On the stability of the Magnus method

Jitse Niesen

Ustaoset, 15 February 2005

Introduction

Anto, Hans et al. wrote in *Acta Numerica* 2000:

> *[M]uch needs to be done in the realm of stability investigations [...] Interesting results abound which cannot yet be fitted into a general theory.*

Introduction

Anto, Hans et al. wrote in *Acta Numerica* 2000:

> *[M]uch needs to be done in the realm of stability investigations [...] Interesting results abound which cannot yet be fitted into a general theory.*

Outline of the talk:

- An example of a stiff equation
- Classical stability for RK-methods
- The behaviour of the Magnus method

The equation

We consider the following linear ODE:

$$y' = \begin{bmatrix} -\mu & 1 \\ \mu^2 - \operatorname{sech}^2 t & -\mu \end{bmatrix} y, \qquad y(-10) = \begin{bmatrix} 1 \\ \mu \end{bmatrix},$$

where $\mu \gg 0$.

The eigenvalues of the matrix on the right-hand side are:

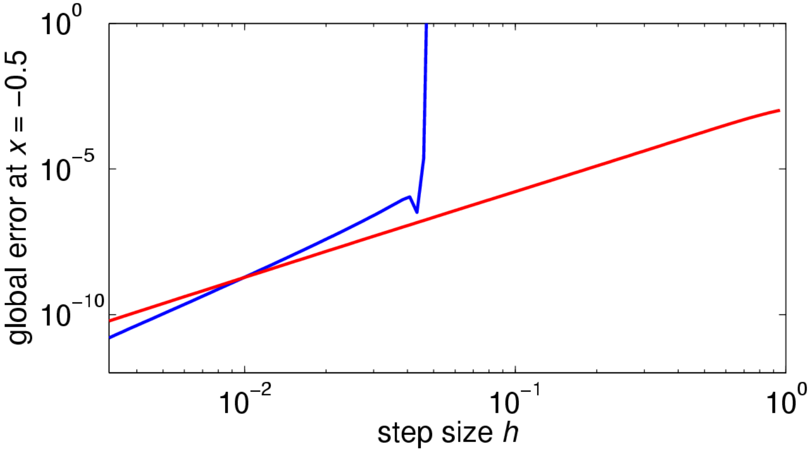
$$\lambda_1 = -\mu + \sqrt{\mu^2 - \operatorname{sech}^2 x} \approx 0 \qquad \text{with } v_1 = \begin{bmatrix} 1 \\ \sqrt{} \end{bmatrix} \approx \begin{bmatrix} 1 \\ \mu \end{bmatrix},$$

$$\lambda_2 = -\mu - \sqrt{\mu^2 - \operatorname{sech}^2 x} \approx -2\mu \quad \text{with } v_2 = \begin{bmatrix} 1 \\ -\sqrt{} \end{bmatrix} \approx \begin{bmatrix} 1 \\ -\mu \end{bmatrix}.$$

So there is one neutral and one very negative eigenvalue, and the solution will approximately follow v_1.

Global error versus step size

We take $\mu = 30$ and solve the equation on $[-10, -0.5]$.



Blue line = RK4: four stages, fourth order, explicit.
Red line = Radau IIA: two stages, third order, implicit.

Outline of the talk

- An example of a stiff equation
- Classical stability for RK-methods
- The behaviour of the Magnus method

A-stability

We restrict ourselves to one-step methods $y_{n+1} = \psi_h(y_n)$.

A-stability theory is based on Dahlquist's test equation $y' = \lambda y$.

$$|y(t)| \le |y(0)| \quad \text{for} \quad t \ge 0 \quad \text{if} \quad \lambda \in \mathbb{C}^- = \{z \in \mathbb{C} : \operatorname{Re} z \le 0\}.$$

Runge–Kutta methods take the form $\phi_h(y) = R(h\lambda)y$.
The stability domain is $S = \{z \in \mathbb{C} : |R(z)| \le 1\}$.

A method is A-stable if the stability domain contains $\mathbb{C}^-$.
For A-stable methods, we have: $|y_n| \le |y_0|$ if $\lambda \in \mathbb{C}^-$.

Explicit Runge–Kutta methods are never A-stable.
All Gauss, Radau and Lobatto methods are A-stable.

B-stability

Suppose that the equation $y' = f(t, y)$ satisfies

$$\mathrm{Re}\langle f(t,y) - f(t,z), y - z\rangle \le 0. \qquad (*)$$

Then the equation is contractive: any two solutions y and z satisfy

$$|y(t) - z(t)| \le |y(0) - z(0)| \quad \text{for} \quad t \ge 0.$$

A method ψ_h is said to be B-stable if $(*)$ implies that

$$|\psi_h(y) - \psi_h(z)| \le |y - z|.$$

All Gauss, Radau and Lobatto IIIC methods are B-stable,
but the Lobatto IIIA and IIIB methods are not B-stable.

AN-stability

Recall condition **(∗)**: $\quad \mathrm{Re}\langle f(t,y) - f(t,z), y - z\rangle \le 0.$

The linear equation $y' = \lambda(t)\, y$ satisfies **(∗)** if $\mathrm{Re}\,\lambda(t) \le 0$.

We say the method is AN-stable if $|\psi_h(y) - \psi_h(z)| \le |y - z|$ for these equations.

AN-stability

Recall condition $(*)$: $\quad \mathrm{Re}\langle f(t,y) - f(t,z), y - z\rangle \le 0.$

The linear equation $y' = \lambda(t)\, y$ satisfies $(*)$ if $\mathrm{Re}\,\lambda(t) \le 0$.

We say the method is AN-stable if $|\psi_h(y) - \psi_h(z)| \le |y - z|$ for these equations.

$$\text{B-stability} \quad \Longrightarrow \quad \text{AN-stability} \quad \Longrightarrow \quad \text{A-stability.}$$

$$\begin{bmatrix} y' = f(t,y) \\ \text{condition } (*) \end{bmatrix} \qquad \begin{bmatrix} y' = \lambda(t)\, y \\ \mathrm{Re}\,\lambda(t) \le 0 \end{bmatrix} \qquad \begin{bmatrix} y' = \lambda y \\ \mathrm{Re}\,\lambda \le 0 \end{bmatrix}$$

For non-confluent RK-methods: AN-stability $\Longleftrightarrow$ A-stability.

B-convergence

Suppose that f satisfies a one-sided Lipschitz condition:

$$\mathrm{Re}\langle f(t,y) - f(t,z), y - z\rangle \le \nu |y - z|^2.$$

Then any two solutions y and z satisfy

$$|y(t) - z(t)| \le |y(0) - z(0)|\, \mathrm{e}^{\nu t} \quad \text{for} \quad t \ge 0.$$

The method is B-convergent of order r if

$$|y_n - y(t_n)| \le h^r \gamma(t_n, \nu) \max_{j=1,\ldots,\ell} \max_{t\in[0,t_n]} |y^{(j)}(t)| \quad \text{for } h\nu < \alpha.$$

The global error can be bounded in terms of ν and derivatives of the exact solution; the stiffness does not enter.

B-stability is a necessary condition for B-convergence.

Outline of the talk

- An example of a stiff equation
- Classical stability for RK-methods
- The behaviour of the Magnus method

Stability and the Magnus methods

Potential problem:
The Magnus series for $y' = A(t)\,y$ is only guaranteed to converge if $\int_t^{t+h} \|A(\tau)\|\,\mathrm{d}\tau < \pi$; this might limit the step size h.

Results are obtained for the following equations:

- oscillatory equations (some eigenvalues on imaginary axis)
  Magnus performs quite well (see work of **Per Christian**, **Simon et al.**, ...)
- Schrödinger equation (∞ eigenvalues near imaginary axis)
  Hochbruck & Lubich consider $y' = -\mathrm{i}(I - \Delta + V(t))y$.
  They find that the above problem does not arise.
- parabolic PDEs (∞ eigenvalues near negative real axis)
  ... as explained by **Mechthild et al.**

Stability and the Magnus methods

$$\text{B-stability} \quad \Longrightarrow \quad \text{AN-stability} \quad \Longrightarrow \quad \text{A-stability.}$$

$$\begin{bmatrix} y' = f(t,y) \\ \text{contractive} \end{bmatrix} \qquad \begin{bmatrix} y' = \lambda(t)\, y \\ \operatorname{Re} \lambda(t) \le 0 \end{bmatrix} \qquad \begin{bmatrix} y' = \lambda y \\ \operatorname{Re} \lambda \le 0 \end{bmatrix}$$

Magnus methods are A-stable and AN-stable, because they solve $y' = \lambda(t)\, y$ exactly.

A linear equation $y' = A(t)\, y$ is contractive if $\mu_2(A) \le 0$, where

$$\mu_2(A) = \lim_{\varepsilon \downarrow 0} \frac{\|I + \varepsilon A\| - 1}{\varepsilon} \qquad \textbf{(logarithmic norm)}$$

Magnus $y_{k+1} = \exp(\Omega)\, y_k$ is B-stable if this implies $\mu_2(\Omega) \le 0$.
It does when $\Omega = \int A(t)\, \mathrm{d}t$ (Magnus-2). Higher orders?

Back to our equation

Consider the fourth-order Magnus method applied to

$$y' = \begin{bmatrix} -\mu & 1 \\ \mu^2 - \operatorname{sech}^2 t & -\mu \end{bmatrix} y, \qquad y(-10) = \begin{bmatrix} 1 \\ \mu \end{bmatrix},$$

where $\mu \gg 0$.

The eigenvalues of the matrix on the right-hand side are:

$$\lambda_1 = -\mu + \sqrt{\mu^2 - \operatorname{sech}^2 x} \approx 0 \qquad \text{with } v_1 = \begin{bmatrix} 1 \\ \sqrt{} \end{bmatrix} \approx \begin{bmatrix} 1 \\ \mu \end{bmatrix},$$

$$\lambda_2 = -\mu - \sqrt{\mu^2 - \operatorname{sech}^2 x} \approx -2\mu \quad \text{with } v_2 = \begin{bmatrix} 1 \\ -\sqrt{} \end{bmatrix} \approx \begin{bmatrix} 1 \\ -\mu \end{bmatrix}.$$

So there is one neutral and one very negative eigenvalue, and the solution will approximately follow v_1.

The exact solution

Define new coordinates by $y = \left[\begin{smallmatrix} 1 & 1 \\ \mu & -\mu \end{smallmatrix}\right] \bar{y}$, then

$$\bar{y}' = \begin{bmatrix} -\frac{1}{2}\mu^{-1}\operatorname{sech}^2 t & -\frac{1}{2}\mu^{-1}\operatorname{sech}^2 t \\ \frac{1}{2}\mu^{-1}\operatorname{sech}^2 t & -2\mu + \frac{1}{2}\mu^{-1}\operatorname{sech}^2 t \end{bmatrix} \bar{y}, \qquad \bar{y}(t_0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

Rationale: The matrix on the left-hand side is almost diagonal.

The exact solution is

$$\bar{y}(t) = \begin{bmatrix} 1 - \frac{1}{2}\mu^{-1}\int_{t_0}^{t}\operatorname{sech}^2\tau\,\mathrm{d}\tau + \mu^{-2}\int \ldots\,\mathrm{d}\tau \\ \frac{1}{4}\mu^{-2}\operatorname{sech}^2 t \end{bmatrix} + \mathcal{O}(\mu^{-3}).$$

To find this, substitute the ansatz

$$\bar{y}(t) = \bar{y}_0(t) + \mu^{-1}\,\bar{y}_1(t) + \mu^{-2}\,\bar{y}_2(t) + \cdots$$

in the equation and equate powers of μ.

The local error

We use Magnus-4 with quadrature at the Gauss–Legendre points:

$$y_{k+1} = \exp(\Omega) y_k, \quad \text{with} \quad \begin{aligned} \Omega &= \tfrac{1}{2} h (A_1 + A_2) - \tfrac{\sqrt{3}}{12} h^2 [A_1, A_2], \\ A_{1,2} &= A\big(t_k + (\tfrac{1}{2} \pm \tfrac{1}{6}\sqrt{3}) h\big). \end{aligned}$$

The local error in the limit $h \to 0$, $\mu h \to \infty$ is

$$\bar{L}_k = \mu^{-1} \begin{bmatrix} h^5(\dots) + \mathcal{O}(h^7, \mu^{-1}) \\ \frac{1}{12} h^2 \operatorname{sech}' t_{k+1/2} + \mathcal{O}(h^4, \mu^{-1}) \end{bmatrix}.$$

So, we have order reduction in the stiff (second) component:
The local error is not h^5 but h^2.

The above formula was found by diagonalizing Ω and with the help of some coffee and perseverance.

The global error

$$\bar{L}_k = \mu^{-1} \begin{bmatrix} h^5(\dots) + \mathcal{O}(h^7, \mu^{-1}) \\ \frac{1}{12} h^2 \operatorname{sech}' t_{k+1/2} + \mathcal{O}(h^4, \mu^{-1}) \end{bmatrix}.$$

The error in the stiff (second) component does not propagate, so the global error is

$$\bar{G}_k = \mu^{-1} \begin{bmatrix} h^4(\dots) + \mathcal{O}(h^6, \mu^{-1}) \\ \frac{1}{12} h^2 \operatorname{sech}' t_{k+1/2} + \mathcal{O}(h^4, \mu^{-1}) \end{bmatrix}.$$

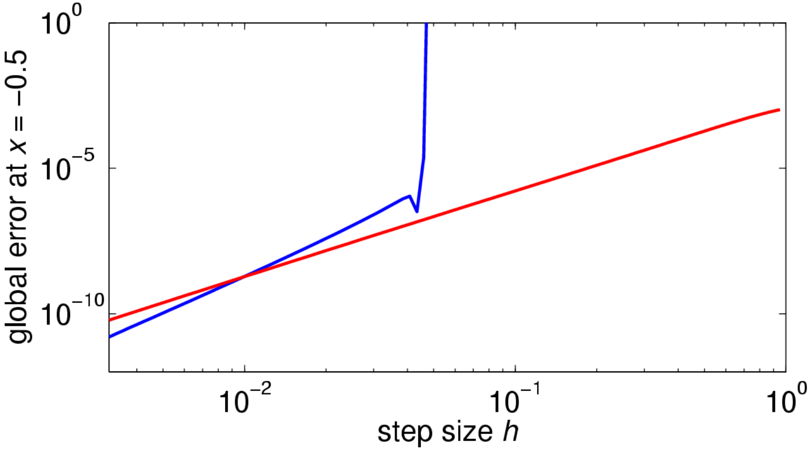
In the original coordinates, this becomes

$$G_k = \begin{bmatrix} \frac{1}{12} \mu^{-1} h^2 \operatorname{sech}' t_{k+1/2} + \mathcal{O}(h^4, \mu^{-2}) \\ \frac{1}{12} h^2 \operatorname{sech}' t_{k+1/2} + \mathcal{O}(h^4, \mu^{-1}) \end{bmatrix}.$$

Hence, the method is second order when $\mu \gg h$.

Global error versus step size

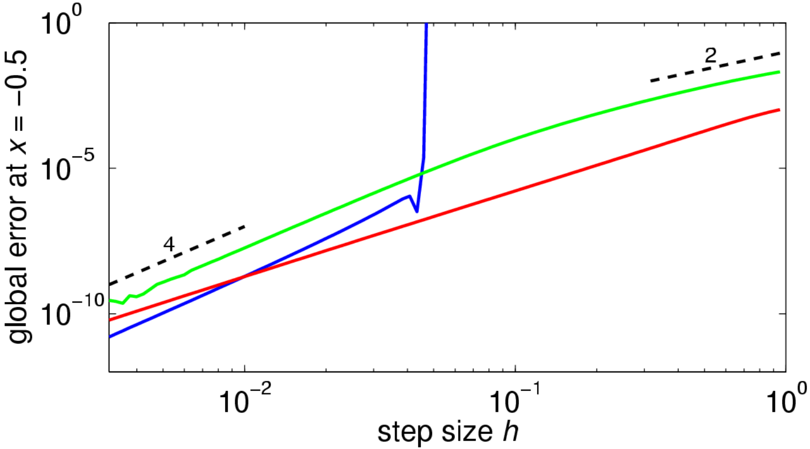
We take $\mu = 30$ and solve the equation on $[-10, -0.5]$.



Blue = RK4; red = 2-stage Radau IIA.

Global error versus step size

We take $\mu = 30$ and solve the equation on $[-10, -0.5]$.



Blue = RK4; red = 2-stage Radau IIA; green = Magnus-4.