

Numerical Solutions to Differential Equations

Lecture Notes #17 — General Linear Methods

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General Linear Methods, I

Butcher, 1966 / Burrage-and-Butcher, 1980

We express a GLM using an $(s + r) \times (s + r)$ matrix:

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

In a GLM we are passing r (scalar, or vector-valued) quantities from the previous step to the following step. In each step, s approximations (stages) to the solution are calculated.

The input at stage n is $y_i^{[n-1]}$, $i = 1, \dots, r$. The stage values Y_i , $i = 1, \dots, s$, are computed, and $F_i = f(Y_i)$, $i = 1, \dots, s$, are the associated derivative values.

The outputs, $y_i^{[n]}$, $i = 1, \dots, r$ are then synthesized from the input-, and derivative-values.

General Linear Methods, II

Butcher, 1966 / Burrage-and-Butcher, 1980

The stage-computations are given by

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

With the quantities $y_j^{[n-1]}$, Y_i , F_i , and $y_i^{[n]}$ being d -dimensional vectors we define, $Y, F \in \mathbb{R}^{s \cdot d}$, and $y^{[n-1]}, y^{[n]} \in \mathbb{R}^{r \cdot d}$:

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \quad F = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_s \end{bmatrix}, \quad y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix},$$

General Linear Methods, I

Butcher, 1966 / Burrage-and-Butcher, 1980

So that in compact notation

$$\begin{bmatrix} Y \\ y^{[n]} \end{bmatrix} = \begin{bmatrix} A \otimes I_d & U \otimes I_d \\ B \otimes I_d & V \otimes I_d \end{bmatrix} \begin{bmatrix} hF \\ y^{[n-1]} \end{bmatrix},$$

where I_d is the $d \times d$ identity matrix, and the Kronecker product is given by

$$A \otimes I_d = \begin{bmatrix} a_{11}I_d & a_{12}I_d & \cdots & a_{1s}I_d \\ a_{21}I_d & a_{22}I_d & \cdots & a_{2s}I_d \\ \vdots & \vdots & & \vdots \\ a_{s1}I_d & a_{s2}I_d & \cdots & a_{ss}I_d \end{bmatrix}.$$

Usually, we simplify the notation:

$$\begin{bmatrix} A \otimes I_d & U \otimes I_d \\ B \otimes I_d & V \otimes I_d \end{bmatrix} \rightarrow \begin{bmatrix} A & U \\ B & V \end{bmatrix}.$$

Matlab Code: Kronecker Product

```
>> A = [11 12 13;21 22 23; 31 32 33]
>> I = eye(5)
>> kron(A,I)
>> kron(I,A)
```

GLM — Equivalence Classes of Methods

Equivalent GLMs

If T is a non-singular $r \times r$ matrix, then the two methods

$$(A, U, B, V) \equiv (A, UT^{-1}, TB, TVT^{-1})$$

are equivalent, but are different computationally.

Specific representations may have computational advantages... We will encounter some examples, but we can imagine that something may be simpler if one or more of UT^{-1} , TB , TVT^{-1} have upper/lower triangular, or diagonal structure.

We will not repeat all the examples of putting known RK and LMMs into GLM form, but will focus on other schemes, or in a few cases, modifications of the straight-forward representations to more efficient GLM-centric form.

Lobatto IIIA, I

The Lobatto- $\{A,B,C\}^*$ methods are related to the Gauss(-Legendre) and Radau- $\{IA,IIA\}$ in that they are *optimal*, with the restriction that *both* endpoints are used; they attain order $p = 2s - 2$.

Example (Lobatto IIIA, $s = 3$, $p = 4$)

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

The method has the natural GLM($s = 3, r = 1$) representation, but noticing the First-Same-As-Last (FSAL) property, it can be written as a GLM($s = 2, r = 2$) scheme...

* There are 4 types of Lobatto schemes: L, L-A^{Ehle-1969}, L-B^{Ehle-1969}, and L-C^{Chipman-1971} ...

Lobatto IIIA, II

Example (Lobatto IIIA, $s = 2$, $p = 4$, $r = 2$)

$$\left[\begin{array}{cc|cc} \frac{1}{3} & -\frac{1}{12} & 1 & \frac{5}{12} \\ \frac{2}{3} & \frac{1}{6} & 1 & \frac{1}{6} \\ \hline \frac{2}{3} & \frac{1}{6} & 1 & \frac{1}{6} \\ 0 & 1 & 0 & 0 \end{array} \right],$$

with $y_1^{[n-1]} \approx y(t_{n-1})$, and $y_2^{[n-1]} \approx hy'(t_{n-1})$ being the input quantities.

Note: Radau-I, Radau-II, and Lobatto-III

Recall the *Legendre polynomials* — $\int_0^1 P_k(x) P_\ell(x) dx = \delta_{k\ell}$:

For an s -stage method of Radau-I, Radau-II, or Lobatto-III type, the c_m -values are taken to be:

- **Radau-I** $c_1 = 0$, and the roots of $P_s(x) + P_{s-1}(x)$; The formula is exact for polynomials up to degree $2s - 2$.
- **Radau-II** $c_s = 1$, and the roots of $P_s(x) - P_{s-1}(x)$; The formula is exact for polynomials up to degree $2s - 2$.
- **Lobatto-III** $c_1 = 0$, $c_s = 1$, and the roots of $P_s(x) - P_{s-2}(x)$; The formula is exact for polynomials up to degree $2s - 3$.

The corresponding b_m values are the integrals of the corresponding Lagrange coefficients, *i.e.*

$$b_m = \int_0^1 L_{s,m}(x) dx, \quad L_{s,m}(x) = \prod_{k=1, k \neq m}^s \frac{x - x_k}{x_m - x_k}$$

Example: 4-stage RK \rightarrow 3-stage GLM

Example (RK($s = 4, p = 4, \text{explicit}$) \rightarrow GLM($s = 3, p = 4, r = 2$))

$$\begin{array}{c|ccc} 0 & & & \\ -\frac{1}{2} & -\frac{1}{2} & & \\ \frac{1}{2} & \frac{3}{4} & -\frac{1}{4} & \\ 1 & -2 & 1 & 2 \\ \hline & \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6} \end{array} \rightarrow \left[\begin{array}{ccc|cc} 0 & 0 & 0 & 1 & 0 \\ \frac{3}{4} & 0 & 0 & 1 & -\frac{1}{4} \\ -2 & 2 & 0 & 1 & 1 \\ \hline \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{array} \right]$$

The second stage is replaced by a quantity from a previous step ($-\frac{1}{2}$) is ($+\frac{1}{2}$) as seen from the preceding point. It's no longer an RK-method, and some stability is lost.

LMMs as GLMs

1 of 4

For a linear k -step method $[\alpha, \beta]$ of the form $\alpha(z) = 1 - z$ [Adams methods], we get in a natural way GLM($s = 1, r = k + 1$), with input approximations

$$y^{[n-1]} = \begin{bmatrix} y(t_{n-1}) \\ h y'(t_{n-1}) \\ h y'(t_{n-2}) \\ \vdots \\ h y'(t_{n-k}) \end{bmatrix}$$

By introducing the right transformation T , it is possible to find an equivalent GLM($s = 1, r = k$)-method.

Note: $\alpha(z) = z^k \rho\left(\frac{1}{z}\right)$, and $\beta(z) = z^k \sigma\left(\frac{1}{z}\right)$; where $\rho(z)$, and $\sigma(z)$ are the polynomials we have so far associated with LMMs.

LMMs as GLMs

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The (A, U, B, V) -matrix representing the method is

$$\begin{bmatrix} \beta_0 & \mathbf{1} & \beta_1 & \beta_2 & \beta_3 & \cdots & \beta_{k-1} & \beta_k \\ \beta_0 & \mathbf{1} & \beta_1 & \beta_2 & \beta_3 & \cdots & \beta_{k-1} & \beta_k \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

Since $y_1^{[n-1]}$ and $y_{k+1}^{[n-1]}$ occur in the same combination — $y_1^{[n-1]} + \beta_k y_{k+1}^{[n-1]}$ in (all) the two places these quantities are used, we can simplify by introducing a transformation T ...

LMMs as GLMs

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$$T = \left[\begin{array}{c|cccccc} 1 & 0 & 0 & \cdots & 0 & \beta_k \\ \hline 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{array} \right]$$

LMMs as GLMs

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The transformed method $(A, UT^{-1}, TB, TTVT^{-1})$ is described by

$$\begin{bmatrix} A & UT^{-1} \\ TB & TTVT^{-1} \end{bmatrix} = \left[\begin{array}{c|cccccc|c} \beta_0 & 1 & \beta_1 & \beta_2 & \beta_3 & \cdots & \beta_{k-1} & \mathbf{0} \\ \beta_0 & \mathbf{1} & \beta_1 & \beta_2 & \beta_3 & \cdots & \beta_{k-1} + \beta_k & \mathbf{0} \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 \end{array} \right]$$

... and we can reduce r from $k + 1$ to k since the last input vector is never used (last column is identically zero.)

Non-RK/LMM Approaches

- Hybrid Methods (Gregg-and-Stetter, 1964) (Butcher, 1965) (Gear, 1965)
 - (B'65) Presents a 7th order RK(multi-stage)+LMM(extended history) scheme.
- Pseudo-RK (Byrne-and-Lambert, 1966)
 - s standard RK+LMM-stages followed by a modified step-assembly using not only “current,” but also past Y_i -values.
- Cyclic Composite Methods (Donelson-and-Hansen, 1971)
 - Two or more LMMs are used in rotation over successive steps: to overcome the conflicting demands of order and stability.

We quietly sweep the huge coefficient matrices under our infinitely expandable rug, see (Butcher, 2008; pp.380–382) for details.

Preconsistency, Consistency, and Stability

Definition (Preconsistency)

A GLM (A, U, B, V) is *preconsistent* if there exists a vector $\tilde{\mathbf{u}}$ such that: $\mathbf{V}\tilde{\mathbf{u}} = \tilde{\mathbf{u}}$, $\mathbf{U}\tilde{\mathbf{u}} = \tilde{\mathbf{1}}$. The vector $\tilde{\mathbf{u}}$ is the *preconsistency vector*.

Definition (Consistency)

A GLM (A, U, B, V) is *consistent* if it is preconsistent with preconsistency vector $\tilde{\mathbf{u}}$ and there exists a vector $\tilde{\mathbf{v}}$ such that:
 $\mathbf{B}\tilde{\mathbf{1}} + \mathbf{V}\tilde{\mathbf{v}} = \tilde{\mathbf{u}} + \tilde{\mathbf{v}}$.

Definition (Stability)

A GLM (A, U, B, V) is '*stable*' if there exists a constant C such that: **for all** $n \geq 1$, $\|V^n\| \leq C$.

Convergence

Theorem (Convergence of GLMs)

A stable and consistent GLM (A, U, B, V) is convergent.

The development of a proof includes introducing the concept of *covariance of methods*, an appropriate quantification of *convergence*, a starting procedure, a Lipschitz condition, showing the necessity of stability, the necessity of consistency, and the proof of a quite gnarly norm-inequality involving the computed quantities... a good 11 pages in (Butcher, 2008; pp 386–396).

Toward Practical Stability Analysis, I

Linear stability analysis follows the same general ideas as for RK and LMMs: we look at the model equation

$$y'(t) = \lambda y(t),$$

and obtain a single-step relation of the form

$$y^{[n]} = M(z)y^{[n-1]},$$

where $z = h\lambda$, and $M(z)$ is an $r \times r$ matrix-valued function of the complex variable z .

Toward Practical Stability Analysis, II

Definition (The Stability Matrix, $M(z)$)

For a GLM (A, U, B, V) , the *stability matrix* is given by:

$$\mathbf{M}(z) = \mathbf{V} + z\mathbf{B}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{U}.$$

Theorem

Let $M(z)$ denote the stability matrix for a GLM. Then, for a linear differential equation $y'(t) = \lambda y(t)$, $y^{[n]} = M(z)y^{[n-1]}$ holds with $z = h\lambda$.

Toward Practical Stability Analysis, III

Definition (Stability function; Stability region)

Let (A, U, B, V) denote a GLM, and $M(z)$ the corresponding stability matrix. The **stability function** for the method is the polynomial $\Phi(w, z)$ given by

$$\Phi(w, z) = \det(wI - M(z))$$

and the **stability region** is the subset of the complex plane such that if z is in this subset then

$$\sup_{n \in \mathbb{N}} \|M(z)^n\| < \infty$$

Toward Practical Stability Analysis, IV

Theorem (Instability region)

The **instability region** for (A, U, B, V) is a subset of the set of points z , such that $\Phi(w, z) = 0$, where $|w| \geq 1$. The instability region is a superset of the points defined by $\Phi(w, z) = 0$, where $|w| > 1$.

This means that points on the boundary of the stability region may or may not be part of it. Often, the *strict stability region* is considered, consisting of $z \in \mathbb{C}$ such that

$$\lim_{n \rightarrow \infty} \|M(z)^n\| = 0.$$

Toward Practical Stability Analysis, IV

Analogous with RK-methods we define:

Definition (A-stability)

A GLM is **A-stable** if $M(z)$ is power-bounded for every z in the left half complex plane.

Definition (L-stability)

A GLM is **L-stable** if it is A-stable and $\rho(M(\infty)) = 0$.

More on Stability Analysis

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Definition (Stability Order)

A method with stability function $\Phi(w, z)$ has **stability order** \tilde{p} if

$$\Phi(e^z, z) = \mathcal{O}(z^{\tilde{p}+1})$$

Theorem (Maximal Stability Order)

For given $\vec{\nu}$, where ν_j is the z -degree of the coefficient of the w^{k-j} of

$$\Phi(w, z) = \sum_{j=0}^k w^{k-j} \sum_{\ell=0}^{\nu_j} \alpha_{j\ell} z^\ell,$$

the maximum possible stability order is given by

$$\tilde{p} = -2 + \sum_{j=0}^k (\nu_j + 1).$$

The concept of the **stability order** leads to a some interesting connections with approximations of exponential functions, and **generalized Padé approximations**.

At least for now, we silently ignore this discussion which leads into some interesting complex analysis on Riemann surfaces; considerations of Homotopy order; and other excitement, including the concepts of non-linear stability, G -stability, and symplectic methods.

On the next few slides we see some stability regions visualized...

GLM ($s=2, p=4, r=2$) from Lobatto-IIIA

$$M(z) = \begin{bmatrix} m_{1,1}(z) & m_{1,2}(z) \\ \frac{6z(z+3)}{2z^2-9z+18} & \frac{z(4z+3)}{2z^2-9z+18} \end{bmatrix}$$

$$m_{1,1}(z) = z \left(\frac{z+3}{2z^2-9z+18} - \frac{3(z-4)}{2z^2-9z+18} \right) + 1$$

$$m_{1,2}(z) = \frac{1}{16} - z \left(\frac{z-5}{2z^2-9z+18} - \frac{4z+3}{6(2z^2-9z+18)} \right)$$

$$\lambda_1(z) = \frac{9z - \sqrt{11z^4 + \frac{159}{2}z^3 + \frac{495}{2}z^2 + 189z + 324 + 4z^2 + 18}}{2(2z^2 - 9z + 18)}$$

$$\lambda_2(z) = \frac{9z + \sqrt{11z^4 + \frac{159}{2}z^3 + \frac{495}{2}z^2 + 189z + 324 + 4z^2 + 18}}{2(2z^2 - 9z + 18)}$$

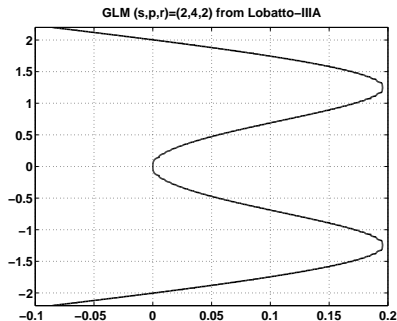
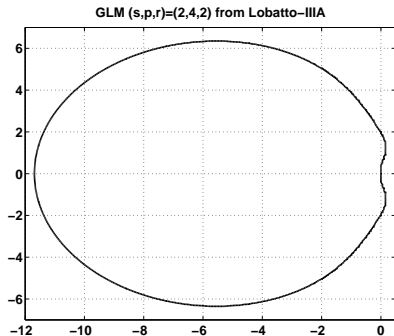
GLM ($s=2, p=4, r=2$) from Lobatto-III A

Figure: Note that Lobatto-III in RK-form is A-stable, but not L-stable.

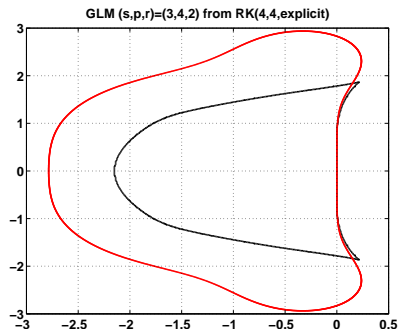
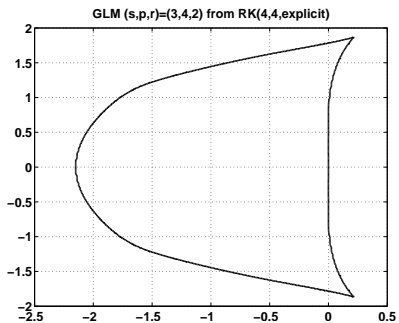
GLM($s=3, p=4, r=2$) derived from Explicit RK($s=p=4$)

$$M(z) = \begin{bmatrix} z \left(\frac{z^2}{4} + \frac{z}{2} + 1 \right) + 1 & -\frac{z^2}{12} \\ z \left(\frac{3z}{4} + 1 \right) & -\frac{z}{4} \end{bmatrix}$$

$$\lambda_1(z) = \frac{3}{8}z - \frac{\sqrt{\frac{1}{16}z^6 + \frac{1}{4}z^5 + \frac{5}{8}z^4 + \frac{17}{12}z^3 + \frac{41}{16}z^2 + \frac{5}{2}z + 1}}{2} + \frac{1}{4}z^2 + \frac{1}{8}z^3 + \frac{1}{2}$$

$$\lambda_2(z) = \frac{3}{8}z + \frac{\sqrt{\frac{1}{16}z^6 + \frac{1}{4}z^5 + \frac{5}{8}z^4 + \frac{17}{12}z^3 + \frac{41}{16}z^2 + \frac{5}{2}z + 1}}{2} + \frac{1}{4}z^2 + \frac{1}{8}z^3 + \frac{1}{2}$$

GLM($s=3, p=4, r=2$) derived from Explicit RK($s=p=4$)



GLM($s=2, p=5, r=5$) from Cycling $m=2$ **unstable** LMM($k=3, p=5$)

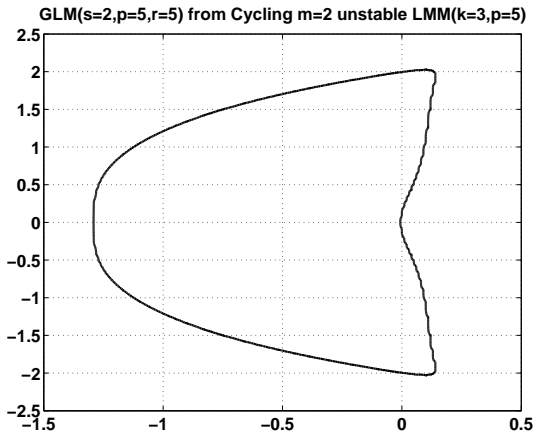
$M(z) \in \mathbb{R}^{5 \times 5}$, $\lambda_1(z) = \lambda_2(z) = 0$, $\lambda_4(z)$ & $\lambda_5(z)$ are "obvious" from $\lambda_3(z)$:

$$\begin{aligned} \lambda_3(z) = & ((\alpha z^2 + \beta z + \gamma)^3 / (27(\delta z^2 - \epsilon z + \gamma)^3) + (((\alpha z^2 + \beta z + \gamma)^3 / (27(\delta z^2 - \epsilon z + \gamma)^3) \\ & + (\zeta z^2 + \eta z) / (2(\delta z^2 - \epsilon z + \gamma)) + ((\theta z^2 + \iota z)(\alpha z^2 + \beta z + \gamma)) / (6(\delta z^2 - \epsilon z + \gamma)^2))^2 \\ & - ((\alpha z^2 + \beta z + \gamma)^2 / (9(\delta z^2 - \epsilon z + \gamma)^2) + (\theta z^2 + \iota z) / (3(\delta z^2 - \epsilon z + \gamma)))^3)^{1/2} \\ & + (\zeta z^2 + \eta z) / (2(\delta z^2 - \epsilon z + \gamma)) + ((\theta z^2 + \iota z)(\alpha z^2 + \beta z + \gamma)) / (6(\delta z^2 - \epsilon z + \gamma)^2))^{1/3} \\ & + ((\alpha z^2 + \beta z + \gamma)^2 / (9(\delta z^2 - \epsilon z + \gamma)^2) + (\theta z^2 + \iota z) / (3(\delta z^2 - \epsilon z + \gamma))) / ((\beta z + \alpha z^2 + \gamma)^3 / (27(\delta z^2 - \epsilon z + \gamma)^3) \\ & + (((\beta z + \alpha z^2 + \gamma)^3 / (27(\delta z^2 - \epsilon z + \gamma)^3) + (\eta z + \zeta z^2) / (\kappa z^2 - \mu z + \nu) + ((\iota z + \theta z^2)(\beta z + \alpha z^2 + \gamma)) / (6(\delta z^2 - \epsilon z + \gamma)^2)))^2 \\ & - ((\beta z + \alpha z^2 + \gamma)^2 / (9(\delta z^2 - \epsilon z + \gamma)^2) + (\iota z + \theta z^2) / (\xi z^2 - \sigma z + \rho))^3)^{1/2} + (\eta z + \zeta z^2) / (\kappa z^2 - \mu z + \nu) \\ & + ((\iota z + \theta z^2)(\beta z + \alpha z^2 + \gamma)) / (6(\delta z^2 - \epsilon z + \gamma)^2))^{1/3} + (\alpha z^2 + \beta z + \gamma) / (3(\delta z^2 - \epsilon z + \gamma)) \end{aligned}$$

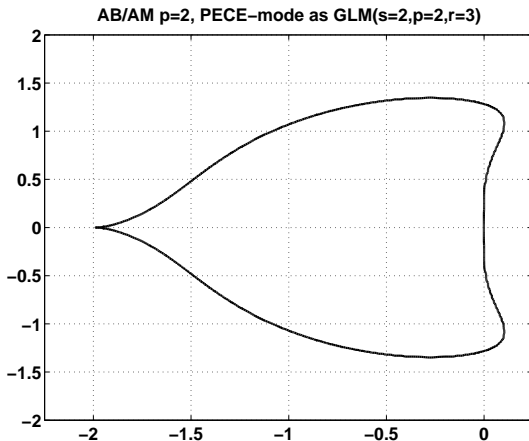
where

$$\begin{aligned} \alpha = 79914749, \quad \beta = 53570682, \quad \gamma = 128589120, \quad \delta = 3396030, \quad \epsilon = 41896998 \\ \zeta = 925085, \quad \eta = 2930598, \quad \theta = 21691476, \quad \iota = 30190842, \quad \kappa = 6792060 \\ \mu = 83793996, \quad \nu = 257178240, \quad \xi = 10188090, \quad \sigma = 125690994, \quad \rho = 385767360 \end{aligned}$$

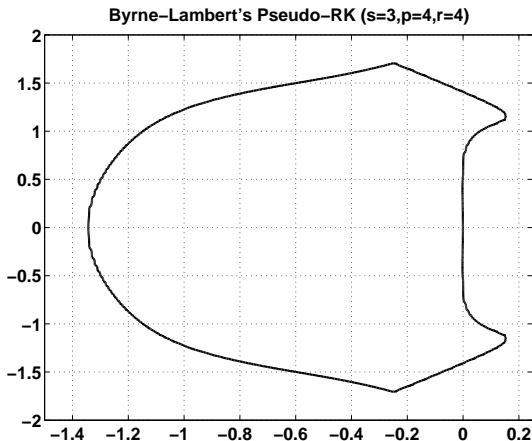
GLM($s=2, p=5, r=5$) from Cycling $m=2$ unstable LMM($k=3, p=5$)



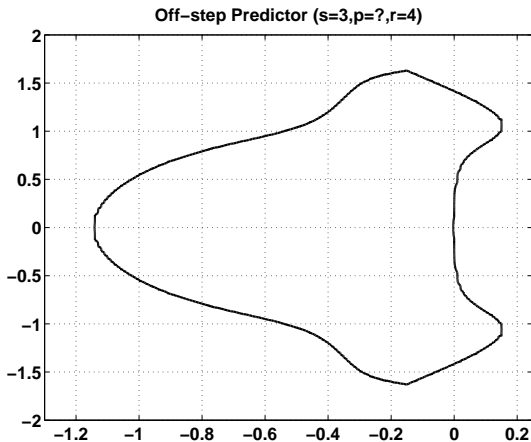
Adams-Bashforth/Moulton($p=2$) in PECE-mode as GLM($s=2,p=2,r=3$)



Bryne-Lambert's Pseudo-RK ($s=3, p=4, r=4$)



Offstep Predictor ($s=3, p=?, r=4$)



The Order of GLMs, I

The r input quantities $y_i^{[n-1]}$ must be defined before we can take a step... The only requirement is that these quantities are computable from an approximation to $y(t_{n-1})$...

We can associate a generalized RK method

$$S_i = \frac{c^{(i)} \mid A^{(i)}}{b_0^{(i)} \mid b^{(i)T}}.$$

We use a sequence $S = \{S_i\}$, $i = 1, \dots, r$ as a *starting method* for the GLM.

Standard RK: $b_0^{(i)} \equiv 1$, the coefficient multiplying y_{n-1} in the assembly stage.

The Order of GLMs, II

Definition

A starting method S defined by a sequence of generalized RK-methods, is **degenerate** if $b_0^{(i)} = 0$, for $i = 1, \dots, r$, and **non-degenerate** otherwise.

SM: (S)tarting + (M)ethod.

ES: (E)xact + (S)tarting

Definition (530B, p.411)

Consider a GLM, M and a non-degenerate starting method S . The method M has order p relative to S if the results found from SM and ES agree to within order $p + 1$.