

Numerical Solutions to Differential Equations

Lecture Notes #16 — Hybrid Methods

Peter Blomgren,
(blomgren.peter@gmail.com)

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720
<http://terminus.sdsu.edu/>

Spring 2015

Outline

1 Hybrid Methods

- Introduction
- Byrne-and-Lambert's Pseudo Runge-Kutta Methods
- Generalized Linear Multistep Methods

2 General Linear Methods

- First Pass: GLM-lite
- GLM-lite: Old Methods, New Notation...
- New Methods, New Notation...

So far we have looked at three strategies for improving on Euler's method

1 Taylor Series Methods

- Best used when the Taylor expansion of $f(t, y(t))$ is available and cheap/easy to compute.
- **Stiffness:** Small stability region. Step-size h very restrictive.

② Runge-Kutta Methods

- When the Taylor expansion of $f(t, y(t))$ is not easily computable (or prohibitively expensive), but multiple evaluation of $f(t, y(t))$ incur a reasonable amount of work, then RK-methods are a good choice.
- **Stiffness:** When the problem is stiff, we have to use fully implicit RK-methods. We have seen that there are A-stable s -stage $2s$ -order methods (Gauss-Legendre) for arbitrary s , as well as L-stable s -stage $(2s-1)$ -order methods (Radau I-A, and II-A).

3 Linear Multistep Methods

- Explicit LMMs only require one new function evaluation per step, making them very competitive (fast and cheap). Used in the predictor-corrector context $P(EC)^\mu$, only $(1+\mu)$ evaluations per step are required.
- The main **drawback** is that LMMs are not self-starting, so we need an RK- or Taylor-series method (possibly with Richardson Extrapolation) to generate enough accurate starting information.
- **Stiffness:** If/when we can live with an $A(\alpha)$ -stable method, implementing efficient LMM-based stiff solvers is quite straightforward (at least up to order 6...)

Strategies

We have 4 fundamental strategies on hand

- 1 Use more derivatives of $y(t)$, (*Taylor series methods*)
- 2 Use more past values, (*Linear Multistep Methods*)
- 3 Use more calculations per step, (*Runge Kutta*)
- 4 Use derivatives of $f(t, y(t))$, (*not used so far**)

Combinations in the literature:

Obreshkov more (past values + derivatives of $y(t)$)
~ LMM + Taylor

Rosenbrock more (derivatives of $y(t)$, and $f(t, y(t))$ +
calculations per step)
~ RK + Taylor + f -derivatives

General Linear more (past values + calculations per step)
~ LMM + RK

- 1960–1970 Combining Runge-Kutta and Linear Multistep Method ideas; use of stage-derivatives (the RK- $k;s$) in previous steps in the formation of the final step. (Byrne and Lambert, 1966)
- 1964–1965 Hybrid Methods (Gragg and Stetter, 1964; Gear, 1965; Butcher, 1965); now “*modified multistep methods*.” (Butcher)
- * The class of multivalued^{LMM}-multistage^{RK} methods are referred to as *General Linear Methods*.

Byrne-and-Lambert's RK+LMM idea boils down to s standard RK-stages (1-2)

$$Y_i = y_{n-1} + h \sum_{j=1}^s a_{ij} k_j^{[n]} \quad (1)$$

$$k_i^{[n]} = f(t_{n-1} + hc_i, Y_i) \quad (2)$$

$$y_n = y_{n-1} + h \left(\sum_{i=1}^s b_{i,0} k_i^{[n]} + \sum_{i=1}^s \bar{b}_{i,1} k_i^{[n-1]} \right) \quad (3)$$

followed by a modified step-assembly (3) using not only “current,” but also past k_j -values.

The associated Butcher array:

\vec{c}	A
	\vec{b}_0^T
	\vec{b}_1^T

or, in general

$$Y_i = y_{n-1} + h \sum_{j=1}^s a_{ij} k_j^{[n]}$$

$$k_i^{[n]} = f(t_{n-1} + hc_i, Y_i)$$

$$y_n = y_{n-1} + h \left(\sum_{i=1}^s b_{i,0} k_i^{[n]} + \sum_{p=1}^P \left(\sum_{i=1}^s \bar{b}_{i,p} k_i^{[n-p]} \right) \right)$$

\vec{c}	A
	\vec{b}_0^T
	\vec{b}_1^T
\vdots	\vdots
	\vec{b}_P^T

The following ($s = 3$)-stage Pseudo-RK method is order ($p = 4$):

0			
$\frac{1}{2}$		$\frac{1}{2}$	
1	$-\frac{1}{3}$	$\frac{4}{3}$	
	$\frac{11}{12}$	$\frac{1}{3}$	$\frac{1}{4}$
	$\frac{1}{12}$	$-\frac{1}{3}$	$-\frac{1}{4}$

Recall (Lecture #5)

Theorem (Butcher, 2008: p.187)

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

Note that Pseudo-RK methods “inherit” the non-self-starting, and difficult-to-change-step-size properties from the LMM framework.

Starting and step-size changes can be handled with “classical” RK-methods, whose order of course must match the Pseudo-RK method in use.

- Generalizes LMM Predictor-Corrector pairs, by inserting additional *predictors*
- Additional predictors, usually, at off-step points

Example (Off-step predictor at $\frac{8}{15} h$ — part 1)

- 1 Predict the value at $t = t_{n-1} + \frac{8}{15} h = t_n - \frac{7}{17} h$ — $y_{n-\frac{7}{15}}^{[p1]}$
- 2 Predict the value at $t = t_n$ — $y_n^{[p2]}$
- 3 Correct the value at $t = t_n$ — $y_n^{[c]}$

Example (Off-step predictor at $\frac{8}{15} h$ — part 2)

$$y_{n-\frac{7}{15}}^{[p1]} = -\frac{529}{3375} y_{n-1} + \frac{3904}{3375} y_{n-2} + h \left(\frac{4232}{3375} f_{n-1} + \frac{1472}{3375} f_{n-2} \right)$$

$$f_{n-\frac{7}{15}}^{[p1]} = f \left(t_n - \frac{7}{15} h, y_{n-\frac{7}{15}}^{[p1]} \right)$$

$$y_n^{[p2]} = \frac{152}{25} y_{n-1} - \frac{127}{25} y_{n-2} + h \left(\frac{189}{92} f_{n-\frac{7}{15}}^{[p1]} - \frac{419}{100} f_{n-1} - \frac{1118}{575} f_{n-2} \right)$$

$$f_n^{[p2]} = f \left(t_n, y_n^{[p2]} \right)$$

$$y_n^{[c]} = y_{n-1} + h \left(\frac{25}{168} f_n^{[p2]} + \frac{3375}{5152} f_{n-\frac{7}{15}}^{[p1]} + \frac{19}{96} f_{n-1} - \frac{1}{552} f_{n-2} \right)$$

Given that r (d -dimensional) quantities are passed from step-to-step, one full step is completed once given the values $\vec{y}^{[n-1]}$ we have computed $\vec{y}^{[n]}$:

$$\vec{y}^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix} \rightarrow \vec{y}^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}$$

using an s -stage method, during the step we compute s stage-values (\vec{Y}_i), and s associated stage derivatives (\vec{F}_i)... We let, \vec{Y} and \vec{F} be the “supervectors” that contain the respective Y_i and F_i sub-vectors.

- As for RK-methods, stages consist of linear combinations of stage-derivatives.
- Additional linear combinations are needed to express the dependence on the *input* information.
- ... and the *output* quantities depend linearly on both the stage derivatives, and the input quantities.

All-in-all, we need 4 matrices to capture the computations of one stage:

$$A = [a_{ij}]_{s,s}, \quad U = [u_{ij}]_{s,r}, \quad B = [b_{ij}]_{r,s}, \quad V = [v_{ij}]_{r,r}.$$

The stage-computations are given by

$$\begin{aligned}
 Y_i &= h \sum_{j=1}^s a_{ij} F_j + \sum_{j=1}^r u_{ij} y_j^{[n-1]}, & i = 1, 2, \dots, s \\
 y_i^{[n]} &= h \sum_{j=1}^s b_{ij} F_j + \sum_{j=1}^r v_{ij} y_j^{[n-1]}, & i = 1, 2, \dots, r
 \end{aligned}$$

or, in more compact notation

$$\begin{aligned}
 Y &= h(A \otimes I_d)F + (U \otimes I_d)y^{[n-1]} \\
 y^{[n]} &= h(B \otimes I_d)F + (V \otimes I_d)y^{[n-1]}
 \end{aligned}$$

In all cases, we can express the GLM using an $(s + r) \times (s + r)$ matrix:

$$\left[\begin{array}{c|c} A_{s,s} & U_{s,r} \\ \hline B_{r,s} & V_{r,r} \end{array} \right]$$

it turns out we can cast quite a few of our well-known schemes in this notation...

$$\left[\begin{array}{c|c} 0 & 1 \\ \hline 1 & 1 \end{array} \right]$$

Euler's Method

$$\left[\begin{array}{c|c} 1 & 1 \\ \hline 1 & 1 \end{array} \right]$$

Implicit Euler

The 2nd order, 2-stage Runge-Kutta, with Butcher array

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

can be expressed as a GLM:

$$\left[\begin{array}{cc|c} 0 & 0 & 1 \\ 1 & 0 & 1 \\ \hline \frac{1}{2} & \frac{1}{2} & 1 \end{array} \right]$$

Old Methods, New Notation... — III

The 3rd order, 3-stage Runge-Kutta, with Butcher array

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

can be expressed as a GLM:

$$\left[\begin{array}{ccc|c} 0 & 0 & 0 & 1 \\ \frac{1}{2} & 0 & 0 & 1 \\ -1 & 2 & 0 & 1 \\ \hline \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 1 \end{array} \right]$$

Old Methods, New Notation... — IV

The 4th order, 4-stage Runge-Kutta, with Butcher array

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

can be expressed as a GLM:

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

2nd order Adams-Bashforth, and Adams-Moulton methods:

$$y_{n+1}^{\text{AB}} = y_n + \frac{h}{2} [3f_n - f_{n-1}]$$

$$y_{n+1}^{\text{AM}} = y_n + \frac{h}{2} [f_{n+1} + f_n]$$

in GLM-notation:

$$\left[\begin{array}{c|ccc} 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ \hline 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array} \right] \quad \left[\begin{array}{c|c} \frac{1}{2} & 1 \\ \hline \frac{1}{2} & 1 \end{array} \right]$$

Old Methods, New Notation... — VI

Uh?!?

$$\left[\begin{array}{c|ccc} 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ \hline 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array} \right]$$

This means,

$$Y_1 = y_1^{[n-1]} + \frac{3}{2}y_2^{[n-1]} - \frac{1}{2}y_3^{[n-1]}$$

solution $y_1^{[n]} = y_1^{[n-1]} + \frac{3}{2}y_2^{[n-1]} - \frac{1}{2}y_3^{[n-1]}$

step-derivative $y_2^{[n]} = hF_1 \equiv \mathbf{f}(Y_1)$

step-derivative $y_3^{[n]} = y_2^{[n-1]}$

Old Methods, New Notation... — VII

2nd order Adams-Bashforth, and Adams-Moulton methods:

$$\left[\begin{array}{c|ccc} 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ \hline 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array} \right] \quad \left[\begin{array}{c|c} \frac{1}{2} & 1 \\ \hline \frac{1}{2} & 1 \end{array} \right]$$

Operating in P(EC)E mode:

$$\left[\begin{array}{cc|ccc} 0 & 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ \frac{1}{2} & 0 & 1 & \frac{1}{2} & 0 \\ \hline \frac{1}{2} & 0 & 1 & \frac{1}{2} & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{array} \right]$$

New Methods, New Notation... — VII

Byrne-Lambert's 4th order 3-stage Pseudo-RK:

0			
$\frac{1}{2}$	$\frac{1}{2}$		
1	$-\frac{1}{3}$	$\frac{4}{3}$	
	$\frac{11}{12}$	$\frac{1}{3}$	$\frac{1}{4}$
	$\frac{1}{12}$	$-\frac{1}{3}$	$-\frac{1}{4}$

GLM:
$$\left[\begin{array}{ccc|ccc} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 1 & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{4}{3} & 0 & 1 & 0 & 0 & 0 \\ \hline \frac{11}{12} & \frac{1}{3} & \frac{1}{4} & 1 & \frac{1}{12} & -\frac{1}{3} & -\frac{1}{4} \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{array} \right]$$

New Methods, New Notation... — VIII

Off-step predictor at $\frac{8}{15} h$ —

$$\text{GLM: } \left[\begin{array}{ccc|cccc} 0 & 0 & 0 & -\frac{529}{3375} & \frac{3904}{3375} & \frac{4232}{3375} & \frac{1472}{3375} \\ \frac{189}{92} & 0 & 0 & \frac{152}{25} & -\frac{127}{25} & -\frac{419}{100} & -\frac{1118}{575} \\ \frac{3375}{5152} & \frac{25}{168} & 0 & 1 & 0 & \frac{19}{96} & -\frac{1}{552} \\ \hline \frac{3375}{5152} & \frac{25}{168} & 0 & 1 & 0 & \frac{19}{96} & -\frac{1}{552} \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{array} \right]$$

The output quantities are:

$$y_1^{[n]} \approx y(t_n),$$

$$y_2^{[n]} \approx y(t_{n-1}),$$

$$y_3^{[n]} \approx h y'(t_n),$$

$$y_4^{[n]} \approx h y'(t_{n-1}).$$