,q,p) \\ \\ 0 \end{pmatrix}, \quad f_2(t,q,p) = \begin{pmatrix} 0 \\ \\ f(t,q,p) \end{pmatrix}.$$

Applying for $s = 2$ the Lobatto IIIA coefficients as $a_{1,ij}$ and the Lobatto IIIB coefficients as $a_{2,ij}$, we obtain again the generalized Newton-Störmer-Verlet-leapfrog method (3). Additive Lobatto methods have been considered in multibody dynamics in (Jay, 1998; Schaub and Simeon, 2003). Additive methods are more general than partitioned methods since partitioned system of ODEs can always be reformulated as a split system of ODEs, but the reverse is false in general.

Lobatto methods for DAEs

An important use of Lobatto methods is for the solution of differential-algebraic equations (DAEs). DAEs consist generally of coupled systems of differential equations and nonlinear relations. They arise typically in mechanics and electrical/electronic circuits simulation. Consider for example a system of DAEs of the form

$$\frac{d}{dt}y = f(t, y, \lambda), \qquad 0 = k(t, y)$$

where $D_y k(t, y) D_\lambda f(t, y, \lambda)$ is nonsingular. Lobatto methods can be applied to this class of problems while preserving their classical order of convergence (Jay, 2003). For example the application of the 2-stage Lobatto IIID method can be expressed as

$$\begin{aligned}
Y_{n1} &= y_n + \frac{h_n}{4}(f(t_n, Y_{n1}, \Lambda_{n1}) - f(t_{n+1}, Y_{n2}, \Lambda_{n2})), \\
Y_{n2} &= y_n + \frac{h_n}{4}(3f(t_n, Y_{n1}, \Lambda_{n1}) + f(t_{n+1}, Y_{n2}, \Lambda_{n2})), \\
y_{n+1} &= y_n + \frac{h_n}{2}(f(t_n, Y_{n1}, \Lambda_{n1}) + f(t_{n+1}, Y_{n2}, \Lambda_{n2})),
\end{aligned}$$

$$0=\frac{1}{2}(k(t_n,Y_{n1})+k(t_{n+1},Y_{n2})),$$

$$0=k(t_{n+1},y_{n+1}).$$

For such DAEs a combination of Gauss and Lobatto coefficients is also considered in (Murua, 1996). Consider now overdetermined system of DAEs (ODAEs) of the form

$$\frac{d}{dt}q=v(t,q,p),\ \frac{d}{dt}p=f(t,q,p,\lambda),\ 0=g(t,q),\ 0=D_tg(t,q)+D_qg(t,q)v(t,q,p) \quad (9)$$

where $D_qg(t,q)D_pv(t,q,p)D_\lambda f(t,q,p,\lambda)$ is nonsingular. Very general Lobatto methods can be applied to this type of ODAEs (Jay, 1998). Hamiltonian and Lagrangian systems with holonomic constraints can be expressed in the form (9). For such ODAEs the application of Lobatto IIIA-IIIB methods can be shown to preserve their classical order of convergence, to be variational integrators, and to preserve a symplectic two-form (Jay, 1996; Leimkuhler and Reich, 2005; Hairer and Wanner, 1996; Hairer et al, 2006). For example the application of the 2-stage Lobatto IIIA-IIIB method reads

$$q_{n+1}=q_n+\frac{h_n}{2}\left(v\left(t_n,q_n,p_{n+1/2}\right)+v\left(t_{n+1},q_{n+1},p_{n+1/2}\right)\right),$$

$$p_{n+1/2}=p_n+\frac{h_n}{2}f\left(t_n,q_n,p_{n+1/2},\Lambda_{n1}\right),$$

$$0=g(t_{n+1},q_{n+1}),$$

$$p_{n+1}=p_{n+1/2}+\frac{h_n}{2}f\left(t_{n+1},q_{n+1},p_{n+1/2},\Lambda_{n2}\right)$$

$$0=D_tg(t_{n+1},q_{n+1})+D_qg(t_{n+1},q_{n+1})v(t_{n+1},q_{n+1},p_{n+1}).$$

Gauss methods with s stages can also be applied in combination with Lobatto methods with $s+1$ stages for this type of ODAEs when $f(t,q,p,\lambda)$ is decomposed in $f(t,q,p)+r(t,q,\lambda)$ and they also possess these aforementioned properties while generally requiring less computational effort (Jay, 2007). For example the application of the midpoint-trapezoidal method (the $(1,1)$-Gauss-Lobatto SPARK method of Jay (2007)) reads

$$Q_{n1}=q_n+\frac{h_n}{2}v(t_{n+1/2},Q_{n1},P_{n1})=\frac{1}{2}(q_n+q_{n+1}),$$

$$P_{n1}=p_n+\frac{h_n}{2}f(t_{n+1/2},Q_{n1},P_{n1})+\frac{h_n}{2}r(t_n,q_n,\Lambda_{n1}),$$

$$q_{n+1} = q_n + h_n v(t_{n+1/2}, Q_{n1}, P_{n1}),$$

$$p_{n+1} = p_n + h_n f(t_{n+1/2}, Q_{n1}, P_{n1}) + h_n \left(\frac{1}{2} r(t_n, q_n, \Lambda_{n1}) + \frac{1}{2} r(t_{n+1}, q_{n+1}, \Lambda_{n2}) \right),$$

$$0 = g(t_{n+1}, q_{n+1}),$$

$$0 = D_t g(t_{n+1}, q_{n+1}) + D_q g(t_{n+1}, q_{n+1}) v(t_{n+1}, q_{n+1}, p_{n+1}).$$

Lobatto methods for some other classes of problems

Lobatto IIIA methods have been considered for boundary value problems (BVP) due to their good stability properties (Ascher et al, 1995; Bashir-Ali et al, 1998). The *MATLAB* code `bvp4c` for BVP is based on 3-stage collocation at Lobatto points, hence it is equivalent to the 3-stage Lobatto IIIA method (Kierzenka and Shampine, 2001). Lobatto methods have also been applied to delay differential equations (DDEs) (Bellen et al, 1999). The combination of Lobatto IIIA and IIIB methods have also been considered for the discrete multisymplectic integration of certain Hamiltonian partial differential equations (PDEs) such as the nonlinear Schrödinger equation and certain nonlinear wave equations (Ryland and McLachlan, 2008).

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