Numerical evaluation of the Evans function by Magnus integration

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Outline

- The Evans function
- Linear non-autonomous ODEs with parameters
- Toy problem: modified Airy equation
- WKB asymptotics and error analysis

Acknowledgments

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1 Linear non-autonomous ODEs with parameters

Example: Sturm–Liouville eigenvalue problem

$$y''(x) + u(x)\,y(x) + \lambda\,y(x) = 0$$

plus boundary conditions, or

$$Y'(x) = \lambda \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} Y + \begin{pmatrix} 0 & 1 \\ -u(x) & 0 \end{pmatrix} Y$$

In general: need to solve IVPs of the form

$$\dot{Y} = A(t,\lambda)\,Y\,, \quad Y(0) = Y_0$$

$$A(t,\lambda) = A_0(t) + \sum_{k=1}^{p} \lambda_k\,A_k(t)$$

2 Application: Reaction diffusion systems

$$U_t = BU_{\xi\xi} + cU_\xi + F(U)$$

Example: Autocatalytic two-component system

$$\begin{aligned} u_t &= \delta u_{\xi\xi} + cu_\xi - uv^m \\ v_t &= v_{\xi\xi} + cv_\xi + uv^m \end{aligned}$$

Front-type boundary conditions

$$\begin{aligned} (u, v) &\to (1, 0) \quad \text{as } x \to -\infty \\ (u, v) &\to (0, 1) \quad \text{as } x \to +\infty \end{aligned}$$

Travelling wave in moving frame

$$U(\xi, t) = U_c(\xi)$$

3 Stability of travelling waves

Perturbation ansatz:

$$U(\xi,t) = U_c(\xi) + \hat{U}(\xi)\,\mathrm{e}^{\lambda t}$$

Plugging this into the reaction-diffusion system

$$U_t = BU_{\xi\xi} + cU_\xi + F(U)$$

yields

$$\lambda\hat{U} = \left[B\partial_{\xi\xi} + c\,I\partial_\xi + DF(U_c(\xi))\right]\hat{U}$$

with $\hat{U}(\xi) \to 0$ as $\xi \to \pm\infty$.

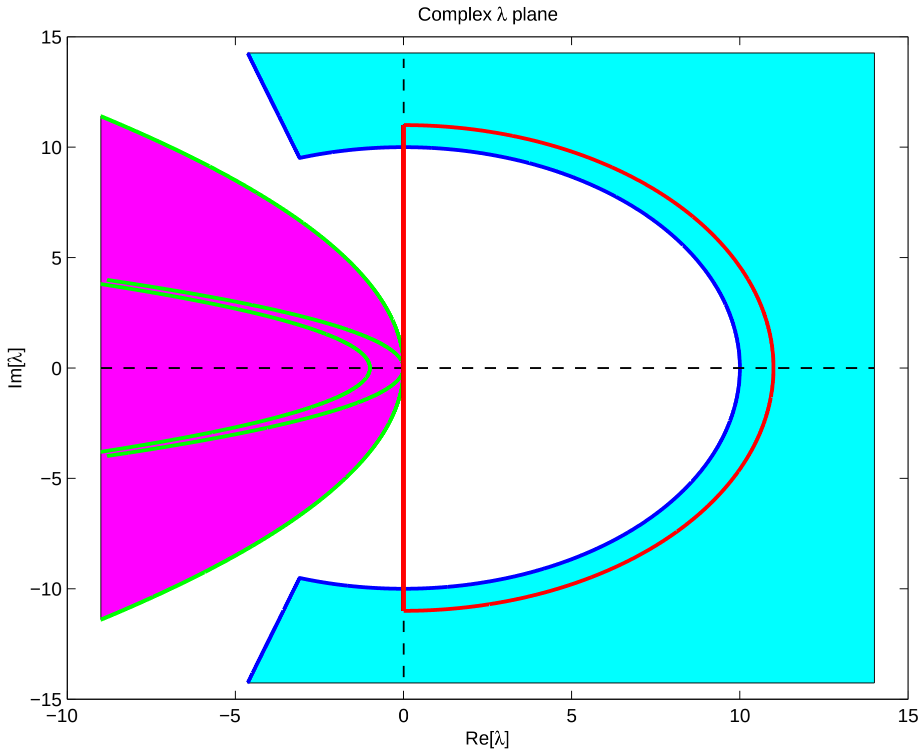
Reformulation

$$Y' = A(\xi,\lambda)\,Y\,,$$

where $Y = (\hat{U}, \hat{U}_\xi)$, and

$$A(\xi,\lambda) = \begin{pmatrix} O & I \\ B^{-1}\big(\lambda - DF(U_c(\xi))\big) & -c\,B^{-1} \end{pmatrix}$$

Spectrum of the linearized travelling wave operator



4 The Evans function

Limiting systems

$$A_\pm(\lambda) = \lim_{\xi\to\pm\infty} A(\xi,\lambda)$$

- Assume A_- has a k-dimensional unstable manifold
- A^+ has an $(2n-k)$-dimensional stable manifold
- Look for intersection under the "evolution" of the BVP

Wronskian

$$\begin{aligned} D(\lambda) &= \mathrm{e}^{-\int_0^\xi \mathrm{Tr}\, A(x,\lambda)\mathrm{d}x} \cdot \det\big(Y_1^-(\xi;\lambda)\cdots Y_k^-(\xi;\lambda)\;\; Y_{k+1}^+(\xi;\lambda)\cdots Y_{2n-k}^+(\xi;\lambda)\big) \\ &= \mathrm{e}^{-\int_0^\xi \mathrm{Tr}\, A(x,\lambda)\mathrm{d}x} \cdot \big(Y_1^- \wedge\cdots\wedge Y_k^-\big)\wedge\big(Y_{k+1}^+\wedge\cdots\wedge Y_{2n-k}^+\big) \\ &\equiv \mathrm{e}^{-\int_0^\xi \mathrm{Tr}\, A(x,\lambda)\mathrm{d}x} \cdot \big(U_-(\xi;\lambda)\wedge U_+(\xi;\lambda)\big) \end{aligned}$$

(Prefactor ensures ξ-independence.)

5 Properties of the Evans function

(Evans, 1975; Alexander, Gardner & Jones, 1990)

- Zeros correspond to eigenvalues
- Order of the zero corresponds to algebraic multiplicity
- Analytic to the right of the essential spectrum
- Can use argument principle to determine number of zeros in the right half plane

Numerical issues

- May want to rescale solution by expected exponential growth
- Computing second most unstable eigenspace is numerically unstable

$\rightarrow$ *Projection methods* or *Exterior product representation*

6 Problem features

- Need to solve the equation for many different parameter values
- System can become oscillatory or stiff
- Potential is slowly varying, and typically computed numerically

Idea

- Use methods that work well for near-autonomous, oscillatory problems: *Magnus integrators*
- Collect all parameter independent parts, and evaluate them in a *precomputation step*

7 Neumann series

$$\dot{S} = A(t)\,S\,, \qquad S(0) = I$$

can be written in integral from as

$$(\mathsf{I} - \mathsf{K}) \circ S \equiv S(t) - \int_0^t A(\tau)\,S(\tau)\,\mathrm{d}\tau = I$$

Neumann series solution

$$\begin{aligned} S(t) &= (\mathsf{I} - \mathsf{K})^{-1} \circ I \\ &= (\mathsf{I} + \mathsf{K} + \mathsf{K}^2 + \mathsf{K}^3 + \dots) \circ I \\ &= I + \int_0^t A(\tau)\,\mathrm{d}\tau + \int_0^t A(\tau_1) \int_0^{\tau_1} A(\tau_2)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1 + \dots \end{aligned}$$

Convergence criterion:

$$\int_0^t \|A(\tau)\|\,\mathrm{d}\tau < \infty$$

$\rightarrow$ *Peano-Baker series*, *Chen-Fleiss series*, *Feynman-Dyson path-ordered exponential*

8 Magnus series

Write $S(t) = \mathrm{e}^{\sigma(t)}$, so that

$$\begin{aligned}
\sigma(t) &= \ln S(t) \\
&= \mathsf{K} \circ I + \big(\mathsf{K}^2 \circ I - \frac{1}{2}(\mathsf{K} \circ I)^2\big) \\
&\quad + \left(\mathsf{K}^3 \circ I - \frac{1}{2}\big((\mathsf{K}^2 \circ I)(\mathsf{K} \circ I) + (\mathsf{K} \circ I)(\mathsf{K}^2 \circ I)\big) + \frac{1}{3}(\mathsf{K} \circ I)^3\right) \\
&\quad + \ldots \\
&\equiv s_1 + s_2 + \ldots
\end{aligned}$$

where

$$\begin{aligned}
s_1 &= \int_0^t A(\tau)\,\mathrm{d}\tau\,, \\
s_2 &= \frac{1}{2}\int_0^t \int_0^{\tau_1} [A(\tau_1), A(\tau_2)]\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1
\end{aligned}$$

$\rightarrow$ *Arieh Iserles*, *Syvert Norsett*, *Antonella Zanna*, *Hans Munthe-Kaas*, *Brynjulf Owren*, *Per Christian Moan*, *Sergio Blanes*, *Fernando Casas*, *Matthias Kawski*

9 Convergence of the Magnus series

The Magnus expansion converges in the Euclidean 2-norm provided

$$\int_0^t \|A(\tau)\| \, \mathrm{d}\tau < \frac{r_0}{\nu}$$

where

$$r_0 = \int_0^{2\pi} \left(2 + \tfrac{1}{2}\tau(1 - \cot(\tfrac{1}{2}\tau))\right)^{-1} \mathrm{d}\tau = 2.173737\ldots$$

and $\nu \leq 2$ is the smallest constant such that

$$\|[A_1, A_2]\| \leq \nu \, \|A_1\| \, \|A_2\|$$

(Moan, 2002).

Rough estimate

$$\int_0^t \|A(\tau)\| \, \mathrm{d}\tau < 1.09$$

guarantees convergence.

10 Precomputation

$$
\begin{aligned}
\mathsf{K}^n \circ I &= (\mathsf{K}_0 + \lambda \mathsf{K}_1 + \mu \mathsf{K}_2)^n \circ I \\
&= \sum_{k=0}^{n} \sum_{j=0}^{k} \left(\sum_{\alpha \in \mathcal{P}(j,k,n)} \mathsf{K}_{\alpha_1} \circ \cdots \circ \mathsf{K}_{\alpha_n} \circ I \right) \lambda^j \, \mu^{k-j} \\
&\equiv \sum_{k=0}^{n} \sum_{j=0}^{k} \Gamma_{j,k,n}(t) \, \lambda^j \, \mu^{k-j}
\end{aligned}
$$

where

$$
\begin{aligned}
\Gamma_{j,k,n}(t) &\equiv \sum_{\alpha \in \mathcal{P}(j,k,n)} \mathsf{K}_{\alpha_1} \circ \cdots \circ \mathsf{K}_{\alpha_n} \circ I \\
\mathcal{P}(j,k,n) &= \text{Permutations}\{\underbrace{0, \ldots, 0}_{n-k}, \underbrace{1, \ldots, 1}_{j}, \underbrace{2, \ldots, 2}_{k-j}\}
\end{aligned}
$$

Precomputation for the Neumann series

$$
\begin{aligned}
S_N^{\text{neu}}(t;\lambda,\mu) &= \sum_{n=0}^{N}\sum_{k=0}^{n}\sum_{j=0}^{k} \Gamma_{j,k,n}(t)\,\lambda^j\,\mu^{k-j} \\
&= \sum_{k=0}^{N}\sum_{j=0}^{k} \Lambda_{j,k}^{N}(t)\,\lambda^j\,\mu^{k-j}
\end{aligned}
$$

where

$$
\Lambda_{j,k}^{N}(t) = \sum_{n=k}^{N} \Gamma_{j,k,n}(t) = \sum_{n=k}^{N} \sum_{\alpha\in\mathcal{P}(j,k,n)} \mathsf{K}_{\alpha_1}\circ\cdots\circ\mathsf{K}_{\alpha_n}\circ I
$$

- Similar expansion for the exponent in the Magnus series
- *But:* Cannot precompute exponentiation
- Other possible splittings?

$\rightarrow$ *Per Christian Moan* 1998

11 Toy problem: a modified Airy equation

$$y''(t) + (1+\lambda)(t^2 + \lambda)\, y(t) = 0$$

or

$$Y' = A_0(t) + \lambda\, A_1\, Y$$

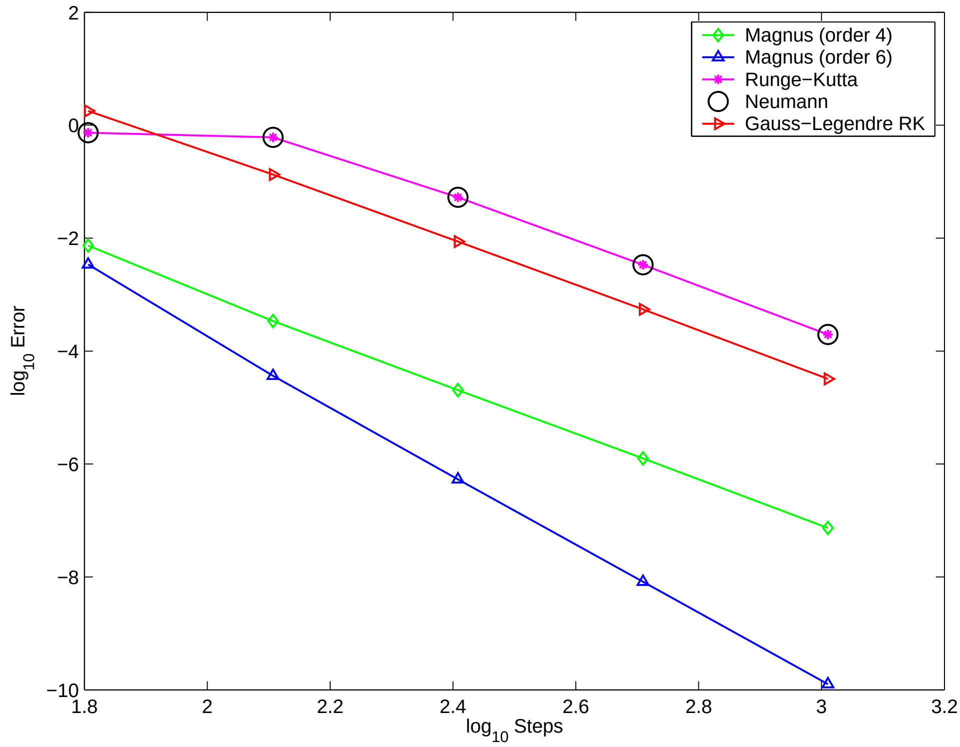
with

$$A_0(t) = \begin{pmatrix} 0 & 1 \\ -t^2 & 0 \end{pmatrix} \quad \text{and} \quad A_1(t) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

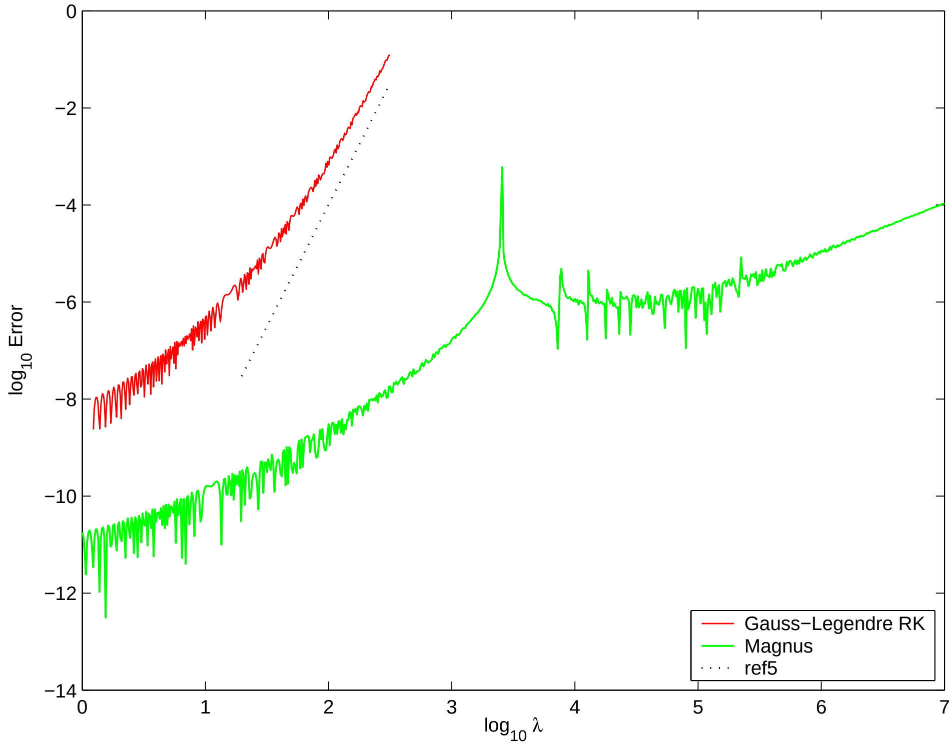
Note:

- For λ large, behaviour is dominated by constant frequency fast oscillations
- *Type A equation* according to Degani and Schiff (2003)
- Quadratic t dependence exposes generic leading order error term for moderate λ

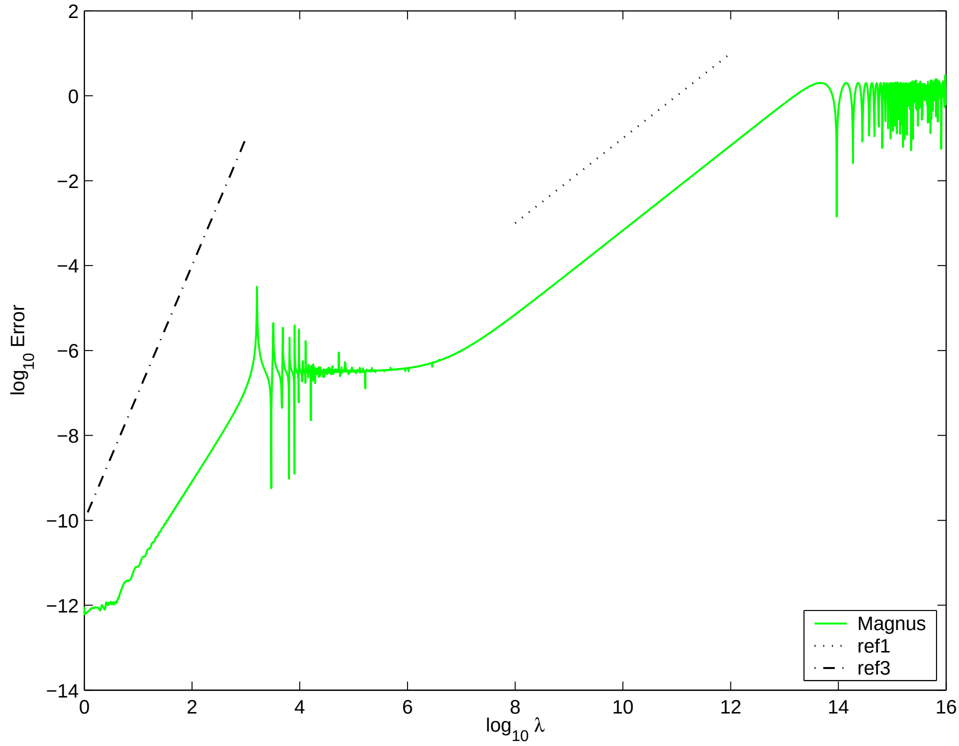
Global error for $\lambda = 1$ at $t = 10$



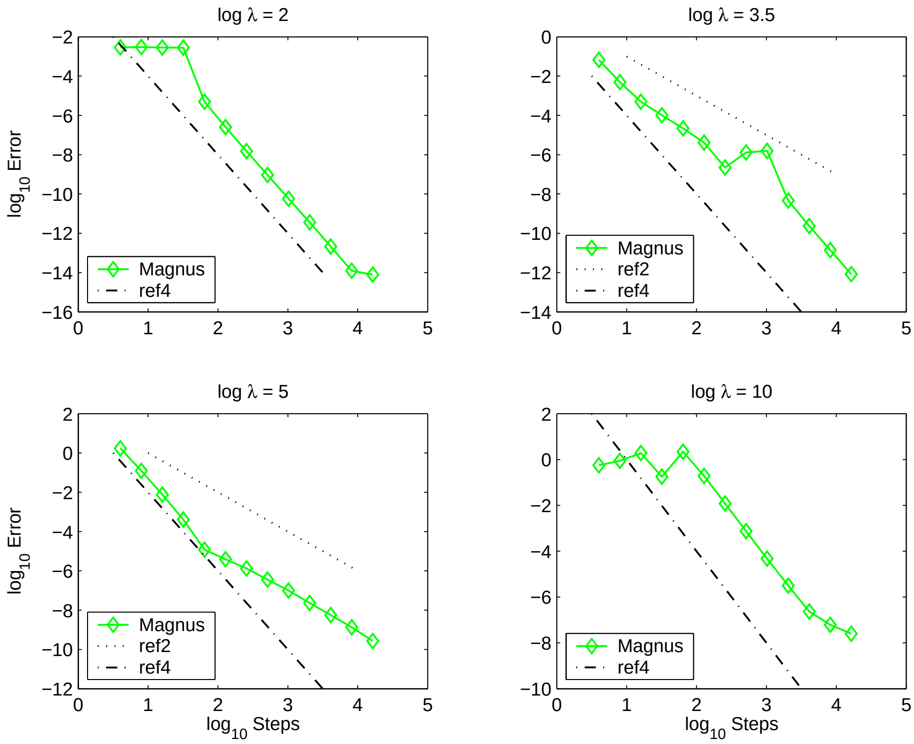
Global error as a function of λ at $t = 10$ with $N = 2^{13}$



Global error as a function of λ at $t = 1$ with $N = 512$



Order reduction when $\log\lambda \approx 5$



12 Classical order

Write

$$A(t+h) = a_0 + a_1 h + a_2 h^2 + \dots$$

where, for the modified Airy equation,

$$a_0 = \begin{pmatrix} 0 & 1+\lambda \\ -(t^2+\lambda) & 0 \end{pmatrix}, \quad a_1 = \begin{pmatrix} 0 & 0 \\ -2t & 0 \end{pmatrix}, \quad a_2 = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}$$

Leading local truncation error for forth order Magnus

$$\begin{aligned} E_2^{\text{mag}} &= \frac{h^5}{720} \left(2\,[a_0,[a_0,a_2]] + 3\,[a_1,[a_1,a_0]] + [a_0,[a_0,[a_0,a_1]]]\right) + \mathcal{O}(h^6) \\ &= \frac{h^5}{720}\, 4(1+\lambda) \begin{pmatrix} 2t(1+\lambda)(t^2+\lambda) & (1+\lambda) \\ -5t^2+\lambda & -2t(1+\lambda)(t^2+\lambda) \end{pmatrix} + \mathcal{O}(h^6) \\ &= \mathcal{O}(h^5)\,\mathcal{O}(\lambda^3) \end{aligned}$$

13 WKB analysis

On the interval $[t, t+h]$, write

$$A(t+h) = C(t) + H(t,h)$$

where $H(t,h) = \mathcal{O}(h)$. Assume that

$$C = XDX^{-1}$$

with X an unitary matrix, i.e. $X^{-1} = X^*$. Factor the flow map

$$S(h) = X\,\mathrm{e}^{Dh}\,\tilde{S}(h)$$

so that

$$\tilde{S}'(h) = \tilde{A}(t,h)\,\tilde{S}(h)$$
$$\tilde{S}(0) = X^{-1}$$

with

$$\tilde{A}(t,h) = \mathrm{e}^{-Dh}\,X^{-1}\,H\,X\,\mathrm{e}^{Dh}$$

14 Modified Magnus – RCMS

The rescaled equation can be used as a basis for a numerical method, usually in the form

$$\hat{S}'(h) = \mathrm{e}^{-Ch}\, H\, \mathrm{e}^{Ch}\, \hat{S}(h)$$

This equation can be solved by Magnus expansion

- "Modified Magnus method" (Iserles, 2002)
- "Right correction Magnus series" (Degani and Schiff, 2003)
- or by Neumann expansion (Iserles, 2004)

This approach is not taken here.

- Interferes with precomputation
- Implementation issues
- Superior behaviour only for very large λ

15 Asymptotic solution for modified Airy

For the modified Airy equation,

$$(1)\qquad \begin{aligned}\tilde{A}(t,h) &= \exp(-Dh)\, X^{-1}\, \hat{a}(t,h)\, X\, \exp(Dh)\\ &= \tfrac{1}{2}\mathrm{i}(2th+h^2)\begin{pmatrix} 1 & \mathrm{e}^{-2\mathrm{i}\mu h} \\ -\mathrm{e}^{2\mathrm{i}\mu h} & -1 \end{pmatrix} + \mathcal{O}\left(\frac{h}{\lambda}\right).\end{aligned}$$

and therefore, the first term of the Magnus expansion is

$$\tilde{s}_1 = \int_0^h \tilde{A}(t,h_1)\,\mathrm{d}h_1 = \tfrac{1}{2}\,\mathrm{i}\left(th^2+\frac{h^3}{3}\right)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \mathcal{O}\left(\frac{h}{\lambda}\right)$$

and therefore

$$S(h) = \exp(Ch)\,\exp\left(\tfrac{1}{2}\left(th^2+\frac{h^3}{3}\right)\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + \mathcal{O}\left(\frac{h}{\lambda}\right)\right)$$

16 Local error indicators for Magnus-4

Recall that

$$S^{\mathrm{mag}}(h) = \mathrm{e}^{s_1+s_2}$$

where

$$s_1 = \int_0^h \big(C + H(h_1)\big)\,\mathrm{d}h_1 = Ch + \mathcal{O}(h^2)$$

$$s_2 = \int_0^h \int_0^{h_1} [C + H(h_1), C + H(h_2)]\,\mathrm{d}h_2\,\mathrm{d}h_1 = \mathcal{O}(h^3\lambda)$$

The exponent is diagonalized by $s_1 + s_2 = X^{\mathrm{mag}} D^{\mathrm{mag}} (X^{\mathrm{mag}})^{-1}$ where

$$D^{\mathrm{mag}} = Dh + \tilde{s}_1 - \frac{\mathrm{i}\lambda t^2 h^5}{72}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} + \text{h.o.t.}$$

$$X^{\mathrm{mag}} = X - \frac{th^2}{6\sqrt{2}}\begin{pmatrix}0 & 0\\ 1 & 1\end{pmatrix} + \text{h.o.t.}$$

17 Local error indicators II

Altogether, we find that

$$S^{\mathrm{mag}}(h) = X \exp\left(D^{\mathrm{mag}}\right) X^{-1} + \frac{th^2}{6} \sin(\mu^{\mathrm{mag}}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \text{h.o.t}$$

The local error $S(h) - S^{\mathrm{mag}}(h)$ has leading order contributions

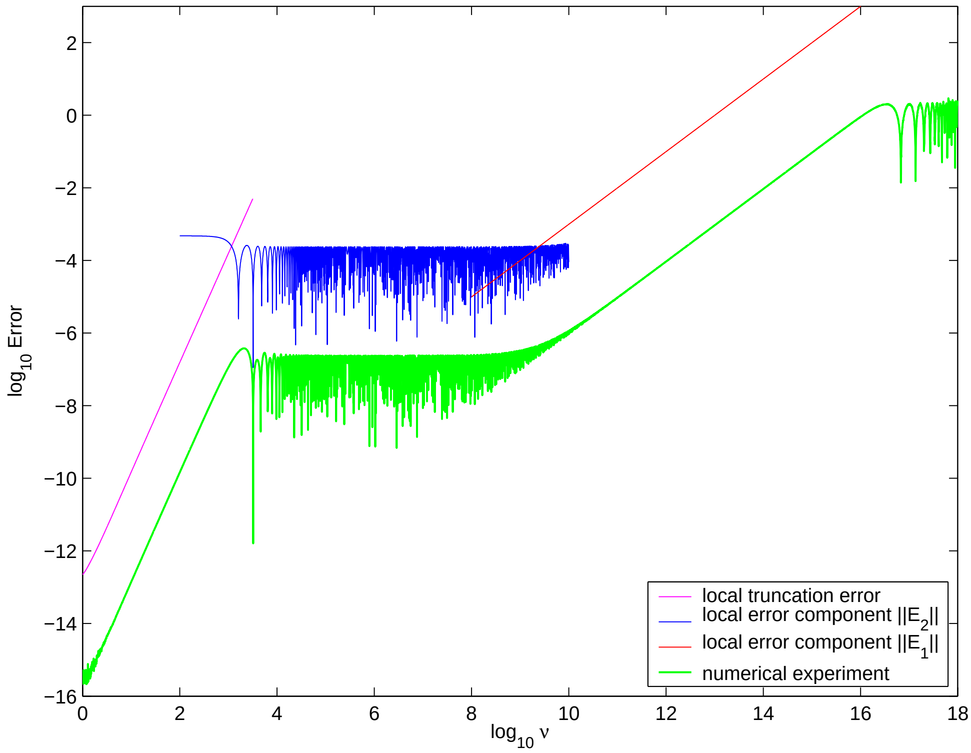
$$E_1^{\mathrm{loc}} \equiv -\frac{\lambda t^2 h^5}{72} \begin{pmatrix} \sin \mu^{\mathrm{mag}} & -\cos \mu^{\mathrm{mag}} \\ \cos \mu^{\mathrm{mag}} & \sin \mu^{\mathrm{mag}} \end{pmatrix}$$

$$E_2^{\mathrm{loc}} \equiv -\frac{th^2}{6} \sin(\mu^{\mathrm{mag}}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$E_3^{\mathrm{loc}} \equiv \frac{th}{\lambda} \sin(\mu^{\mathrm{mag}}) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \frac{th}{2\lambda} \begin{pmatrix} \cos(2\mu h - \mu^{\mathrm{mag}}) & \sin(2\mu h - \mu^{\mathrm{mag}}) \\ \sin(2\mu h - \mu^{\mathrm{mag}}) & -\cos(2\mu h - \mu^{\mathrm{mag}}) \end{pmatrix}$$

$$E_4^{\mathrm{loc}} \equiv \frac{\mathrm{i}t}{4\lambda^2} \begin{pmatrix} \sin(\mu^{\mathrm{mag}} - 2\mu h) - \sin \mu^{\mathrm{mag}} & \cos(\mu^{\mathrm{mag}} - 2\mu h) - \cos \mu^{\mathrm{mag}} \\ \cos(\mu^{\mathrm{mag}} - 2\mu h) - \cos \mu^{\mathrm{mag}} & -\sin(\mu^{\mathrm{mag}} - 2\mu h) + \sin \mu^{\mathrm{mag}} \end{pmatrix}$$

Local error indicators for the modified Airy equation



18 Global error indicators for Magnus-4

$$
\begin{aligned}
E^{\text{global}} &= S(0,T) - S^{\text{mag}}(0,T) \\
&= \prod_{N-1}^{n=0} \left(S^{\text{mag}}(t_n, t_{n+1}) + E_n^{\text{loc}}\right) - \prod_{N-1}^{n=0} S^{\text{mag}}(t_n, t_{n+1}) \\
&= \sum_{n=0}^{N-1} S^{\text{mag}}(t_{n+1}, T)\, E_n^{\text{loc}}\, S^{\text{mag}}(0, t_n) + \mathcal{O}\left(\|E^{\text{loc}}\|^2/h\right)
\end{aligned}
$$

Notice that

$$
\begin{aligned}
S^{\text{mag}}(0,T) &= \prod_{n=N-1}^{0} X^{\text{mag}}(t_n)\, \exp\bigl(D^{\text{mag}}(t_n)\bigr)\, \left(X^{\text{mag}}(t_n)\right)^{-1} \\
&= X\, \exp\bigl(D^{\text{mag}}(0,T)\bigr)\, X^{-1} + \text{h.o.t.}
\end{aligned}
$$

therefore

$$
E^{\text{global}} \approx X \left[\sum_{n=0}^{N-1} \exp\bigl(D^{\text{mag}}(t_{n+1},T)\bigr)\, X^{-1} E_n^{\text{loc}}\, X \exp\bigl(D^{\text{mag}}(0,t_n)\bigr)\right] X^{-1}
$$

19 Global error indicators II

For example, the local error term E_2^{loc} contributes globally

$$E^{\text{global}} = \frac{h^2}{6} X \left[\sum_{n=0}^{N-1} t_n \sin\big(\mu^{\text{mag}}(t_n)\big) \begin{pmatrix} 0 & \exp(\mathrm{i}\sigma_n) \\ \exp(-\mathrm{i}\sigma_n) & 0 \end{pmatrix} \right] X^{-1} + \text{h.o.t.}$$

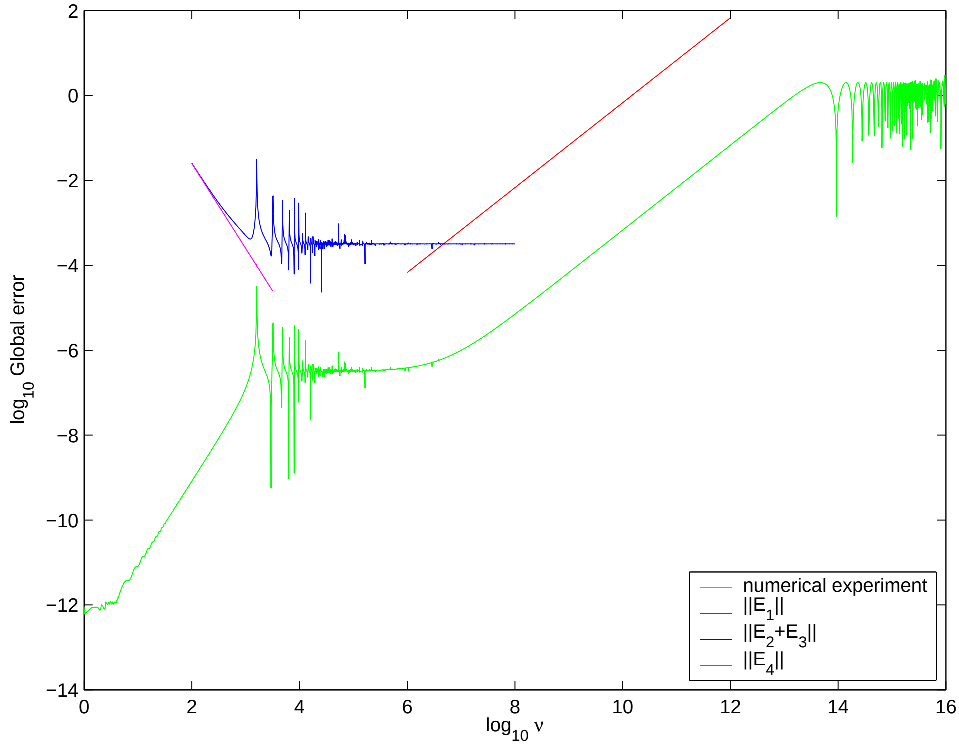
where

$$\sigma_n = 2t_n\lambda - (T+h)\lambda + f(t_n) + \mathcal{O}(h)$$

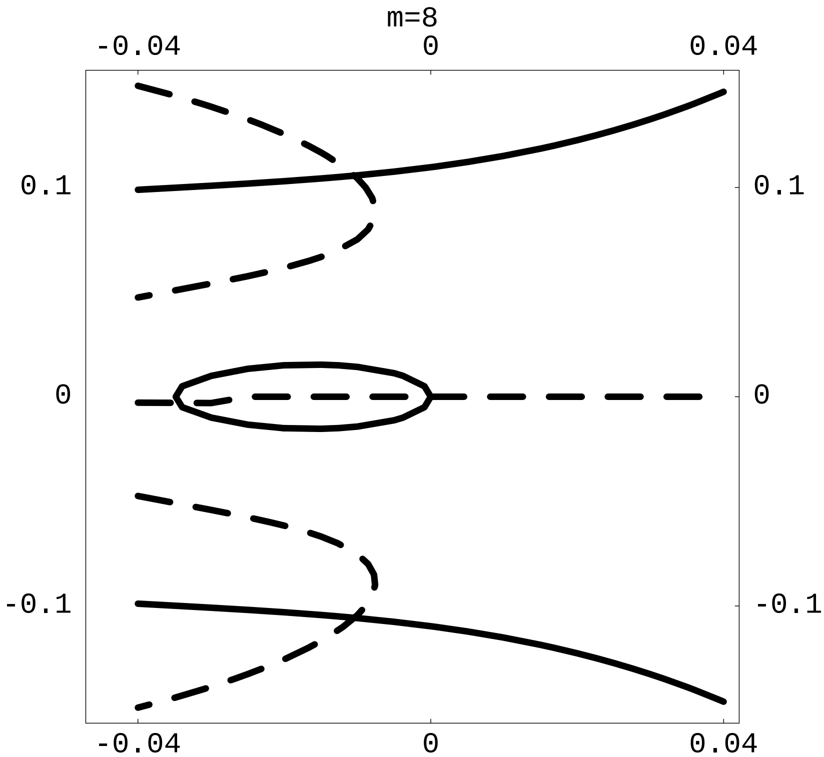
To the same order of approximation, this corresponds to an oscillatory integral of the type

$$h \ \text{bdd}(h,\lambda) \int_0^T g(t)\, \mathrm{e}^{-2\,\mathrm{i}\lambda t}\, \mathrm{d}t = \mathcal{O}\left(\frac{h}{\lambda}\right)$$

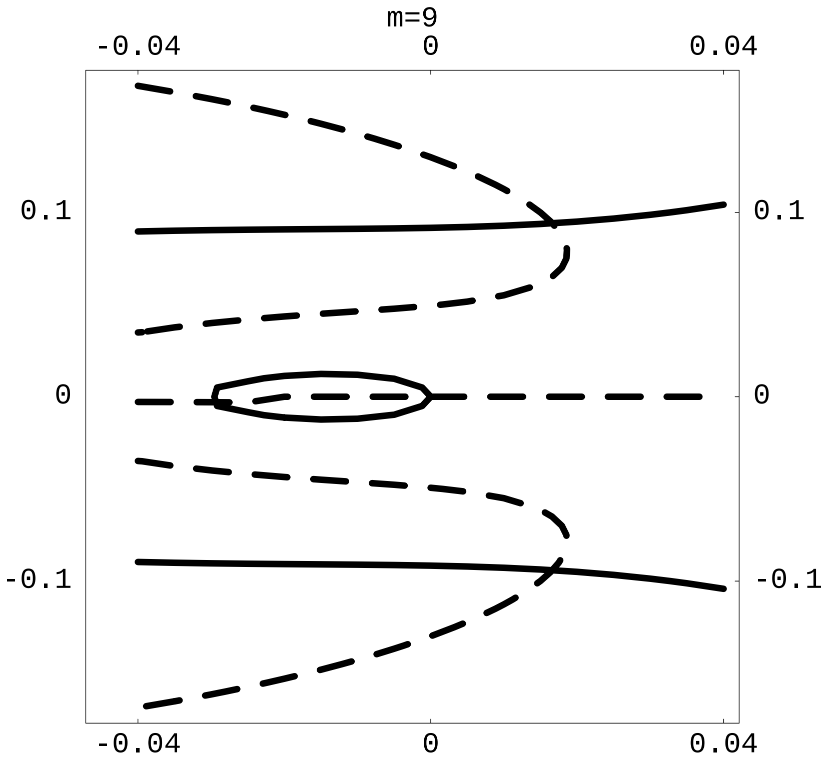
Global error indicators for the modified Airy equation



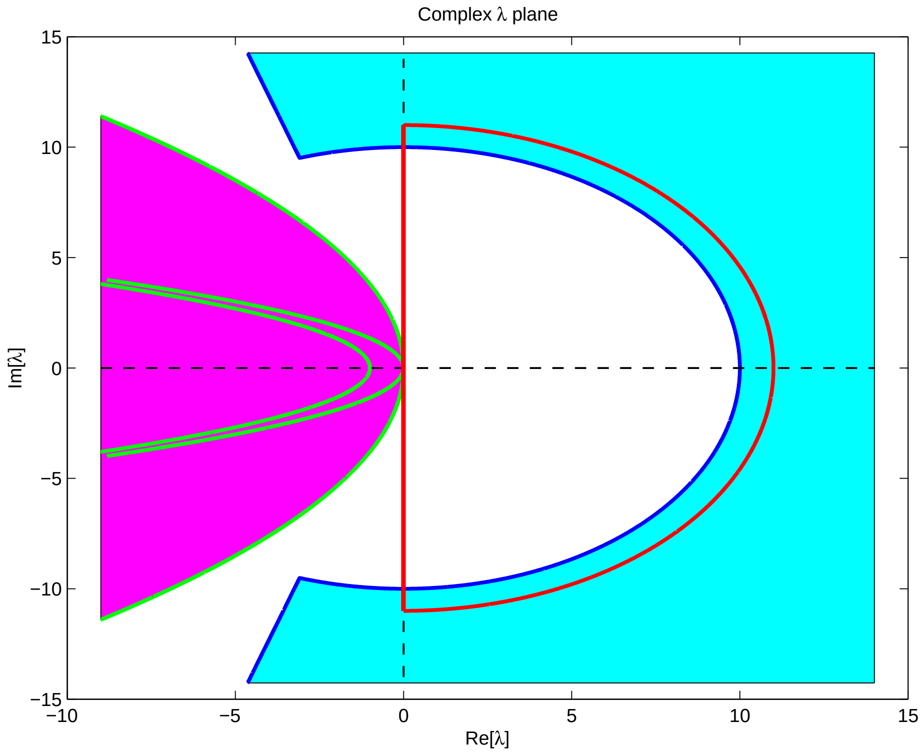
Real problem: stability of travelling wave



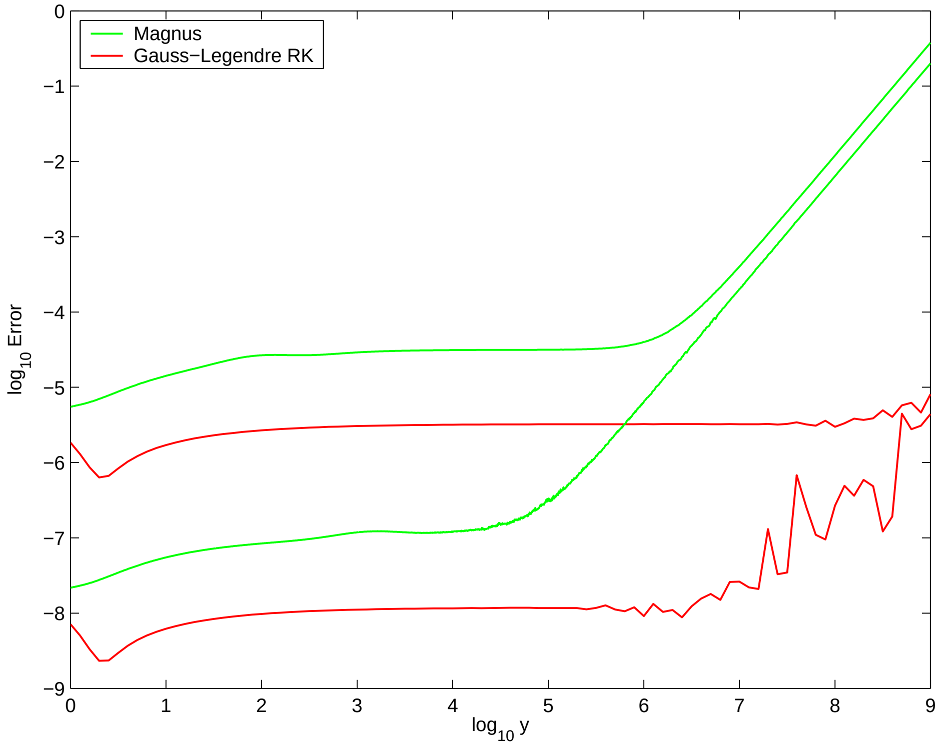
Real problem: stability of travelling wave



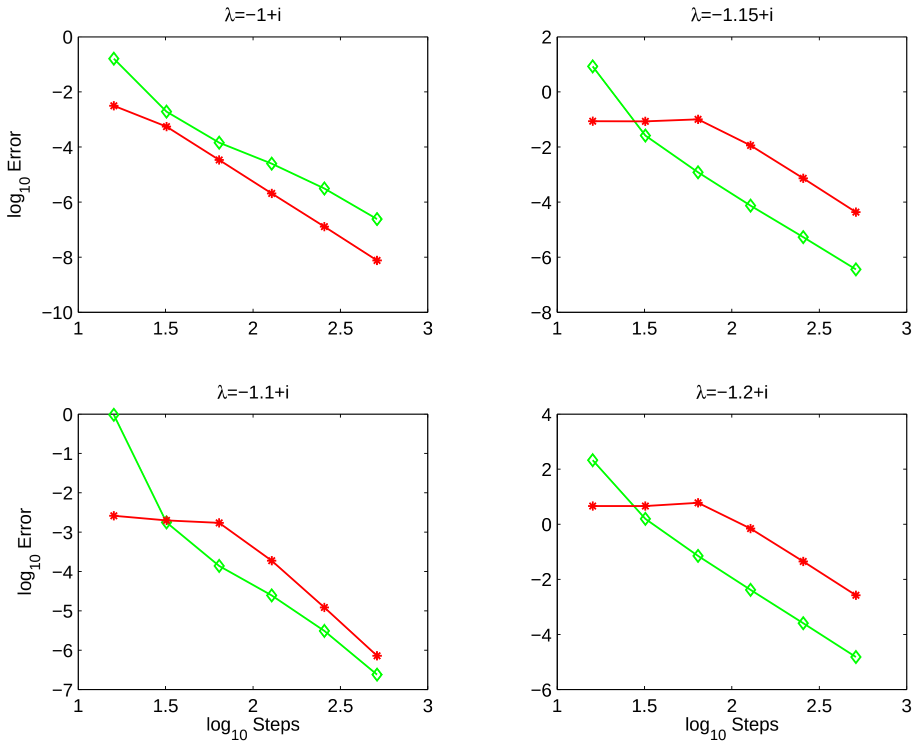
Spectrum of the linearized travelling wave operator



Error behaviour in the stiff regime ($N = 128, 512$)



Error behaviour in the oscillatory regime



20 Performance comparison

Near the ground state

- Magnus works well
- Implicit/Explicit Runge–Kutta perform better

In the stiff regime ($\lambda = \mathrm{i}y$ for y large)

- Magnus works well in the interesting regime
- Implicit RK performs better
- Explicit RK cannot be used

In the oscillatory regime (near the essential spectrum)

- Magnus is the best
- Explicit RK clearly worse than implicit RK

21 Conclusions

Magnus integrators offer

- Unconditional stability
- Superior performance in highly oscillatory regimes
- Possibility of *a priori* stepsize control

Would I recommend Magnus?

- If higher bound states exist or are suspected
- If implementation time does not matter (e.g. for library codes)
- Generally, if good splitting methods can be found ($\rightarrow$ Jitse Niesen)
- Discontinuous potentials?