## Numerical Solutions to Differential Equations

## Lecture Notes \#17 - General Linear Methods

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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 $y_{i}^{[n-1]}, i=1, \ldots, r$. The stage values $Y_{i}$, $i=1, \ldots, s$, are computed, and $F_{i}=f\left(Y_{i}\right), i=1, \ldots, s$, are the associated derivative values.

The outputs, $y_{i}^{[n]}, i=1, \ldots, r$ at then synthesized from the input-, and derivative-values.
(1) General Linear Methods

- Introduction (w/Review)
- Examples: Runge-Kutta Methods as GLMs
- Examples: LMMs as GLMs
(2) GLMs, ctd.
- Unconventional methods
- Some Theory
- Stability RegionsThe Order of GLMs

General Linear Methods, II
The stage-computations are given by

$$
\begin{aligned}
Y_{i} & =h \sum_{j=1}^{s} a_{i j} F_{j}+\sum_{j=1}^{r} u_{i j} y_{j}^{[n-1]}, \\
y_{i}^{[n]} & =h \sum_{j=1}^{s} b_{i j} F_{j}+\sum_{j=1}^{r} v_{i j} y_{j}^{[n-1]},
\end{aligned} \quad i=1,2, \ldots, s, r, r l
$$

With the quantities $y_{i}^{[n-1]}, Y_{i}, F_{i}$, and $y_{i}^{[n]}$ being $d$-dimensional vectors we define, $Y, F \in \mathbb{R}^{s \cdot d}$, and $y^{[n-1]}, y^{[n]} \in \mathbb{R}^{r \cdot d}$ :

$$
Y=\left[\begin{array}{c}
Y_{1} \\
Y_{2} \\
\vdots \\
Y_{s}
\end{array}\right], \quad F=\left[\begin{array}{c}
F_{1} \\
F_{2} \\
\vdots \\
F_{s}
\end{array}\right], \quad y^{[n-1]}=\left[\begin{array}{c}
y_{1}^{[n-1]} \\
y_{2}^{[n-1]} \\
\vdots \\
y_{r}^{[n-1]}
\end{array}\right], \quad y^{[n]}=\left[\begin{array}{c}
y_{1}^{[n]} \\
y_{2}^{[n]} \\
\vdots \\
y_{r}^{[n]}
\end{array}\right]
$$

So that in compact notation

$$
\left[\begin{array}{c}
Y \\
y^{[n]}
\end{array}\right]=\left[\begin{array}{ll}
A \otimes I_{d} & U \otimes I_{d} \\
B \otimes I_{d} & V \otimes I_{d}
\end{array}\right]\left[\begin{array}{c}
h F \\
y^{[n-1]}
\end{array}\right],
$$

where $I_{d}$ is the $d \times d$ identity matrix, and the Kronecker product is given by

$$
A \otimes I_{d}=\left[\begin{array}{cccc}
a_{11} I_{d} & a_{12} l_{d} & \cdots & a_{1 s} I_{d} \\
a_{21} I_{d} & a_{22} l_{d} & \cdots & a_{2 s} l_{d} \\
\vdots & \vdots & & \vdots \\
a_{s 1} l_{d} & a_{s 2} l_{d} & \cdots & a_{s s} I_{d}
\end{array}\right] .
$$

Matlab Code: Kronecker Product

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

Usually, we simplify the notation:

$$
\left[\begin{array}{ll}
A \otimes I_{d} & U \otimes I_{d} \\
B \otimes I_{d} & V \otimes I_{d}
\end{array}\right] \rightarrow\left[\begin{array}{cc}
A & U \\
B & V
\end{array}\right]
$$

## GLM - Equivalence Classes of Methods

## Equivalent GLMs

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

$$
(A, U, B, V) \equiv\left(A, U T^{-1}, T B, T V T^{-1}\right)
$$

are equivalent, but are different computationally.
Specific representations may have computational advantages... We will encounter some examples, but we can imagine that something my be simpler if one or more of $U T^{-1}, T B, T V T^{-1}$ 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- $\{, \mathrm{A}, \mathrm{B}, \mathrm{C}\}^{*}$ methods are related to the Gauss(-Legendre) and Radau- $\{\mathrm{IA}, \mathrm{IIA}\}$ in that they are optimal, with the restriction that both endpoints are used; they attain order $p=2 s-2$.

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



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

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

Recall the Legendre polynomials - $\int_{0}^{1} P_{k}(x) P_{\ell}(x) d x=\delta_{k \ell}$ :
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 $2 s-2$.
- 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 $2 s-2$.
- 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 $2 s-3$.

The corresponding $b_{m}$ values are the integrals of the corresponding Legrange coefficients, i.e.

$$
b_{m}=\int_{0}^{1} L_{s, m}(x) d x, \quad L_{s, m}(x)=\prod_{k=1, k \neq m}^{s} \frac{x-x_{k}}{x_{m}-x_{k}}
$$



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

LMMs as GLMs

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

$$
y^{[n-1]}=\left[\begin{array}{c}
y\left(t_{n-1}\right) \\
h y^{\prime}\left(t_{n-1}\right) \\
h y^{\prime}\left(t_{n-2}\right) \\
\vdots \\
h y^{\prime}\left(t_{n-k}\right)
\end{array}\right]
$$

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

The $(A, U, B, V)$-matrix representing the method is
$\left[\begin{array}{c|ccccccc}\beta_{0} & \mathbf{1} & \beta_{1} & \beta_{2} & \beta_{3} & \cdots & \beta_{k-1} & \beta_{\mathbf{k}} \\ \hline \beta_{0} & \mathbf{1} & \beta_{1} & \beta_{2} & \beta_{3} & \cdots & \beta_{k-1} & \beta_{\mathbf{k}} \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0\end{array}\right]$

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

The transformed method $\left(A, U T^{-1}, T B, T V T^{-1}\right)$ is described by $\left[\begin{array}{cc}A & U T^{-1} \\ T B & T V T^{-1}\end{array}\right]=\left[\begin{array}{c|cccccc|c}\beta_{0} & 1 & \beta_{1} & \beta_{2} & \beta_{3} & \cdots & \beta_{k-1} & \mathbf{0} \\ \hline \beta_{0} & \mathbf{1} & \beta_{1} & \beta_{2} & \beta_{3} & \cdots & \beta_{\mathbf{k}-\mathbf{1}}+\beta_{\mathbf{k}} & \mathbf{0} \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0\end{array}\right]$
... and we can reduce $r$ from $k+1$ to $k$ since the last input vector is never used (last column is identically zero.)

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

General Linear Methods

## 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.

Definition (Preconsistency)
A GLM $(A, U, B, V)$ is preconsistent if there exists a vector $\tilde{u}$ 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 $n \geq 1,\left\|V^{n}\right\| \leq C$.

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

$$
y^{\prime}(t)=\lambda y(t)
$$

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 $z$.

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).

General Linear Methods

Toward Practical Stability Analysis, II

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

For a GLM $(A, U, B, V)$, the stability matrix is given by:
$\mathbf{M}(\mathbf{z})=\mathbf{V}+\mathbf{z B}(\mathbf{I}-\mathbf{z A})^{\mathbf{- 1}} \mathbf{U}$.

Theorem
Let $M(z)$ denote the stability matrix for a GLM. Then, for a linear differential equation $y^{\prime}(t)=\lambda y(t), y^{[n]}=M(z) y^{[n-1]}$ holds with $z=h \lambda$.

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

$$
\Phi(w, z)=\operatorname{det}(w l-M(z))
$$

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

$$
\sup _{n \in \mathbb{N}}\left\|M(z)^{n}\right\|<\infty
$$

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 $\rho(M(\infty))=0$.

## 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

$$
\lim _{n \rightarrow \infty}\left\|M(z)^{n}\right\|=0
$$

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

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

Theorem (Maximal Stability Order)
For given $\vec{\nu}$, where $\nu_{j}$ is the $z$-degree of the coefficient of the $w^{k-j}$ of

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

the maximum possible stability order is given by

$$
\tilde{p}=-2+\sum_{j=0}^{k}\left(\nu_{j}+1\right)
$$

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



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

GLM ( $\mathrm{s}=2, \mathrm{p}=4, \mathrm{r}=2$ ) from Lobatto-IIIA

$$
\begin{gathered}
M(z)=\left[\begin{array}{cc}
m_{1,1(z)} & m_{1,2}(z) \\
\frac{6 z(z+3)}{2 z^{2}-9 z+18} & \frac{z 4 z+3)}{2 z^{2}-9 z+18}
\end{array}\right] \\
m_{1,1}(z)=z\left(\frac{z+3}{2 z^{2}-9 z+18}-\frac{3(z-4)}{2 z^{2}-9 z+18}\right)+1 \\
m_{1,2}(z)=\frac{1}{16}-z\left(\frac{z-5}{2 z^{2}-9 z+18}-\frac{4 z+3}{6\left(2 z^{2}-9 z+18\right)}\right) \\
\lambda_{1}(z)=\frac{9 z-\sqrt{11 z^{4}+\frac{159}{2} z^{3}+\frac{495}{2} z^{2}+189 z+324}+4 z^{2}+18}{2\left(2 z^{2}-9 z+18\right)} \\
\lambda_{2}(z)=\frac{9 z+\sqrt{11 z^{4}+\frac{159}{2} z^{3}+\frac{495}{2} z^{2}+189 z+324}+4 z^{2}+18}{2\left(2 z^{2}-9 z+18\right)}
\end{gathered}
$$

General Linear Methods

GLM $(s=3, p=4, r=2)$ derived from Explict $\operatorname{RK}(s=p=4)$

$$
\begin{gathered}
M(z)=\left[\begin{array}{cc}
z\left(\frac{z^{2}}{4}+\frac{z}{2}+1\right)+1 & -\frac{z^{2}}{12} \\
z\left(\frac{3 z}{4}+1\right) & -\frac{z}{4}
\end{array}\right] \\
\lambda_{1}(z)=\frac{3}{8} z-\frac{\sqrt{\frac{1}{16} z^{6}+\frac{1}{4} z^{5}+\frac{5}{8} z^{4}+\frac{17}{12} z^{3}+\frac{41}{16} z^{2}+\frac{5}{2} z+1}}{2}+\frac{1}{4} z^{2}+\frac{1}{8} z^{3}+\frac{1}{2} \\
\lambda_{2}(z)=\frac{3}{8} z+\frac{\sqrt{\frac{1}{16} z^{6}+\frac{1}{4} z^{5}+\frac{5}{8} z^{4}+\frac{17}{12} z^{3}+\frac{41}{16} z^{2}+\frac{5}{2} z+1}}{2}+\frac{1}{4} z^{2}+\frac{1}{8} z^{3}+\frac{1}{2}
\end{gathered}
$$



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


$$
\begin{aligned}
& M(z) \in \mathbb{R}^{5 \times 5}, \lambda_{1}(z)=\lambda_{2}(z)=0, \lambda_{4}(z) \& \lambda_{5}(z) \text { are "obvious" from } \lambda_{3}(z): \\
& \lambda_{3}(z)=\left(\left(\alpha z^{2}+\beta z+\gamma\right)^{3} /\left(27\left(\delta z^{2}-\epsilon z+\gamma\right)^{3}\right)+\left(\left(\left(\alpha z^{2}+\beta z+\gamma\right)^{3} /\left(27\left(\delta z^{2}-\epsilon z+\gamma\right)^{3}\right)\right.\right.\right. \\
&+\left(\zeta z^{2}+\eta z\right) /\left(\left(\delta\left(\delta z^{2}-\epsilon z+\gamma\right)\right)+\left(\left(\theta z^{2}+\iota z\right)\left(\alpha z^{2}+\beta z+\gamma\right)\right) /\left(6\left(\delta z^{2}-\epsilon z+\gamma\right)^{2}\right)\right)^{2} \\
& \quad-\left(\left(\left(\alpha z^{2}+\beta z+\gamma\right)^{2} /\left(9\left(\delta z^{2}-\epsilon z+\gamma\right)^{2}\right)+\left(\theta z^{2}+\iota z\right) /\left(3\left(\delta z^{2}-\epsilon z+\gamma\right)\right)\right)^{3}\right)^{1 / 2} \\
&+\left.\left(\zeta z^{2}+\eta z\right) /\left(2\left(\delta z^{2}-\epsilon z+\gamma\right)\right)+\left(\left(\theta z^{2}+\iota z\right)\left(\alpha z^{2}+\beta z+\gamma\right)\right) /\left(6\left(\delta z^{2}-\epsilon z+\gamma\right)^{2}\right)\right)^{1 / 3} \\
&+\left(\left(\alpha z^{2}+\beta z+\gamma\right)^{2} /\left(9\left(\delta z^{2}-\epsilon z+\gamma\right)^{2}\right)+\left(\theta z^{2}+\iota z\right) /\left(3\left(\delta z^{2}-\epsilon z+\gamma\right)\right)\right) /\left(\left(\beta z+\alpha z^{2}+\gamma\right)^{3} /\left(27\left(\delta z^{2}-\epsilon z+\gamma\right)^{3}\right)\right. \\
&+\left(\left(\left(\beta z+\alpha z^{2}+\gamma\right)^{3} /\left(27\left(\delta z^{2}-\epsilon z+\gamma\right)^{3}\right)+\left(\eta z+\zeta z^{2}\right) /\left(\kappa z^{2}-\mu z+\nu\right)+\left(\left(\iota z+\theta z^{2}\right)\left(\beta z+\alpha z^{2}+\gamma\right)\right) /\left(6\left(\delta z^{2}-\epsilon z+\gamma\right)^{2}\right)\right)^{2}\right. \\
&-\left(\left(\beta z+\alpha z^{2}+\gamma\right)^{2} /\left(9\left(\delta z^{2}-\epsilon z+\gamma\right)^{2}\right)+\left(\iota z+\theta z^{2}\right) /\left(\xi z^{2}-\sigma z+\rho\right)\right)^{1 / 2}+\left(\eta z+\zeta z^{2}\right) /\left(\kappa z^{2}-\mu z+\nu\right) \\
&+\left.\left(\left(\iota z+\theta z^{2}\right)\left(\beta z+\alpha z^{2}+\gamma\right)\right) /\left(6\left(\delta z^{2}-\epsilon z+\gamma\right)^{2}\right)\right)^{1 / 3}+\left(\alpha z^{2}+\beta z+\gamma\right) /\left(3\left(\delta z^{2}-\epsilon z+\gamma\right)\right) \\
& \text { where } \quad \alpha=79914749, \quad \beta=53570682, \quad \gamma=128589120, \quad \delta=3396030, \quad \epsilon=41896998 \\
& \zeta=93793996, \quad \nu=257178240, \quad \xi=10188090, \quad \sigma=125690994, \quad \rho=385767360
\end{aligned}
$$

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



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 $y\left(t_{n-1}\right) \ldots$
We can associate a generalized RK method

$$
S_{i}=\begin{array}{c|c}
c^{(i)} & A^{(i)} \\
\hline b_{0}^{(i)} & b^{(i) T}
\end{array}
$$

We use a sequence $S=\left\{S_{i}\right\}, i=1, \ldots, r$ as a starting method for the GLM.

Standard RK: $b_{0}^{(i)} \equiv 1$, the coefficient multiplying $y_{n-1}$ in the assembly stage.

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


General Linear Methods

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 $i=1, \ldots, r$, 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 $S M$ and $E S$ agree to within order $p+1$.

