

Numerical evaluation of the Evans function by Magnus integration

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Nairo Aparicio, Simon Malham & Marcel Oliver

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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Referee

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

$$\begin{aligned} \dot{Y} &= A(t, \lambda) Y, \quad Y(0) = Y_0 \\ A(t, \lambda) &= A_0(t) + \sum_{k=1}^p \lambda_k A_k(t) \end{aligned}$$

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

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

Travelling wave in moving frame

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

3 Stability of travelling waves

Perturbation ansatz:

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

Plugging this into the reaction-diffusion system

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

yields

$$\lambda \hat{U} = [B\partial_{\xi\xi} + cI\partial_\xi + DF(U_c(\xi))] \hat{U}$$

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

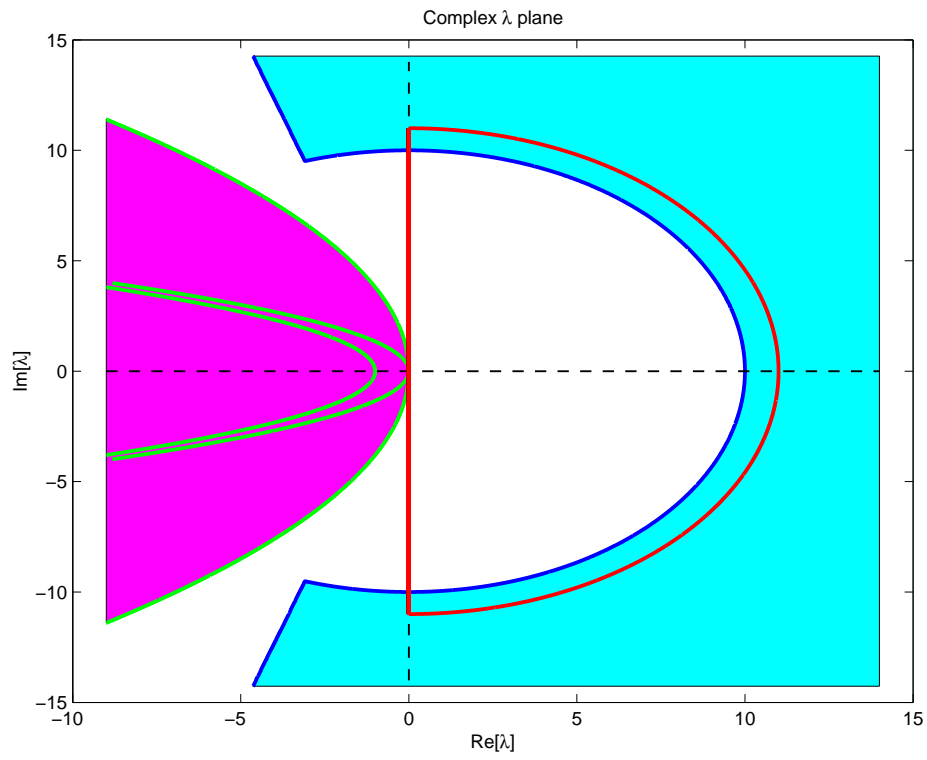
Reformulation

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

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

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

Spectrum of the linearized travelling wave operator



4 The Evans function

Limiting systems

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

- 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

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

(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

→ *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

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

can be written in integral form as

$$(I - K) \circ S \equiv S(t) - \int_0^t A(\tau) S(\tau) d\tau = I$$

Neumann series solution

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

Convergence criterion:

$$\int_0^t \|A(\tau)\| d\tau < \infty$$

→ *Peano-Baker series, Chen-Fleiss series, Feynman-Dyson path-ordered exponential*

8 Magnus series

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

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

where

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

→ *Arieh Iserles, Syvert Norsett, Antonella Zanna, Hans Munthe-Kaas, Brynjulf Owren, Per Christian Moan, Sergio Blanes, Fernando Casas, Matthias Kowski*

9 Convergence of the Magnus series

The Magnus expansion converges in the Euclidean 2-norm provided

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

where

$$r_0 = \int_0^{2\pi} \left(2 + \frac{1}{2}\tau(1 - \cot(\frac{1}{2}\tau))\right)^{-1} \, d\tau = 2.173737\dots$$

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

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

(Moan, 2002).

Rough estimate

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

guarantees convergence.

10 Precomputation

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

where

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

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

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

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

→ *Per Christian Moan 1998*

11 Toy problem: a modified Airy equation

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

or

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

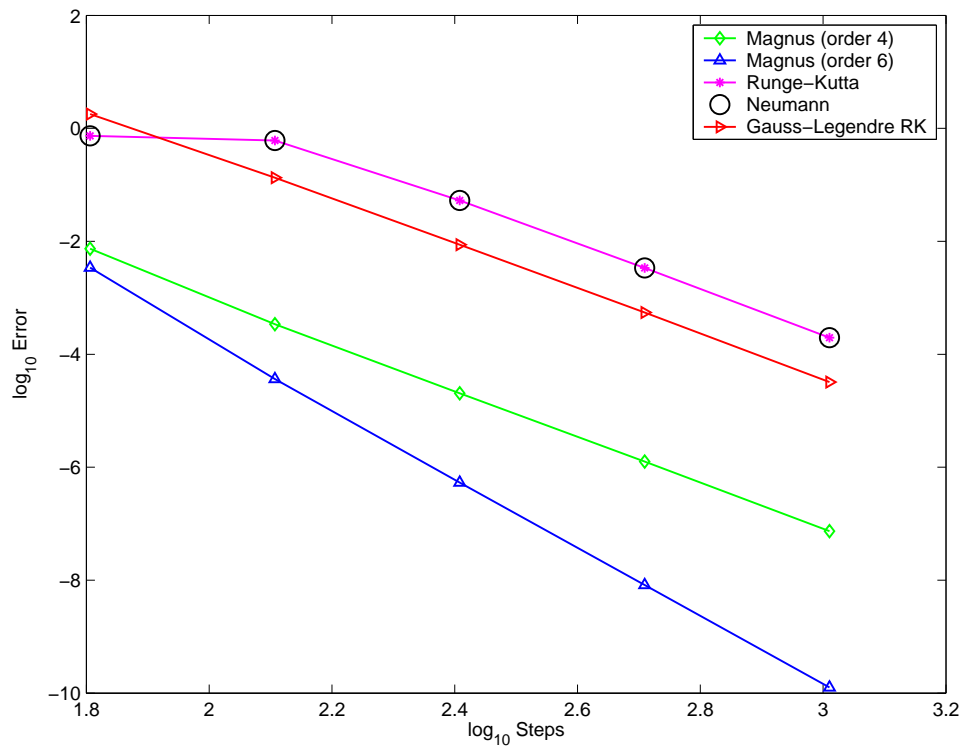
with

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

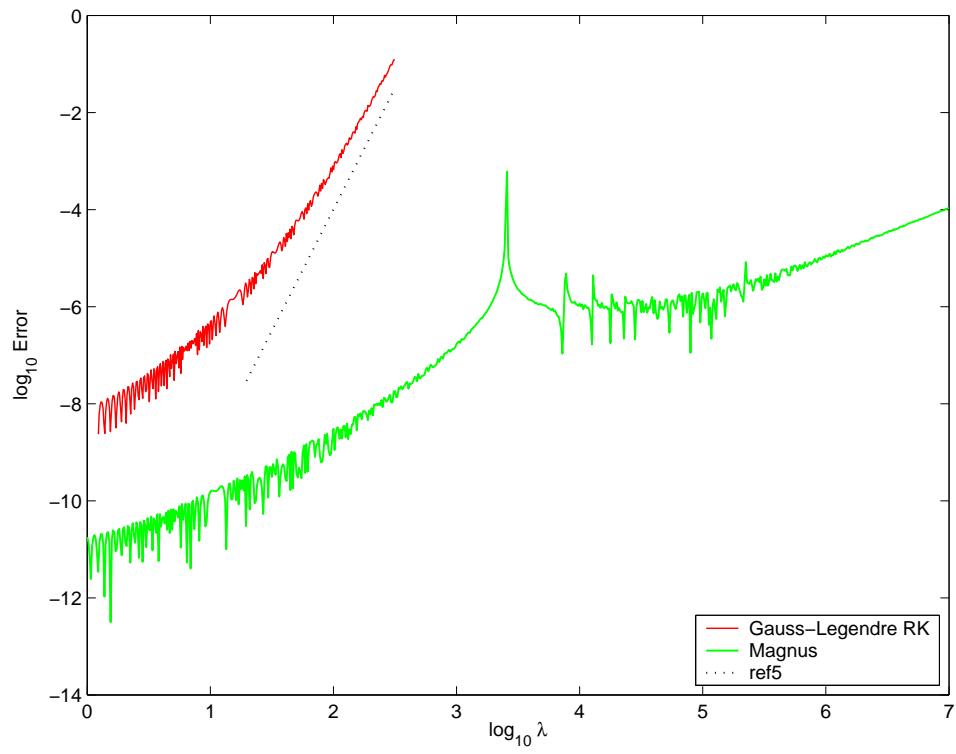
Note:

- 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

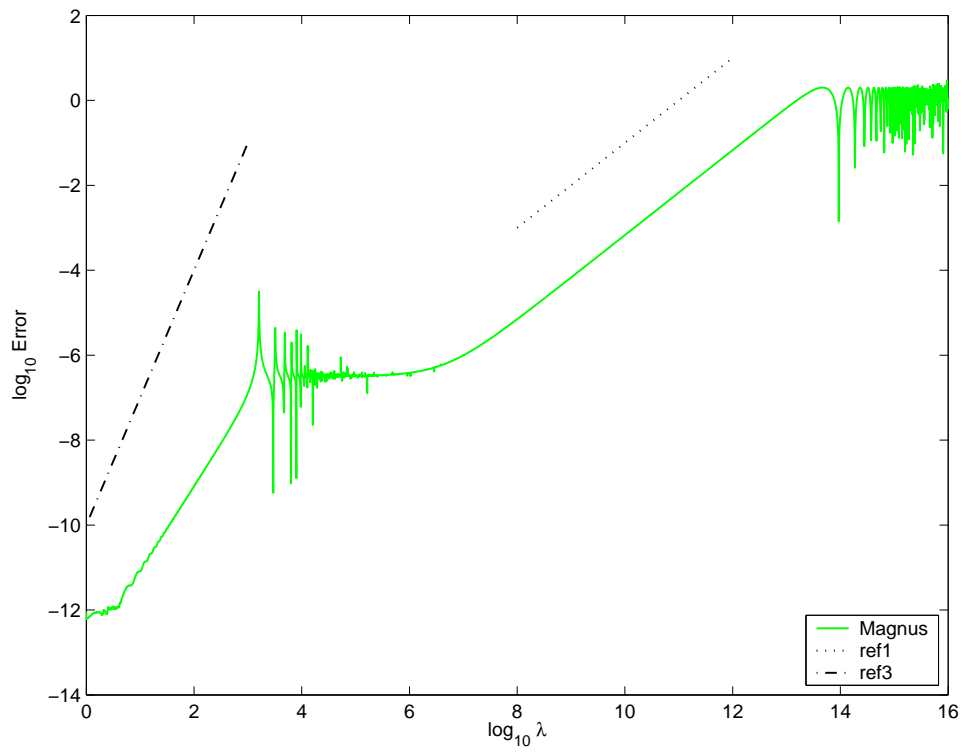
Global error for $\lambda = 1$ at $t = 10$



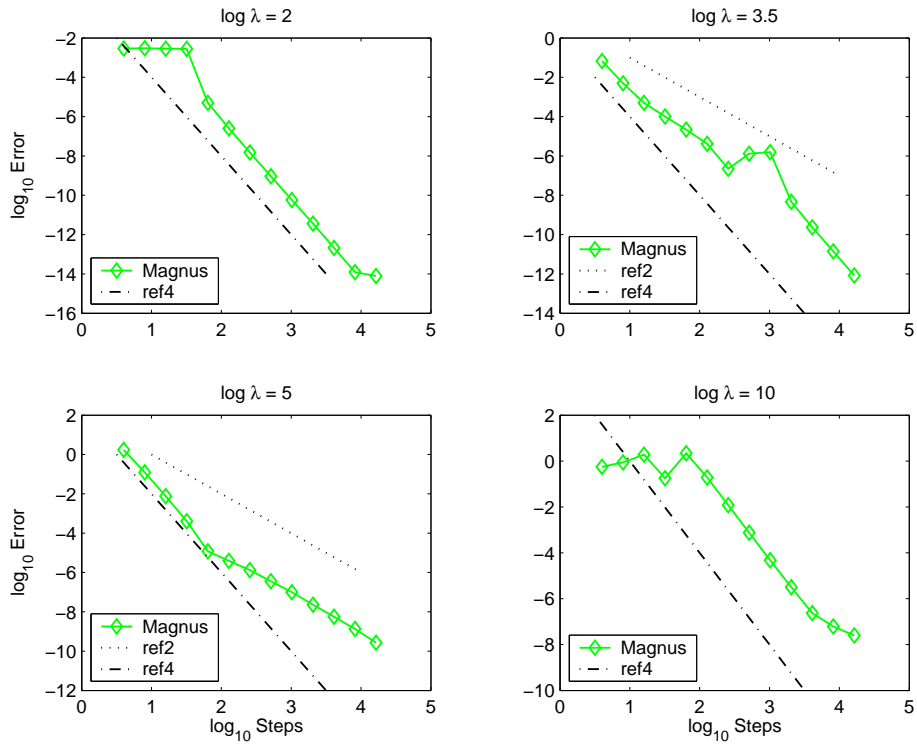
Global error as a function of λ at $t = 10$ with $N = 2^{13}$



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 fourth order Magnus

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

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

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

so that

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

with

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

14 Modified Magnus – RCMS

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

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

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,

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

and therefore, the first term of the Magnus expansion is

$$\tilde{s}_1 = \int_0^h \tilde{A}(t, h_1) dh_1 = \frac{1}{2}i \left(th^2 + \frac{h^3}{3} \right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \mathcal{O}\left(\frac{h}{\lambda}\right)$$

and therefore

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

16 Local error indicators for Magnus-4

Recall that

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

where

$$\begin{aligned} s_1 &= \int_0^h (C + H(h_1)) dh_1 = Ch + \mathcal{O}(h^2) \\ s_2 &= \int_0^h \int_0^{h_1} [C + H(h_1), C + H(h_2)] dh_2 dh_1 = \mathcal{O}(h^3\lambda) \end{aligned}$$

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

$$\begin{aligned} D^{\text{mag}} &= Dh + \tilde{s}_1 - \frac{i\lambda t^2 h^5}{72} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \text{h.o.t.} \\ X^{\text{mag}} &= X - \frac{th^2}{6\sqrt{2}} \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix} + \text{h.o.t.} \end{aligned}$$

17 Local error indicators II

Altogether, we find that

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

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

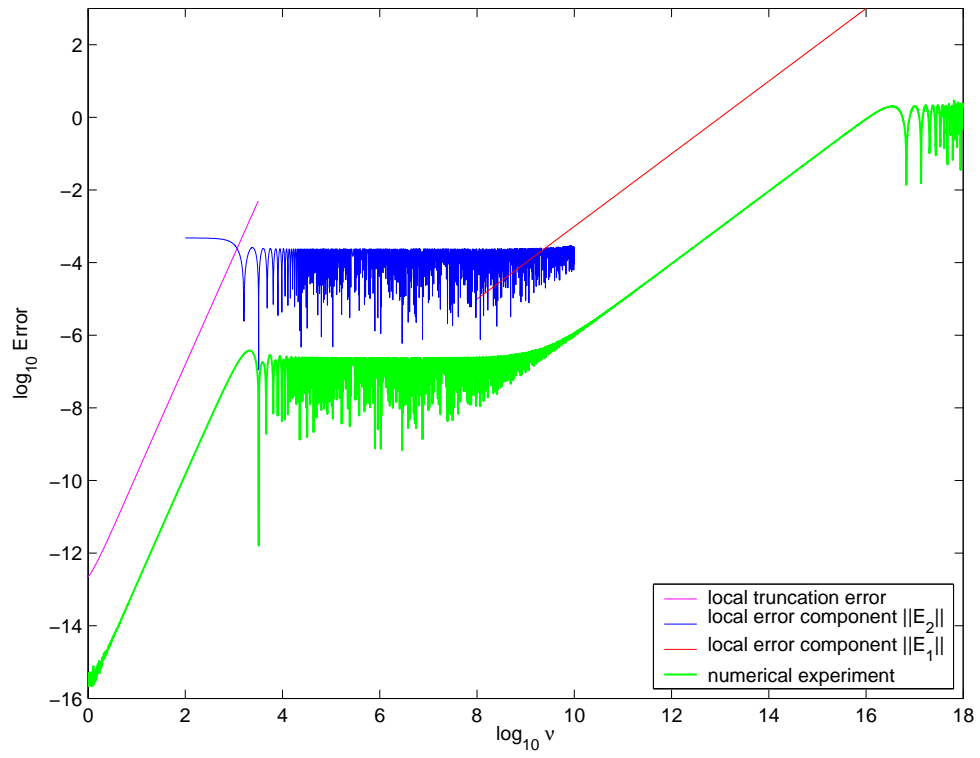
$$E_1^{\text{loc}} \equiv -\frac{\lambda t^2 h^5}{72} \begin{pmatrix} \sin \mu^{\text{mag}} & -\cos \mu^{\text{mag}} \\ \cos \mu^{\text{mag}} & \sin \mu^{\text{mag}} \end{pmatrix}$$

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

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

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

Local error indicators for the modified Airy equation



18 Global error indicators for Magnus-4

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

Notice that

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

therefore

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

19 Global error indicators II

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

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

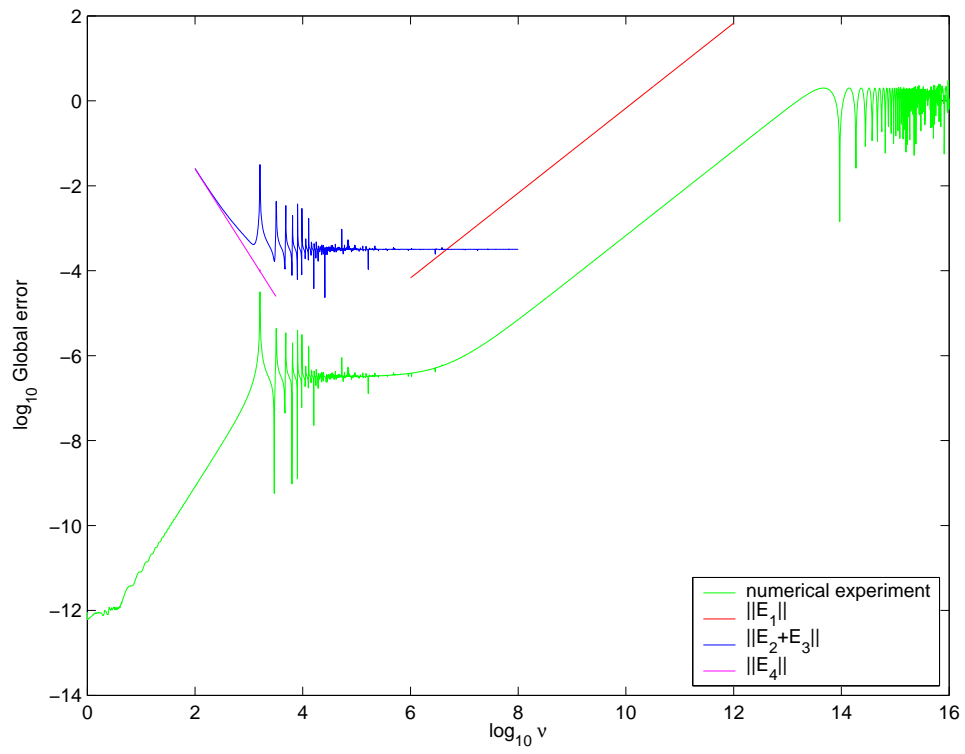
where

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

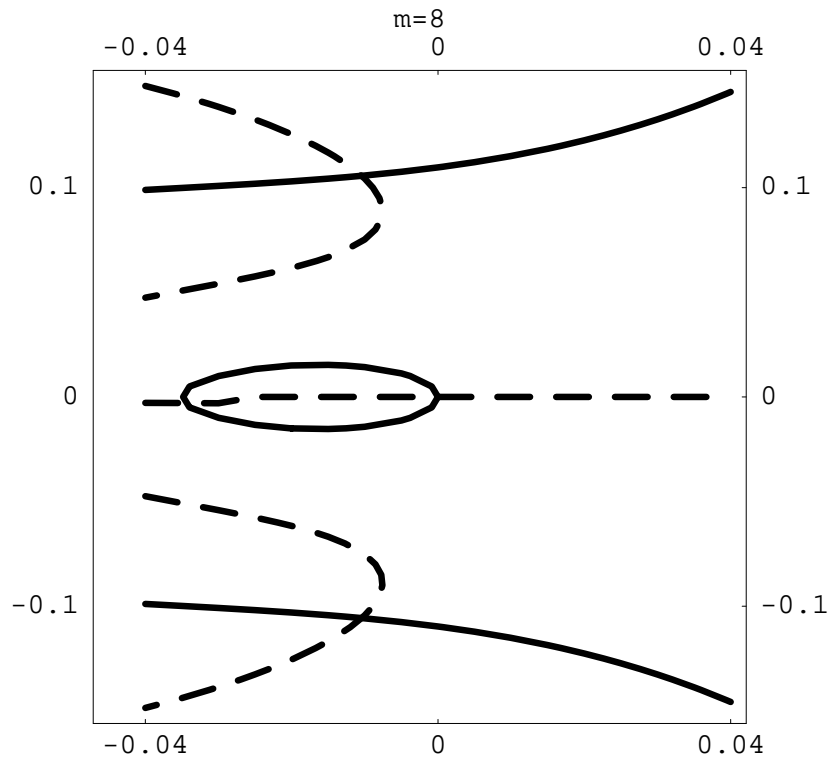
To the same order of approximation, this corresponds to an oscillatory integral of the type

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

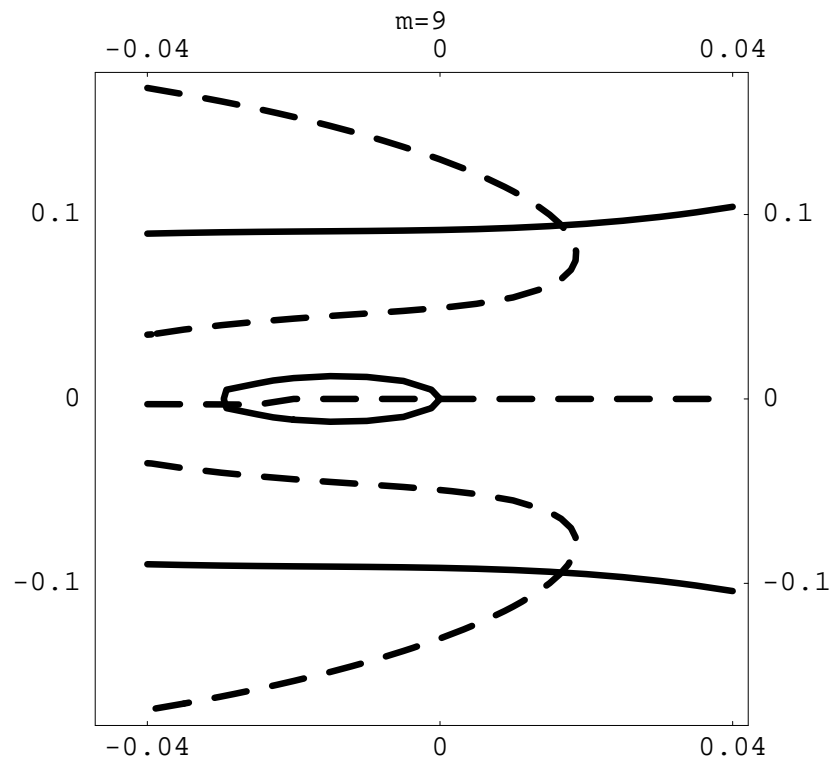
Global error indicators for the modified Airy equation



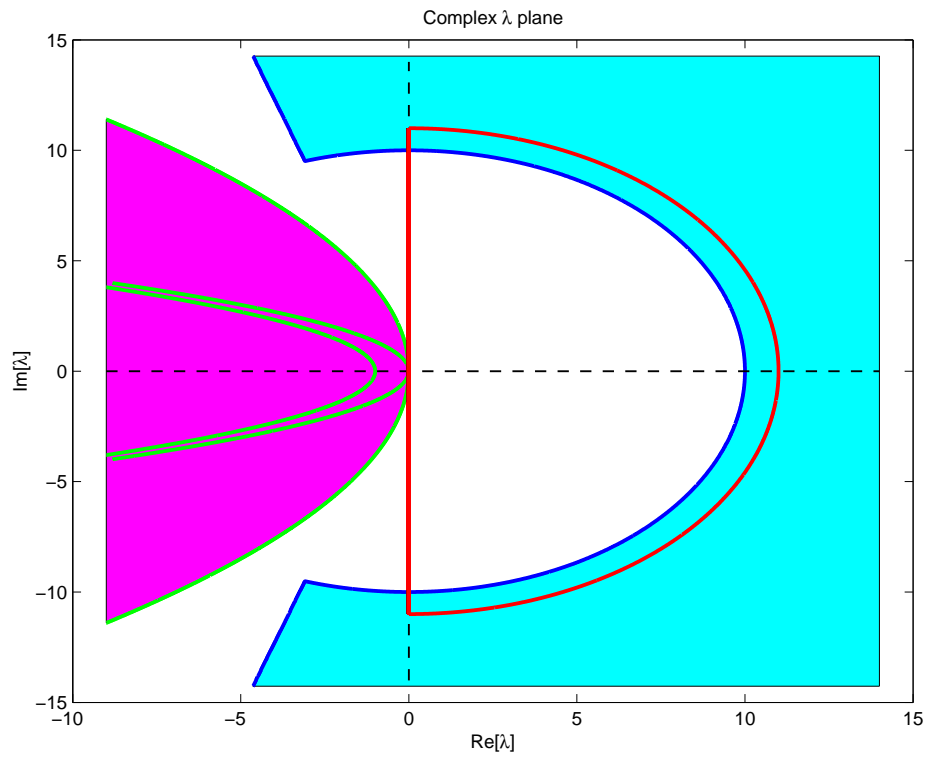
Real problem: stability of travelling wave



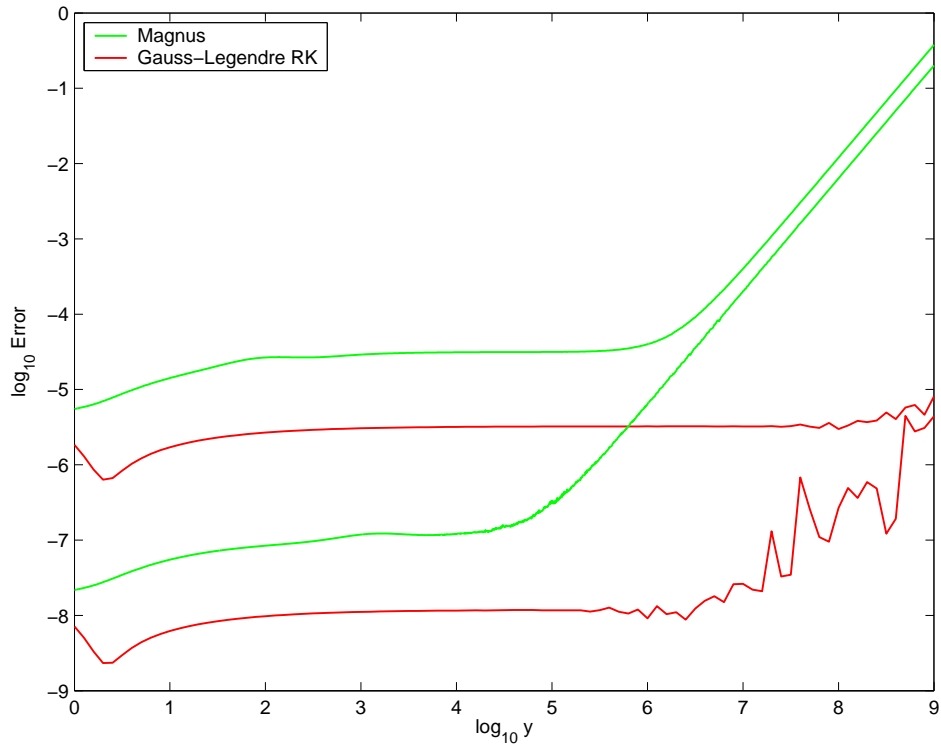
Real problem: stability of travelling wave



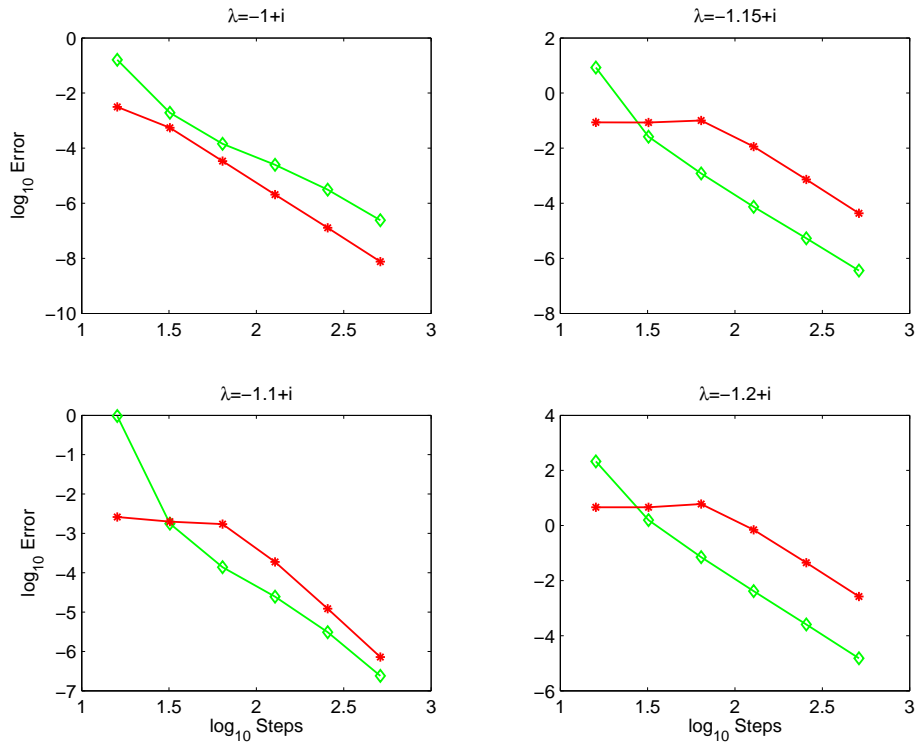
Spectrum of the linearized travelling wave operator



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 ($\lambda = iy$ 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 (→ Jitse Niesen)
- Discontinuous potentials?