Order reduction in stability computations using the Magnus method

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Overview

- Background: Stability of travelling waves
- The model equation
- The fourth-order Magnus method
- The oscillatory regime
- The stiff regime
- Conclusions
Background: Stability for travelling waves

Consider a reaction–diffusion equation of the form

\[ u_t = u_{xx} + f(u), \quad u(x, t) \in \mathbb{R}^n, \ x \in \mathbb{R}. \tag{\star} \]

Assume that the PDE supports a travelling wave solution

\[ u(t, x) = u_*(\xi) \quad \text{where} \ \xi = x - ct. \]

We are interested in the stability of this travelling wave.

\[ ^{1}\text{Sandstede, in: Fiedler (ed.), } \textit{Handbook of Dynamical Systems II}, 2002. \]
Background: Stability for travelling waves

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(*)&

Assume that the PDE supports a travelling wave solution

\[ u(t, x) = u_*(\xi) \quad \text{where} \quad \xi = x - ct. \]

We are interested in the stability of this travelling wave. Let \( u = u_* + \hat{u} \) be a perturbation.

PDE (*)& in travelling frame:

\[ u_t = u_{\xi\xi} + cu_\xi + f(u) \]

Travelling wave equation:

\[ 0 = u''_* + cu'_* + f(u_*) \]

Subtracting:

\[ \hat{u}_t = \hat{u}_{\xi\xi} + c\hat{u}_\xi + f(u_* + \hat{u}) - f(u_*) \]

Linearized stability analysis:

\[ \hat{u}_t = \hat{u}_{\xi\xi} + c\hat{u}_\xi + f'(u_*) \hat{u} \]

Set \( \hat{u}(\xi, t) = e^{\lambda t} \bar{u}(\xi) \) to get:

\[ \lambda \bar{u} = \bar{u}_{\xi\xi} + c\bar{u}_\xi + f'(u_*) \bar{u} \]  

(*)&

Wave is unstable if (*)& has any solution with \( \text{Re} \, \lambda > 0. \)

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Background: A simple shooting method

We want to solve the boundary value problem

$$\ddot{\bar{u}} + c\dot{\bar{u}} + f'(u_*(x)) \bar{u} = \lambda \bar{u}, \quad \bar{u}(x) \to 0 \text{ as } x \to \pm\infty.$$ 

Convert this problem to first-order form:

$$y' = \begin{bmatrix} 0 & 1 \\ \lambda - f'(u_*(x)) & c \end{bmatrix} y, \quad y(x) \to 0 \text{ as } x \to \pm\infty.$$ 

Shooting method: Solve this equation on $(-\infty, 0]$ and $[0, +\infty)$ and see whether the solutions match at $x = 0$. Subtract multiple of identity matrix to counter exponential growth.

Here, we concentrate on the regime where $|\lambda|$ is large.

For simplicity, assume that $u$ is scalar (and hence, $y \in \mathbb{C}^2$). In this case, the above simple method is usually not the best,

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The model equation

As an example, consider the PDE \( u_t = \frac{1}{6} (u_{xx} + 2u^3 - u) \). \(^3\)

This equation supports the stationary pulse

\[
\begin{align*}
u_*(x, t) = \text{sech } x = \frac{2}{e^x + e^{-x}}.
\end{align*}
\]

The resulting boundary value problem is

\[
y' = \begin{bmatrix} 0 & 1 \\ \lambda + \frac{1}{6} - \text{sech}^2 x & 1 \end{bmatrix} y, \quad y(x) \to 0 \text{ as } x \to \pm\infty.
\]

This problem is particularly simple to analyse because

- \( u_* \) is a pulse: the limits \( x \to -\infty \) and \( x \to +\infty \) coincide;
- \( u_* \) is stationary: the speed \( c \) vanishes;
- \( u_* \) has an analytic expression.

The oscillatory and stiff regimes

\[ y' = A(x; \lambda) y, \quad \text{where} \quad A(x; \lambda) = \begin{bmatrix} 0 & 1 \\ \lambda + \frac{1}{6} - \text{sech}^2 x & 0 \end{bmatrix} \]

We suppose that \(|\lambda|\) is large.

In the limit \(x \to \pm \infty\), the eigenvalues of \(A\) are

\[ \pm \mu \quad \text{with} \quad \mu = \sqrt{\lambda + \frac{1}{6}}, \]

so we can distinguish two regimes:

- If \(\lambda\) is negative, \(A\) has purely imaginary eigenvalues, so the equation is oscillatory.

- If \(\text{arg} \lambda \in (-\pi + \varepsilon, \pi - \varepsilon)\), one eigenvalue has positive real part and one has negative real part. We need to cancel out the former, so replace \(A\) with \(A - \mu I\). Now, the equation is stiff.
The Magnus method

Numerical methods based on the Magnus expansion perform well on Sturm–Liouville problems.\textsuperscript{4} Furthermore, they preserve some geometrical structure in the case where \( u \) is a vector.

The standard fourth-order Magnus method for

\[ y' = A(x)y \]

is given by the following formula\textsuperscript{5,6}

\[
y_1 = \exp\left(\frac{1}{2} h (A(x_-) + A(x_+)) - \frac{\sqrt{3}}{12} h^2 [A(x_-), A(x_+)]\right) y_0.
\]

where \( x_- = x_0 + \left(\frac{1}{2} - \frac{1}{6} \sqrt{3}\right) h \), \( x_+ = x_0 + \left(\frac{1}{2} + \frac{1}{6} \sqrt{3}\right) h \).

\textsuperscript{6}Hairer, Lubich & Wanner, Geometric Numerical Integration, 2004.
The oscillatory regime

The equation that we want to solve is

\[ y' = \begin{bmatrix} 0 & 1 \\ \mu^2 - \text{sech}^2 x & 0 \end{bmatrix} y, \quad \text{where } \mu \in i\mathbb{R}, |\mu| \gg 1. \]

The matrix on the right has large, purely imaginary eigenvalues. Hence, the solution will oscillate very fast.

Magnus performs well on this kind of problems.\(^7,8,9\)

Analysis goes as follows:

- Approximate exact solution with WKB;
- Approximate numerical solution by diagonalizing \( \Omega \);
- Subtract to get the local error;
- Combine local errors to get the global error.

\(^7\)Iserles, On the global error . . ., *BIT* 42(3), 2002.
Global error versus $\mu$

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

Blue: Gauss–Legendre; red: Magnus (both 4th order).

Solid: stepsize $h = 0.01$; dashed: $h = 0.005$
The stiff regime

The equation that we want to solve is

\[ y' = \begin{bmatrix} -\mu & 1 \\ \mu^2 - \text{sech}^2 x & -\mu \end{bmatrix} y, \quad \text{where } \text{Re} \mu > 0, \ |\mu| \gg 1. \]

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

\[ \lambda_1 = -\mu + \sqrt{\mu^2 - \text{sech}^2 x} \approx 0 \quad \text{with } v_1 = \begin{bmatrix} 1 \\ \sqrt{-} \end{bmatrix} \approx \begin{bmatrix} 1 \\ \mu \end{bmatrix}, \]

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

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

We will take the initial condition \( y(x) = v_1 \) as \( x \to -\infty \).
The exact solution

Define new coordinates by \( y = \begin{bmatrix} 1 & 1 \\ \mu & -\mu \end{bmatrix} \bar{y} \), then

\[
\bar{y}' = \begin{bmatrix}
-\frac{1}{2} \mu^{-1} \text{sech}^2 t & -\frac{1}{2} \mu^{-1} \text{sech}^2 t \\
\frac{1}{2} \mu^{-1} \text{sech}^2 t & -2\mu + \frac{1}{2} \mu^{-1} \text{sech}^2 t
\end{bmatrix} \bar{y}, \quad \bar{y}(t_0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.
\]

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

The exact solution is

\[
\bar{y}(t) = \left[ 1 - \frac{1}{2} \mu^{-1} \int_{t_0}^{t} \text{sech}^2 \tau \, d\tau + \mu^{-2} \int \ldots \int \right] + \mathcal{O}(\mu^{-3}).
\]

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 \( \mu \).
The error committed by the Magnus method

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

$$\bar{L}_k = \mu^{-1} \left[ \frac{1}{12} h^2 \text{sech}' t_{k+1/2} + O(h^4, \mu^{-1}) \right].$$

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

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

$$\bar{G}_k = \mu^{-1} \left[ \frac{1}{12} h^2 \text{sech}' t_{k+1/2} + O(h^4, \mu^{-1}) \right].$$

In the original coordinates, this becomes

$$G_k = \left[ \frac{1}{12} \mu^{-1} h^2 \text{sech}' t_{k+1/2} + O(h^4, \mu^{-2}) \right].$$

Hence, the method is second order when $\mu \gg h$. 
Global error versus step size

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

Blue: Gauss–Legendre; red: Magnus (both 4th order).
Conclusions and other remarks

- As reported before, Magnus method outperforms Runge–Kutta methods for oscillatory linear systems.
- Magnus methods perform not so well in the “classical stiff” case, where one eigenvalue is negative and large in modulus. In our example, the error of Magnus-4 is a factor $|\text{eval}|^{1/2}$ larger than that of Gauss–Legendre.
- The standard fourth-order Magnus method is not B-stable. (B-stability = preservation of contractivity)
- The computation sketched in this talk has been generalized to arbitrary wave profiles $u_*$ and speeds $c$, under the assumption that the limits $\lim_{x \to \pm \infty} u_*(x)$ exist.

$$y' = \begin{bmatrix} -\mu \\ \mu^2 - f'(u_*(x)) \\ c - \mu \end{bmatrix} y, \quad y(x) \to 0 \text{ as } x \to \pm \infty.$$ 

- The case where $u$ is a vector has not been tackled.