Hybrid Methods General Linear Methods

Numerical Solutions to Differential Equations Lecture Notes #16 — Hybrid Methods

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Spring 2015

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

2 General Linear Methods

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- New Methods, New Notation...



In the Rear-view Mirror I

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

- 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 2*s*-order methods (Gauss-Legendre) for arbitrary *s*, as well as L-stable *s*-stage (2*s*-1)-order methods (Radau I-A, and II-A).

In the Rear-view Mirror III

O 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 $P(EC)^{\mu}$, 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(α)-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

- **()** Use more derivatives of y(t), (Taylor series methods)
- Output State St
- Use more calculations per step, (Runge Kutta)
- Use derivatives of f(t, y(t)), (not used so far*)

Combinations in the literature:

 $\begin{array}{l} \mathsf{Obreshkov} & \mathsf{more} \ (\mathsf{past} \ \mathsf{values} + \mathsf{derivatives} \ \mathsf{of} \ y(t)) \\ & \sim \mathsf{LMM} + \mathsf{Taylor} \end{array}$

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

 $\begin{array}{l} \mbox{General Linear more (past values + calculations per step)} \\ & \sim \mbox{LMM + RK} \end{array}$

- 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^{LMM}-multistage^{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)

$$Y_{i} = y_{n-1} + h \sum_{j=1}^{s} a_{ij} k_{j}^{[n]}$$
(1)

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

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

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

The associated Butcher array:



Pseudo Runge-Kutta Methods, II

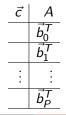
Byrne-and-Lambert

or, in general

$$Y_{i} = y_{n-1} + h \sum_{j=1}^{s} a_{ij} k_{j}^{[n]}$$

$$k_{i}^{[n]} = f(t_{n-1} + hc_{i}, Y_{i})$$

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





Pseudo Runge-Kutta Methods, III

Byrne-and-Lambert

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

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

Recall (Lecture #5)

Theorem (Butcher, 2008: p.187)

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

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

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



Hybrid Methods General Linear Methods Generalized Linear Multistep Methods

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

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

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

Hybrid Methods General Linear Methods Keneral Linear Methods

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

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

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.

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

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:

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



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

General Linear Methods, III

Butcher, 1966 / Burrage-and-Butcher, 1980

The stage-computations are given by

$$Y_{i} = h \sum_{j=1}^{s} a_{ij}F_{j} + \sum_{j=1}^{r} u_{ij}y_{j}^{[n-1]}, \quad i = 1, 2, ..., s$$

$$y_{i}^{[n]} = h \sum_{j=1}^{s} b_{ij}F_{j} + \sum_{j=1}^{r} v_{ij}y_{j}^{[n-1]}, \quad i = 1, 2, ..., r$$

or, in more compact notation

$$Y = h(A \otimes I_d)F + (U \otimes I_d)y^{[n-1]}$$

$$y^{[n]} = h(B \otimes I_d)F + (V \otimes I_d)y^{[n-1]}$$

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

Old Methods, New Notation... - I

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

$$\begin{bmatrix} A_{s,s} & U_{s,r} \\ B_{r,s} & V_{r,r} \end{bmatrix}$$

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





Old Methods, New Notation... — II

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

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

can be expressed as a GLM:

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 1 \\ \hline \frac{1}{2} & \frac{1}{2} & 1 \end{bmatrix}$$



Old Methods, New Notation... — III

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

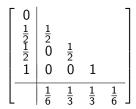
can be expressed as a GLM:

Γ	0	0	0	1
	$\frac{1}{2}$	0	0	1
	$-\overline{1}$	2	0	1
	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$	1



Old Methods, New Notation... — IV

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



can be expressed as a GLM:

Γ	0	0	0	0	1
	$\frac{1}{2}$	0	0	0	1
	Ō	$\frac{1}{2}$	0	0	1
	0	Ō	1	0	1
Ľ	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$	1

Old Methods, New Notation... – V

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

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

in GLM-notation:

$$\begin{bmatrix} 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ \hline 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{2} & 1 \\ \hline \frac{1}{2} & 1 \end{bmatrix}$$

Old Methods, New Notation... — VI

Uh?!?

٥ ٦	1	$\frac{3}{2}$	$-\frac{1}{2}$
0	1	$\frac{3}{2}$	$-\frac{1}{2}$
1	0	Ō	$-\frac{1}{2}$ 0
0	0	1	0]

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
$$y_{2}^{[n]} = h F_{1} \equiv \mathbf{f}(\mathbf{Y}_{1})$$
step-derivative
$$y_{3}^{[n]} = y_{2}^{[n-1]}$$

Old Methods, New Notation... — VII

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

$$\begin{bmatrix} 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ \hline 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{2} & 1 \\ \hline \frac{1}{2} & 1 \end{bmatrix}$$

Operating in P(EC)E mode:

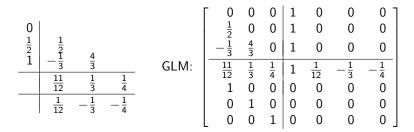
$$\begin{bmatrix} 0 & 0 & 1 & \frac{3}{2} & -\frac{1}{2} \\ \frac{1}{2} & 0 & 1 & \frac{1}{2} & 0 \\ \hline \frac{1}{2} & 0 & 1 & \frac{1}{2} & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$



Hybrid Methods General Linear Methods, New Notation... New Methods, New Notation...

New Methods, New Notation... — VII

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



Hybrid Methods	First Pass: GLM-lite		
General Linear Methods	GLM-lite: Old Methods, New Notation		
	New Methods, New Notation		

New Methods, New Notation... — VIII

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

	0	0	0	$-\frac{529}{3375}$	$\frac{3904}{3375}$	$\frac{4232}{3375}$	$\frac{1472}{3375}$
GLM:	<u>189</u> 92	0	0	<u>152</u> 25	$-\frac{127}{25}$	$-\frac{419}{100}$	$-\frac{1118}{575}$
	$\frac{3375}{5152}$	$\frac{25}{168}$	0	1	0	$\frac{19}{96}$	$-\frac{1}{552}$
	<u>3375</u> 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
	L 0	0	0	0	0	1	0]

The output quantities are:

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