Explicit General Linear Methods with quadratic stability

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The problem

Ordinary Differential Equations of first order

$$\begin{cases} y'(t) = f(y), & t \in [t_0, T] \\ y(t_0) = y_0, \end{cases}$$

$f : \mathbb{R}^m \to \mathbb{R}^m$, $y_0 \in \mathbb{R}^m$.

model a huge number of phenomena, like

- the growth of populations and of infectious diseases [1],
- phenomena in the field of medicine and genetics [2],
- economic processes [3]

[1] Norberto *et al* (2005), Zhao (2003), Jamrog *et al* (2006)

[2] Beuter *et al* (2002), Iyengar (2008), Spencer *et al* (2004), Varnai *et al* (2004), S.Yamasaki *et al* (2009)

[3] Gregory *et al* (2004)

Numerical solution of ODEs

Numerical simulation of real problems modeled by systems of ODEs needs for methods which are:

- accurate
- efficient
- reliable, i.e. capable of facing with 'difficult' problems, like moderately and highly stiff problems
- ...

General Linear Methods

$t_0 < t_1 < \cdots < t_N = T,\ t_n - t_{n-1} = h$

$0 \leq c_1 < \ldots < c_s \leq 1$ collocation abscissae

GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{V}, \mathbf{B})$

$$\begin{cases} Y_i^{[n]} &= h\sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \quad i = 1,\ldots,s, \\ y_i^{[n]} &= h\sum_{j=1}^{s} b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \quad i = 1,\ldots,r, \end{cases}$$

- $Y_i^{[n]} \approx y(t_{n-1} + c_i h)$ with order **q**
- $y_i^{[n]} \approx$ linear combinat. of the derivatives of the solution at t_n, with order **p**
- **s** internal stages, **r** external stages

Representation of GLM in vector form

Vector form in the scalar case

$$\left[\begin{array}{c} Y^{[n]} \\ y^{[n]} \end{array}\right] = \left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] \left[\begin{array}{c} hF\left(Y^{[n]}\right) \\ y^{[n-1]} \end{array}\right]$$

$$y^{[n]} = \left[\begin{array}{c} y_1^{[n]} \\ \vdots \\ y_r^{[n]} \end{array}\right], \quad Y^{[n]} = \left[\begin{array}{c} Y_1^{[n]} \\ \vdots \\ Y_s^{[n]} \end{array}\right], \quad F(Y^{[n]}) = \left[\begin{array}{c} f\left(Y_1^{[n]}\right) \\ \vdots \\ f\left(Y_s^{[n]}\right) \end{array}\right].$$

Explicit methods:	$\mathbf{A}$ strictly lower triangular;
Singly Implicit methods:	$\mathbf{A}$ lower triangular with $diag(\mathbf{A}) = (\lambda \ldots \lambda)$

Examples of GLM: Runge Kutta methods

$$\begin{cases} Y_i^{[n]} & = y_{n-1} + h \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}), \quad i = 1, 2 \dots, s, \\ y_n & = y_{n-1} + h \sum_{j=1}^{s} b_j f(Y_j^{[n]}), \end{cases}$$

can be represented in GLM form with $r = 1$ external stage:

Runge-Kutta methods

abscissae vector: $(c_1, \dots, c_s)$ and coefficients matrix:

$$\left[\begin{array}{c|c} A & e \\ \hline b^T & 1 \end{array} \right]$$

with $e = (1, \dots, 1)^T \in \mathbb{R}^s$.

Examples of GLM: linear multistep methods

$$y_n = \sum_{j=1}^{k} \alpha_j y_{n-j} + h \sum_{j=0}^{k} \beta_j f(y_{n-j}), \quad n = k, \ldots, N$$

can be represented as a GLM with $r = 2k$ and $s = 1$:

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cccccccc} \beta_0 & \alpha_1 & \ldots & \alpha_{k-1} & \alpha_k & \beta_1 & \ldots & \beta_{k-1} & \beta_k \\ \hline \beta_0 & \alpha_1 & \ldots & \alpha_{k-1} & \alpha_k & \beta_1 & \ldots & \beta_{k-1} & \beta_k \\ 0 & 1 & \ldots & 0 & 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & 0 & 0 & \ldots & 0 & 0 \\ 1 & 0 & \ldots & 0 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & \ldots & 0 & 0 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & 0 & 0 & \ldots & 1 & 0 \end{array}\right]$$

Order and stage order

We assume that there exist $q_k = (q_{1k}, \ldots, q_{rk})^T$, $k = 1, \ldots, p$:

$$y_i^{[n-1]} = \sum_{k=0}^{p} q_{ik} h^k y^{(k)}(t_{n-1}) + O(h^{p+1}), \quad i = 1, \ldots, r$$

Definitions

The GLM has order **p** and stage order **q** if

$$y_i^{[n]} = \sum_{k=0}^{p} q_{ik} h^k y^{(k)}(t_n) + O(h^{p+1}), \quad i = 1, \ldots, r.$$

$$Y_i^{[n]} = y(t_{n-1} + c_i h) + O(h^{q+1}), \quad i = 1, \ldots, s$$

Order conditions

Zero-stability: $\|V^n\| \leq C, \quad \forall n = 1, 2, ...$

Theorem (Butcher 1993)

The GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ has order p and stage order $q = p$ iff:

$$\begin{aligned} e^{\mathbf{c}z} &= z\mathbf{A}e^{\mathbf{c}z} + \mathbf{U}w(z) + O(z^{p+1}) \\ e^{z}w(z) &= z\mathbf{B}e^{\mathbf{c}z} + \mathbf{V}w(z) + O(z^{p+1}), \end{aligned}$$

where $e^{cz} = [e^{c_1 z}, \ldots, e^{c_s z}]$ and $w(z) = \sum_{k=0}^{p} q_k z^k$.

Similar order conditions hold for $q = p - 1$.

order conditions $\Longrightarrow$ conditions on the coefficients matrices

Order conditions (*cont.*)

As a matter of fact, from the previous theorem follows that the GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ has order p and stage order $q = p$ iff

$$\mathbf{U}\mathbf{q_0} = \mathbf{e}, \qquad \mathbf{V}\mathbf{q_0} = \mathbf{q_0}, \qquad \text{(preconsistency conditions)},$$

where $\mathbf{e} = (1, \dots, 1)^T$ and

$$\frac{\mathbf{c}^k}{k!} - \mathbf{A}\frac{\mathbf{c}^{k-1}}{(k-1)!} - \mathbf{U}\mathbf{q_k} = 0, \qquad k = 1, \dots, p$$

$$\sum_{l=0}^{k} \frac{\mathbf{q_{k-l}}}{l!} - \mathbf{B}\frac{\mathbf{c}^{k-1}}{(k-1)!} - \mathbf{V}\mathbf{q_k} = 0 \quad k = 1, \dots, p$$

Linear stability

Linear test equation:

$$y'(t) = \xi y(t), \qquad t \geq 0,$$

$\xi \in \mathbb{C}, \Re\xi < 0$. Applying the GLM method $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ we get:

$$y^{[n]} = \mathbf{M}(z)y^{[n-1]}, \qquad n \geq 1, \qquad z = h\xi.$$

Stability matrix $M(z)$ and stability function $p(w, z)$

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

$$p(w, z) = \det(w\mathbf{I} - \mathbf{M}(z)).$$

The method is said *absolutely stable* for $z \in \mathbb{C}$ if $p(w, z)$ has roots of modulus < 1. The *region of absolute stability* is the set of all the points $z \in \mathbb{C}$ such that the method is stable.

GLM:

Advantages

- furnish a general formulation of classical methods
- have more free parameters of classical methods, which allow to construct new classes of methods with desirable properties of accuracy, stability, efficiency

Present limitations

- only some classes of GLM have been completely analyzed (as DIMSIM, IRKS)
- not yet known *general* conditions to impose to a GLM in order to obtain optimal stability properties together with high accuracy

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to construct optimal GLM methods, in particular

Aim

Explicit GLM with large stability regions

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Methods with special stability functions

Methods with *special* stability functions

- GLM in Nordsieck form with
  Inherent Runge-Kutta Stability
  (Butcher('00,'06), B.& Wright('03), Wright ('02), B.& Jackiewicz('04))
- GLM of type two-step Runge-Kutta with
  Inherent Quadratic Stability
  (Conte, D'Ambrosio, Jackiewicz (2010))

Runge Kutta Stability (RKS)

Definition

A GLM in Nordsieck form with order $p = q$ and $r = s = p + 1$ possesses RK stability if the stability function $p(w, z)$ has the special form

$$p(w, z) = w^p(w - R(z))$$

Th1: $R(z) = \exp(z) + O(z^{p+1})$
Th2: A Runge-Kutta method of order p has stability matrix which reduces to the stability function $R_{RK}(z) = \exp(z) + O(z^{p+1})$.

stability behavior of GLM with RKS
similar to Runge-Kutta methods

Inherent Runge-Kutta stability (IRKS)

Definition

A GLM possesses the IRKS property if $Ve_1 = e_1$ (preconsistency), $p(w,0) = \det(wI - V) = w^p(w-1)$ and there exist $\mathbf{X}$ s.t.:

$$\mathbf{BA} \equiv \mathbf{XB} \qquad \text{and} \qquad \mathbf{BU} \equiv \mathbf{XV} - \mathbf{VX}$$

where $\mathbf{F} \equiv \mathbf{G}$ if $\mathbf{F} = \mathbf{G}$ except for the first row.

Inherent Runge-Kutta stability (2)

Theorem 1

IRKS $\Longrightarrow$ Runge-Kutta stability

In particular $p(w,z) = w^p(w - R(z))$, with

$$R(z) = 1 + z + \frac{z^2}{2} + \cdots + \frac{z^p}{p!} + \eta\frac{z^{p+1}}{(p+1)!}.$$

Also, the error constant of the method is $E = \dfrac{1-\eta}{(p+1)!}$, so the free parameter η can be used to balance stability and accuracy.

Inherent Runge-Kutta stability (2)

Theorem 2

The matrix $\mathbf{X}$ in the definition of IRKS is a doubly companion matrix and has this form:

$$\mathbf{X} = \begin{bmatrix} -\alpha_1 & \cdots & -\alpha_p & -\alpha_{p+1} - \beta_{p+1} \\ 1 & \cdots & 0 & -\beta_p \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 1 & -\beta_1 \end{bmatrix}$$

where $\beta_1, \ldots, \beta_p$ are the error constants of the external stages:

$$y_i^{[n]} = h^{i-1} y^{(i-1)}(t_n) - \beta_{p+2-i} h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2}),$$

$i = 2, \ldots, p+1.$

Construction of IRKS methods

- Butcher and Wright ('03) developed a theory on doubly companion matrices, which led to an *algorithm* to construct IRKS GLM based only on linear operation, with as input the collocation abscissa $c_1, \ldots, c_s$ and the free parameters $\eta, \beta_1, \ldots, \beta_p$;
- B& Jackiewicz ('04) studied how to choose the free parameters in order to balance stability and accuracy;
- Explicit IRKS GLM: stability regions larger than corresponding Runge-Kutta methods;
- Diagonally Implicit IRKS GLM: found classes of A-stable and L-stable methods.

How to improve RKS results?

Relax *the conditions on the stability function*
by Quadratic Stability

Conte, D'Ambrosio and Jackiewicz ('10) introduced QS for the class of Two-step Runge-Kutta methods, giving the following

Definition

The GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ with $\sigma(A) = \{\lambda\}$, possesses Quadratic stability (QS) if the stability function $p(w, z)$ has the special form

$$p(w, z) = w^{s-2}((1 - \lambda z)^s w^2 - p_1(z)w + p_0(z))$$

Inherent quadratic stability (IQS)

Definition

A two-step Runge-Kutta method possesses the IQS property if exists $\mathbf{X}$ s.t.:

$$\mathbf{BA} \equiv \mathbf{XB} \quad \text{and} \quad \mathbf{BU} \equiv \mathbf{XV} - \mathbf{VX}$$

where $\mathbf{F} \equiv \mathbf{G}$ if $\mathbf{F} = \mathbf{G}$ except for the first **two** rows.

Theorem

For the class of two-step Runge-Kutta methods,

IQS $\Longrightarrow$ **quadratic stability**

Conte, D'Ambrosio and Jackiewicz ('10) found classes of $A-$stable and $L-$stable IQS two-step Runge-Kutta methods up to order 8.

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to construct optimal GLM methods, in particular

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Explicit GLM in Nordsieck form with large stability regions

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Methods with Quadratic Stability

Explicit GLM in Nordsieck form with QS

$$\begin{cases} Y_i^{[n]} = h\sum_{j=1}^{i-1} a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} z_j^{[n-1]}, & i = 1, 2 \dots, s, \\ z_i^{[n]} = h\sum_{j=1}^{s} b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} z_j^{[n-1]}, & i = 1, 2 \dots, r, \end{cases}$$

$Y_i^{[n]} \approx (t_n + c_i h)$ of order q
$z^{[n]} \approx z(t,h)$ of order p (Nordsieck vector), i.e.

$$z(t,h) = \begin{bmatrix} y(t) \\ hy'(t) \\ \vdots \\ h^{r-1} y^{(r-1)}(t) \end{bmatrix}.$$

Other assumptions:

$r = s \qquad p = q = s - 1$

$$\mathbf{A} = \begin{bmatrix} 0 & & & & \\ a_{21} & 0 & & & \\ a_{31} & a_{32} & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ a_{s,1} & a_{s,2} & \cdots & a_{s,s-1} & 0 \end{bmatrix}, \quad \mathbf{V} = \begin{bmatrix} 1 & v_{12} & \cdots & v_{1r} \\ 0 & 0 & \cdots & v_{2r} \\ \vdots & & \ddots & \vdots \\ 0 & & \ddots & v_{r-1,r} \\ 0 & 0 & \cdots & 0 \end{bmatrix}.$$

$\sigma(V) = \{1\} \quad \Longrightarrow \quad$ the method is zero-stable

Quadratic stability

Definition

An explicit GLM method possesses quadratic stability property if its stability polynomial $p(w,z)$ has the form:

$$p(w,z) = w^{s-2}\big(w^2 - p_{s-1}(z)w + p_{s-2}(z)\big),$$

where

$$p_{s-1}(z) = 1 + p_{s-1,1}z + p_{s-1,2}z^2 + \cdots + p_{s-1,s}z^s,$$

$$p_{s-2}(z) = p_{s-2,1}z + p_{s-2,2}z^2 + \cdots + p_{s-2,s}z^s.$$

Inherent Quadratic Stability

Definition

A GLM possesses the Inherent Quadratic stability (IQS) property if there exist a matrix $\mathbf{X}$ s.t.:

$$\mathbf{BA} \equiv \mathbf{XB} \qquad \text{and} \qquad \mathbf{BU} \equiv \mathbf{XV} - \mathbf{VX}$$

where $\mathbf{F} \equiv \mathbf{G}$ if $\mathbf{F} = \mathbf{G}$ except for the first *two* rows.

Theorem 1

Inherent Quadratic stability $\Longrightarrow$ **Quadratic stability**

Inherent Quadratic Stability (*cont.*)

Theorem 2

Assume that the GLM possesses IQS. Then the matrix **X** has this form:

$$\mathbf{X} = \left[\begin{array}{ccccc|c} x_{1,1} & x_{1,2} & x_{1,3} & \cdots & x_{1,s-1} & x_{1,s} \\ x_{2,1} & x_{2,2} & x_{2,3} & \cdots & x_{2,s-1} & x_{2,s} \\ \hline 0 & 1 & 0 & \cdots & 0 & x_{3,s} \\ 0 & 0 & 1 & \cdots & 0 & x_{4,s} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & x_{s,s} \end{array}\right],$$

$x_{3,s}, \ldots, x_{s,s}$ **free parameters**

Order conditions

Theorem 1 (Butcher '93; B&Jackiewicz '93)

The GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ in Nordsieck form has order p and stage order $q = p$ iff:

$$
\begin{aligned}
e^{cz} &= zAe^{cz} + U\phi(z) + O(z^{p+1}) \\
e^{z}\phi(z) &= zBe^{cz} + V\phi(z) + O(z^{p+1}),
\end{aligned}
$$

where $e^{cz} = [e^{c_1 z}, \dots, e^{c_s z}]$ and $\phi(z) = [1 \quad z \quad z^2 \dots z^p]$.

Order conditions

Theorem 2

If the GLM $(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ in Nordsieck form has order p and stage order $q = p$, then

$$\mathbf{U} = \mathbf{C} - \mathbf{ACK} \qquad \mathbf{V} = \mathbf{F} - \mathbf{BCK}$$

$$\mathbf{C} = \begin{bmatrix} \mathbf{e} & \mathbf{c} & \frac{\mathbf{c}^2}{2!} & \dots & \frac{\mathbf{c}^p}{p!} \end{bmatrix}$$

$$\mathbf{K} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} 1 & 1 & \frac{1}{2!} & \cdots & \frac{1}{p!} \\ 0 & 1 & 1 & \cdots & \frac{1}{(p-1)!} \\ 0 & 0 & 1 & \cdots & \frac{1}{(p-2)!} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

Representation formulae

From the theorem 2 we have **U** and the first $s-1$ columns of **B**:

Theorem

$$\tilde{B} = \Big(\left[\begin{array}{ccc} f_2 & \cdots & f_s \end{array}\right] - \left[\begin{array}{ccc} v_2 & \cdots & v_s \end{array}\right] - b_s\,\tilde{c} \Big)\tilde{C}^{-1}.$$

where

$$\mathbf{B} = \left[\begin{array}{c|c} \tilde{B} & b_s \end{array}\right], \quad \tilde{B} \in \mathbb{R}^{s\times(s-1)}, \quad b_s \in \mathbb{R}^s,$$

$$\mathbf{F} = \left[\begin{array}{cccc} f_1 & f_2 & \cdots & f_s \end{array}\right], \quad \mathbf{V} = \left[\begin{array}{cccc} v_1 & v_2 & \cdots & v_s \end{array}\right]$$

$$\tilde{C} = \begin{bmatrix} 1 & c_1 & \cdots & \frac{c_1^{p-1}}{(p-1)!} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & c_{s-1} & \cdots & \frac{c_{s-1}^{p-1}}{(p-1)!} \end{bmatrix}, \quad \tilde{c} = \left[1 \; c_s \; \frac{c_s^2}{2} \ldots \frac{c_{s-1}^{p-1}}{(p-1)!}\right]$$

Search for GLM with IQS

Assumed collocation abscissae $c = (c_1, \dots, c_s)$ fixed, we have

order conditions $\Longrightarrow$ a class of GLM methods depending on

$$m = (\mathbf{A}, \mathbf{V}, b_s)$$

b_s =last column of $\mathbf{B}$

Free parameters in the search

$$m = (\mathbf{A}, \mathbf{V}, b_s) \quad \text{and} \quad x = (x_{3s}, \dots, x_{ss})^T,$$

used to ask for:

- Inherent Quadratic Stability: $\mathbf{BA} \equiv \mathbf{XB}$, $\mathbf{BU} \equiv \mathbf{XV} - \mathbf{VX}$
- Maximizing the area of the stability region: $area(m)$

Search for GLM with IQS (*cont.*)

IQS: $\mathbf{BA} \equiv \mathbf{XB}$, $\mathbf{BU} \equiv \mathbf{XV} - \mathbf{VX}$, so we define:

$$\begin{aligned} Q_1(m,x) &= \|(\mathbf{BA} - \mathbf{XB})(3:s,:)\|_F, \\ Q_2(m,x) &= \|(\mathbf{BU} - \mathbf{XV} + \mathbf{VX})(3:s,:)\|_F \end{aligned}$$

and search (m,x) which maximize

objective function

$$f(m,x) = -area(m) + K(Q_1(m,x) + Q_2(m,x)),$$

$K \approx 10^{12}$ penalty constant

This approach works well only for $s \leq 4$

Second approach: ask for Quadratic Stability

First step: find an *optimal* quadratic pol. $q_{op}(w,z)$

$$q_{op}(w,z) = w^{s-2}(w^2 + q_{s-1}(z)w + q_{s-2}(z)),$$

$$\begin{aligned} q_{s-1}(z) &= 1 + q_{s-1,1}z + \cdots + q_{s-1,s}z^s, \\ q_{s-2}(z) &= q_{s-2,1}z + \cdots + q_{s-2,s}z^s, \end{aligned}$$

which

- satisfies the same conditions as the stability polynomial of a GLM of order $p = q = s - 1$
- has maximum area of stability region

Second approach: ask for Quadratic Stability (*cont.*)

Second step: find a GLM with stability polynomial $p(w,z) \approx q_{op}(w,z)$

Find a GLM defined by $m = (\mathbf{A}, \mathbf{V}, b_s)$ with stablity pol.

$$p(w,z) = w^s + p_{s-1}(z)w^{s-1} + \cdots + p_1(z)w + p_0(z),$$

p_j pol. of degree s, with m minimizing the objective function:

$$f(m) = \text{distance between } p(w,z) \text{ and } q_{op}(w,z).$$

where the distance is the norm of the difference of the coefficients.

Low accuracy reached $\Longrightarrow$ stability regions notably smaller than that of $q_{op}(w,z)$

Second approach: ask for Quadratic Stability (*cont.*)

Third step: find a GLM with stability pol. $p(w,z) \approx q_{op}(w,z)$

Using output m of the second step as a starting guess, find a GLM defined by $m = (\mathbf{A}, \mathbf{V}, b_s)$ with stability pol.

$$p(w,z) = w^s + p_{s-1}(z)w^{s-1} + \cdots + p_1(z)w + p_0(z),$$

with m solution of the nonlinear system:

$$\begin{cases} p_{s-1,k} = q_{s-1,k}, \quad p_{s-2,k} = q_{s-2,k}, \quad k = 1, \ldots, s, \\ p_{j,k} = 0, \quad j = 0, \ldots, s-3, \; k = 1, \ldots, s. \end{cases}$$

$q := q_{op}, \quad p_j(z) = p_{js}z^s + \ldots + p_{j1}z + p_{j0}.$

High accuracy reached $\Longrightarrow$ same stability regions of $q_{op}(w,z)$

Efficient computation of stability polynomial coefficients

The computational kernel of our search is
– minimization problem of $f(m)$
– solution of a nonlinear system $g(m) = 0$

evaluation of $f(m)$ or $g(m) \Longrightarrow$ *computation of the coefficients of $p(w, z)$*

so we need for:

- a representation formula for the coefficients of $p(w, z)$
- an efficient technique for the implementation of such formula

Representation formula for the coefficients of $p(w, z)$

$$p(w,z) = w^s + p_{s-1}(z)w^{s-1} + \cdots + p_1(z)w + p_0(z), \;\; p_j(z) = \sum_{k=0}^{s} p_{jk} z^k$$

By the Fourier series approach (Butcher and Jackiewicz '96):

$$p_{jk} = \frac{1}{N_1 N_2} \sum_{\mu=0}^{N_1-1} \sum_{\nu=0}^{N_2-1} w_\mu^{-j} z_\nu^{-k} p(w_\mu, z_\nu), \quad j,k = 0,1,\ldots,s-1.$$

$$w_\mu = \exp\left(-\frac{2\pi\mu\, i}{N_1}\right), \quad z_\nu = \exp\left(-\frac{2\pi\nu\, i}{N_2}\right)$$

Comp. cost $O(s^2 N_1 N_2)$ flops and $O(N_1 N_2)$ eval. of $p(w, z)$

fast Fourier transform technique

By the representation formula we have:

$$\forall j, \quad p_{jk} = \frac{1}{N_2}\sum_{\nu=0}^{N_2-1} G_{j,\nu}\exp\left(\frac{2\pi\nu k\, i}{N_2}\right), k = 0,\dots,s,$$

$$\forall \nu, \quad G_{j,\nu} = \frac{1}{N_1}\sum_{\mu=0}^{N_1-1} p(w_\mu, z_\nu)\exp\left(\frac{2\pi\mu j\, i}{N_1}\right), \quad j = 0,\dots,s,$$

$(p_{j0},\dots,p_{js})$=first $(s+1)$ elements of IDFT of $(G_{j,0},\dots,G_{j,N_2-1})$

$(G_{\nu,0},\dots,G_{\nu,s-1})$=first s el. IDFT of $(p(w_0,z_\nu),\dots,p(w_{N_1-1},z_\nu))$

IDFT= inverse discrete Fourier transform

Algorithm for the coefficients of $p(w, z)$ by FFT

for $\nu = 0 : N_2 - 1$

$(G_{\nu,0}, \dots, G_{\nu,s-1}) =$ first s components of IDFT of $(p(w_0, z_\nu), \dots, p(w_{N_1-1}, z_\nu))$

endfor

for $j = 0 : s - 1$

$(p_{j0}, \dots, p_{js}) =$ first $(s+1)$ components of IDFT of $(G_{j,0}, \dots, G_{j,N_2-1})$

endfor

use of fast Fourier Transform algorithm for the IDFTs

fast Fourier transform technique: cost

Computing the IDFTs by the FFT algorithm we have:

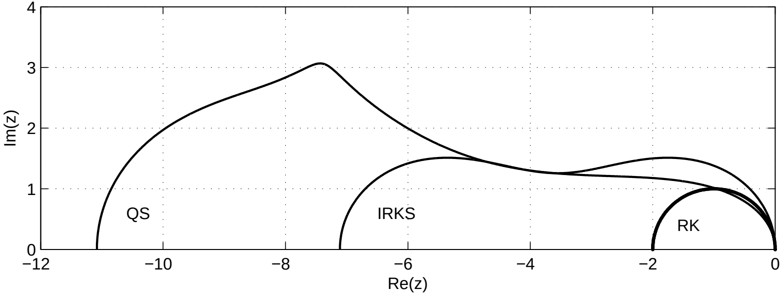
reduction of the computational cost

$$\frac{s^2 N}{(s+N)\log(N)}, \quad N = \max(N_1, N_2).$$

for example, if $s = 5, N = 16$, the reduction is about 5.

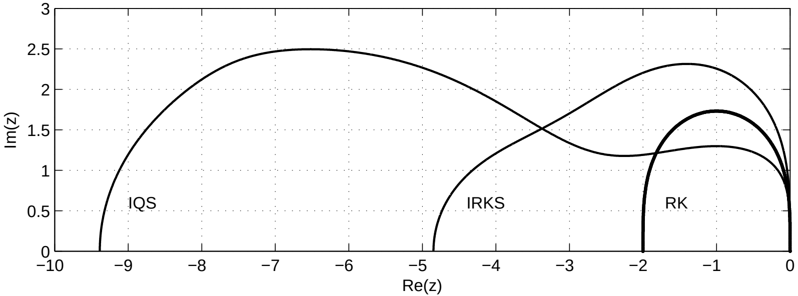
Examples of methods with IQS/QS

$s = 2, p = 1$



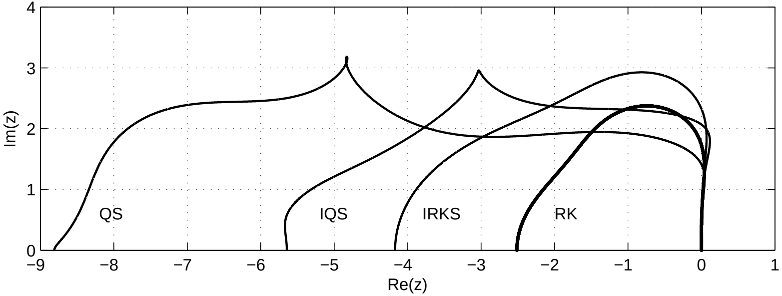
IQS:	Area 35.06	Constant error: 0.6605
IRKS:	Area ≈ 18	Constant error: 0.3594

s=3, p=2



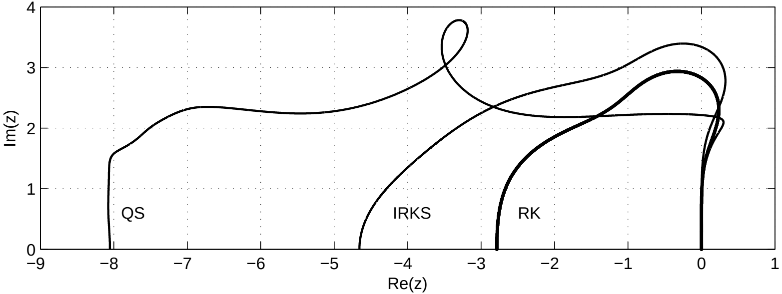
IQS:	Area 32.28	Constant error: 0.2019
IRKS:	Area $\approx$ 18	Constant error: 0.0885

s=4, p=3



QS:	Area: 35.09	Constant error: 0.0623
IQS:	Area: 22.85	Constant error: 0.0187
IRKS:	Area: 18.16	Constant error: 0.1667

s=5, p=4



QS:	Area 36.53	Constant error: 0.0126
IRKS:	Area 21.81	Constant error: 0.0033

Contents

Conclusions

Explicit GLM in Nordsieck form with QS

- IQS sufficient condition for QS
- constructive procedure for IQS/QS GLM based on minimization and on the solution of nonlinear systems
- efficient computation of the stability polynomial coefficients
- stability regions considerably larger than corresponding IRKS methods for $s = 1, 2, 3, 4, 5$ and $p = s - 1$

Future developments

- higher order explicit GLM and implicit GLM with QS/IQS
- theoretical analysis to derive a constructive algorithm for IQS GLM based only on linear operations
- implementation in a variable-step and/or variable-order code