Numerical Solutions to Differential Equations

Lecture Notes #16 — Hybrid Methods

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In the Rear-view Mirror I

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.

In the Rear-view Mirror II

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).

In the Rear-view Mirror III

3. Linear Multistep Methods
   - Explicit LMMs only require one new function evaluation per step, making then very competitive (fast and cheap). Used in the predictor-corrector context P(EC)^μ, 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 straight forward (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 $y(t)$)
$\sim$ LMM + Taylor

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

General Linear more (past values + calculations per step)
$\sim$ LMM + RK

History

1960 – 1970 Combining Runge-Kutta and Linear Multistep Method ideas; use of stage-derivatives (the RK-k_is) 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 multivalue$^{\text{LMM}}$-multistage$^{\text{RK}}$ methods are refered to as *General Linear Methods*.

Pseudo Runge-Kutta Methods, I

Byrne-and-Lambert

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

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

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

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

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

The associated Butcher array:

$$\begin{array}{c|c} \vec{c} & A \\ \hline & \vec{b}_0^T \\ \hline & \vec{b}_1^T \end{array}$$

Pseudo Runge-Kutta Methods, II — Byrne-and-Lambert

or, in general

$$\begin{aligned} Y_i &= y_{n-1} + h \sum_{j=1}^{s} a_{ij} k_j^{[n]} \\ k_i^{[n]} &= f(t_{n-1} + hc_i, Y_i) \\ y_n &= y_{n-1} + h \left(\sum_{i=1}^{s} b_{i,0} k_i^{[n]} + \sum_{p=1}^{P} \left(\sum_{i=1}^{s} \overline{b}_{i,p} k_i^{[n-p]} \right) \right) \end{aligned}$$

$$\begin{array}{c|c} \vec{c} & A \\ \hline & \vec{b}_0^T \\ \hline & \vec{b}_1^T \\ \hline \vdots & \vdots \\ \hline & \vec{b}_P^T \end{array}$$

Pseudo Runge-Kutta Methods, III — Byrne-and-Lambert

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

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -\frac{1}{3} & \frac{4}{3} & \\ \hline & \frac{11}{12} & \frac{1}{3} & \frac{1}{4} \\ \hline & \frac{1}{12} & -\frac{1}{3} & -\frac{1}{4} \end{array}$$

Recall (Lecture #5)

Theorem (Butcher, 2008: p.187)

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

Pseudo Runge-Kutta Methods, IV — Byrne-and-Lambert

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.

Generalized Linear Multistep Methods, I — a.k.a Hybrid Methods / Modified LMMs

- 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 $t = t_n$ — $y_n^{[c]}$

Generalized Linear Multistep Methods, II

a.k.a Hybrid Methods / Modified LMMs

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

$$
\begin{aligned}
y^{[p1]}_{n-\frac{7}{15}} &= -\frac{529}{3375}\, y_{n-1} + \frac{3904}{3375}\, y_{n-2} + h\left(\frac{4232}{3375}\, f_{n-1} + \frac{1472}{3375}\, f_{n-2}\right) \\
f^{[p1]}_{n-\frac{7}{15}} &= f\left(t_n - \frac{7}{15}\, h,\; y^{[p1]}_{n-\frac{7}{15}}\right) \\
y^{[p2]}_{n} &= \frac{152}{25}\, y_{n-1} - \frac{127}{25}\, y_{n-2} + h\left(\frac{189}{92}\, f^{[p1]}_{n-\frac{7}{15}} - \frac{419}{100}\, f_{n-1} - \frac{1118}{575}\, f_{n-2}\right) \\
f^{[p2]}_{n} &= f\left(t_n,\; y^{[p2]}_{n}\right) \\
y^{[c]}_{n} &= y_{n-1} + h\left(\frac{25}{168}\, f^{[p2]}_{n} + \frac{3375}{5152}\, f^{[p1]}_{n-\frac{7}{15}} + \frac{19}{96}\, f_{n-1} - \frac{1}{552}\, f_{n-2}\right)
\end{aligned}
$$

General Linear Methods, I

Butcher, 1966 / Burrage-and-Butcher, 1980

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 $\vec{y}^{[n]}$:

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

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.

General Linear Methods, II

Butcher, 1966 / Burrage-and-Butcher, 1980

- 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:

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

General Linear Methods, III

Butcher, 1966 / Burrage-and-Butcher, 1980

The stage-computations are given by

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

or, in more compact notation

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

Old Methods, New Notation... — I

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

Old Methods, New Notation... — II

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:

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

Old Methods, New Notation... — V

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

$$
\begin{aligned}
y_{n+1}^{AB} &= y_n + \frac{h}{2}\left[3f_n - f_{n-1}\right] \\
y_{n+1}^{AM} &= y_n + \frac{h}{2}\left[f_{n+1} + f_n\right]
\end{aligned}
$$

in GLM-notation:

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

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,

$$
\begin{aligned}
& Y_1 &&= y_1^{[n-1]} + \frac{3}{2}y_2^{[n-1]} - \frac{1}{2}y_3^{[n-1]} \\
\text{solution}\quad & y_1^{[n]} &&= y_1^{[n-1]} + \frac{3}{2}y_2^{[n-1]} - \frac{1}{2}y_3^{[n-1]} \\
\text{step-derivative}\quad & y_2^{[n]} &&= h\,F_1 \equiv \mathbf{f}(\mathbf{Y}_1) \\
\text{step-derivative}\quad & y_3^{[n]} &&= y_2^{[n-1]}
\end{aligned}
$$

Old Methods, New Notation... — VII

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

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

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:

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

New Methods, New Notation... — VIII

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

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

The output quantities are:

$y_1^{[n]} \approx y(t_n)$,
$y_2^{[n]} \approx y(t_{n-1})$,
$y_3^{[n]} \approx h\, y'(t_n)$,
$y_4^{[n]} \approx h\, y'(t_{n-1})$.