The effect of exponential fitting on the stability of numerical methods for solving first order IVPs

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Outline

Exponential fitting

Aim : To build numerical methods which perform very good when the solution has a known exponential of trigonometric behaviour.

How : start from linear functional(s) and impose that for some linear function space $\mathcal{S}$ the method produces exact results.

example : $\mathcal{S} = \langle \cos \omega x, \sin \omega x, 1, x, x^2, \ldots, x^{n-2} \rangle$

The parameter ω, which is either real (trigonometric case) or purely imaginary (exponential case), needs to be determined!

A model problem

Consider the initial value problem

$$y'' + \omega^2 y = g(y) \qquad y(a) = y_a \qquad y(a) = y'_a \, .$$

If $|g(y)| \ll |\omega^2 y|$ then

$$y(x) \approx \alpha \cos(\omega x + \phi)$$

To mimic this oscillatory behaviour, we construct methods which yield exact results when the solution is of trigonometric (in the complex case : exponential) type.

These methods are called Exponentially-fitted methods.

Example : Numerov method

$$y'' = f(y) \qquad y(a) = y_a \qquad y(b) = y_b$$

classical Numerov method :

$$y_{n+1} - 2\,y_n + y_{n-1} = \frac{1}{12}\,h^2\,\left(f(y_{n+1}) + 10\,f(y_n) + f(y_{n-1})\right)$$

$$n = 1,\,2,\,\ldots,\,N \qquad h = \frac{b-a}{N+1}$$

Construction :

impose $\mathcal{L}[z(x);h] = 0$ for $z(x) \in \mathcal{S} = \langle 1,\,x,\,x^2,\,x^3,\,x^4\rangle$ where

$$\begin{aligned}\mathcal{L}[z(x);h] := {} & z(x+h) + a_0\,z(x) + a_{-1}\,z(x-h)\\ & -h^2\left(b_1\,z''(x+h) + b_0\,z''(x) + b_{-1}\,z''(x-h)\right)\end{aligned}$$

$$\mathcal{L}[z(x);h] = -\frac{1}{240}h^6\,z^{(6)}(x) + \mathcal{O}(h^8) \qquad \Longrightarrow \text{order } 4$$

EF Numerov method

Construction : impose $\mathcal{L}[z(x);h] = 0$ for $z(x) \in \mathcal{S}$ with

$$\mathcal{S} = \langle 1, x, x^2, \sin(\omega x), \cos(\omega x) \rangle$$

$$\text{or } \mathcal{S} = \langle 1, x, x^2, \exp(\mu x), \exp(-\mu x) \rangle \qquad \mu := \mathrm{i}\,\omega$$

$$\begin{aligned}\mathcal{L}[z(x);h] := {} & z(x+h) + a_0 z(x) + a_{-1} z(x-h) \\ & - h^2 \left(b_1 z''(x+h) + b_0 z''(x) + b_{-1} z''(x-h) \right)\end{aligned}$$

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left(\lambda f(y_{n-1}) + (1 - 2\lambda) f(y_n) + \lambda f(y_{n+1}) \right)$$

$$\begin{aligned}\lambda &= \frac{1}{4\sin^2\frac{\theta}{2}} - \frac{1}{\theta^2} = \frac{1}{12} + \frac{1}{240}\theta^2 + \frac{1}{6048}\theta^4 + \dots && \theta := \omega h \\ &= -\frac{1}{4\sinh^2\frac{\nu}{2}} + \frac{1}{\nu^2} = \frac{1}{12} - \frac{1}{240}\nu^2 + \frac{1}{6048}\nu^4 + \dots && \nu := \mu h\end{aligned}$$

Choice of ω

It is very important to attribute an appropriate value to ω!

This can be done by a

- local optimization procedure based on the minimisation of the local truncation error (lte)
  ω is step-dependent

- by a global optimization procedure to preserve certain geometric properties (periodicity, energy, ...)
  ω is constant over the interval of integration

EF Numerov method

$$\mathcal{S} = \langle 1, x, x^2, \sin(\omega x), \cos(\omega x) \rangle$$

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left(\lambda f(y_{n-1}) + (1 - 2\lambda) f(y_n) + \lambda f(y_{n+1})\right)$$

$$\mathcal{L}[z(x); h] = -\frac{1}{240} h^6 \left(z^{(6)}(x) + \omega^2 z^{(4)}(x) \right) + \mathcal{O}(h^8) \qquad \Longrightarrow \text{order } 4$$

$$\text{local optimization} : y_n^{(6)} + \omega_n^2 y_n^{(4)} = 0$$

EF Numerov method

$$\mathcal{S} = \langle 1, x, x^2, \sin(\omega x), \cos(\omega x)\rangle$$

$$y_{n+1} - 2y_n + y_{n-1} = h^2\,(\lambda f(y_{n-1}) + (1-2\lambda) f(y_n) + \lambda f(y_{n+1}))$$

$$\text{local optimization} : y_n^{(6)} + \omega_n^2 y_n^{(4)} = 0$$

- if $\omega_n^2 > 0$ we locally fit to $\langle 1, x, x^2\rangle$ and

  $$\langle \sin(\omega_n x), \cos(\omega_n x)\rangle = \langle \exp(i\,\omega_n x), \exp(-i\,\omega_n x)\rangle$$

- if $\omega_n^2 = -\nu_n^2 < 0$ we locally fit to $\langle 1, x, x^2\rangle$ and

  $$\langle \sinh(\nu_n x), \cosh(\nu_n x)\rangle = \langle \exp(\nu_n x), \exp(-\nu_n x)\rangle$$

- if $\omega_n^2 = 0$ we locally fit to $\langle 1, x, x^2, x^3, x^4\rangle$

EF methods

In the past decades, various research groups have constructed modified versions of well-known methods

- for first-order problems $y' = f(t, y)$
  - linear multistep methods (e.g. Adams-type, ...)
  - Runge-Kutta methods (e.g. collocation-type, ...)
  - ...
- for second-order problems $y'' = f(t, y)$
  - linear multistep methods (e.g. Störmer-Cowell type, ...)
  - Runge-Kutta-Nystrom methods
  - ...

EF Runge-Kutta methods of collocation type (Gauss, LobattoIIIA, ...)

$$\begin{cases} \mathcal{L}_i[y(x);h] = y(x+c_i h) - y(x) - h\displaystyle\sum_{j=1}^{s} a_{ij}\, y'(x+c_j h) \\ \qquad\qquad\qquad i = 1,\dots,s \\ \mathcal{L}[y(x);h] = y(x+h) - y(x) - h\displaystyle\sum_{i=1}^{s} b_i\, y'(x+c_i h)\,. \end{cases}$$

A fitting space $\mathcal{S}$ is introduced such that $\forall u \in \mathcal{S}$

$$\begin{cases} \mathcal{L}_i[u(x);h] = 0 \qquad i = 1,\dots,s \\ \mathcal{L}[u(x);h] = 0 \end{cases}$$

Trapezoidal rule

$$\mathcal{S} = \langle 1, x, x^2 \rangle$$

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

$$y_{n+1} - y_n = \frac{h}{2} \left(f(x_n,\, y_n) + f(x_{n+1},\, y_{n+1}) \right)$$

$$\mathrm{lte}_{TR} = -\frac{h^3}{12} y^{(3)}(x_n) + \mathcal{O}(h^4)$$

Exponentially-fitted trapezoidal rule fitted to $\mathcal{S} = \langle 1, \sin(\omega x), \cos(\omega x) \rangle$

$$
\begin{array}{c|cc}
0 & 0 & 0 \\
1 & \frac{\tan(\omega h/2)}{\omega h} & \frac{\tan(\omega h/2)}{\omega h} \\
\hline
 & \frac{\tan(\omega h/2)}{\omega h} & \frac{\tan(\omega h/2)}{\omega h}
\end{array}
$$

$$
y_{n+1} - y_n = \frac{\tan(\omega h/2)}{\omega h} h \left(f(x_n, y_n) + f(x_{n+1}, y_{n+1}) \right)
$$

$$
\mathrm{lte}_{EFTR} = -\frac{h^3}{12} \left(y^{(3)}(x_n) + \omega^2 y'(x_n) \right) + \mathcal{O}(h^4)
$$

Explicit EF Runge-Kutta methods

$$
\begin{cases}
\mathcal{L}_i[y(x);h] = y(x+c_i\,h) - \gamma_i\,y(x) - h\displaystyle\sum_{j=1}^{i-1} a_{ij}\,y'(x+c_j\,h) \\
\qquad\qquad i = 1,\ldots,s \\
\mathcal{L}[y(x);h] = y(x+h) - \gamma\,y(x) - h\displaystyle\sum_{i=1}^{s} b_i\,y'(x+c_i\,h)\,.
\end{cases}
$$

For each stage and for the outer stage, fitting spaces $\mathcal{S}_i$ and $\mathcal{S}$ are introduced such that

$$
\begin{cases}
\mathcal{L}_i[u(x);h] = 0 \quad \forall u \in \mathcal{S}_i \qquad i = 1,\ldots,s \\
\mathcal{L}[u(x);h] = 0 \quad \forall u \in \mathcal{S}
\end{cases}
$$

Explicit Euler method

$$\mathcal{S} = \langle 1, x \rangle$$

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$

$$y_{n+1} = y_n + h\, f(x_n,\, y_n)$$

$$\text{lte}_{Euler} = -\frac{h^2}{2} y^{(2)}(x_n) + \mathcal{O}(h^3)$$

Explicit Euler method fitted to $\mathcal{S} = \langle \sin(\omega x), \cos(\omega x) \rangle$

$$\begin{array}{c|c|c} 0 & 0 & 0 \\ \hline & \cos(\omega h) & \frac{\sin(\omega h)}{\omega h} \end{array}$$

$$y_{n+1} = \cos(\omega h)\, y_n + h\, \frac{\sin(\omega h)}{\omega h}\, f(x_n, y_n)$$

$$\mathrm{lte}_{Euler,EF} = -\frac{h^2}{2}(y^{(2)}(x_n) + \omega^2 y(x_n)) + \mathcal{O}(h^3)$$

An explicit 2-stage RK method

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array}$$

- the second stage is fitted to $\langle 1, x \rangle$
- the outer stage is fitted to $\langle 1, x, x^2 \rangle$.

An EF explicit 2-stage RK method

$$
\begin{array}{c|c|cc}
0 & 0 & 0 & 0 \\
1/2 & \cos(\omega h/2) & \frac{\sin(\omega h/2)}{\omega h} & 0 \\
\hline
 & 1 & 0 & \frac{\sin(\omega h/2)}{\omega h/2}
\end{array}
$$

- the second stage is fitted to $\langle \cos(\omega x), \sin(\omega x) \rangle$
- the outer stage is fitted to $\langle 1, \cos(\omega x), \sin(\omega x) \rangle$.

Linear stability theory

The linear stability properties for both classical methods and EF methods are studied by means of linear test equations

- for first order problems : $y' = \lambda y$, $\lambda \in \mathbb{C}^-$
  - If $\lambda \in \mathbb{C}^-$ then $y(t) \to 0$ when $t \to \infty$.
  - For which values of h does $y_n \to 0$ as $n \to \infty$?
- for second order problems : $y'' + \lambda^2 y = 0$
  - If $\lambda \in \mathbb{R}$ then $y(t)$ is periodic.
  - For which values of h is $\{y_n | n = 0, 1 \ldots\}$ periodic?

Results on linear stability for EF methods

- for second order problems :
  much papers are devoted to the construction of P-stable methods or to the construction of methods with a large interval of periodicity
- for first order problems :
  almost nothing about stability
  Maybe it is assumed that an EF method inherits the properties from the underlying classical method. However this is only true for small values of ω.
  Some examples will illustrate this

Explicit Euler method

$$\mathcal{S} = \langle 1, x \rangle$$

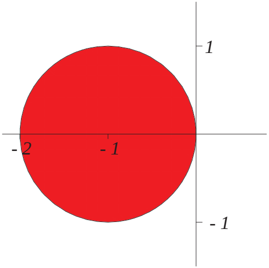
$$y_{n+1} = y_n + h\,f(x_n, y_n)$$

Applying this method to $y' = \lambda y$, $\lambda \in \mathbb{C}$ gives

$$y_{n+1} = (1 + h\,\lambda)\,y_n = R(\lambda\,h)\,y_n$$

$$R(z) = 1 + z$$

$\mathcal{R}$: region in complex z-plane for which $|R(z)| < 1$



EF explicit Euler method fitted to $\mathcal{S} = \langle \exp(\omega_1 x), \exp(\omega_2 x) \rangle$

Let ω_1 and ω_2 be both real or complex conjugate.

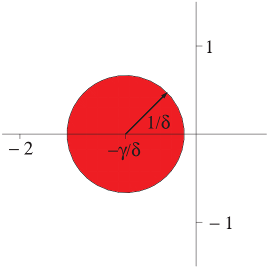
$$y_{n+1} = \gamma(\omega_1 h, \omega_2 h)\, y_n + h\, \delta(\omega_1 h, \omega_2 h)\, f(x_n, y_n)$$

Applying this method to $y' = \lambda y$ gives

$$y_{n+1} = R(\omega_1 h, \omega_2 h, \lambda h)\, y_n$$

$$R(a, b; z) = \gamma(a, b) + z\, \delta(a, b)$$

$\mathcal{R}_{(a,b)}$: region in complex z-plane for which $|R(z)| < 1$



$\mathcal{R}_{(\omega_1 h, \omega_2 h)}$

EF explicit Euler method fitted to $\mathcal{S} = \langle \sin(\omega x), \cos(\omega x) \rangle$

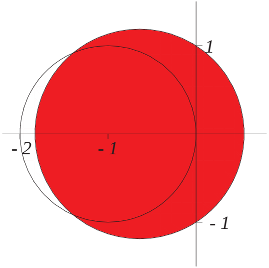
$$\omega_1 h = i\,\omega\,h = i\,\beta \qquad \omega_2 h = -i\,\omega\,h = -i\,\beta$$

$$y_{n+1} = \cos(\beta)\,y_n + h\,\frac{\sin(\beta)}{\beta}\,f(x_n, y_n)$$

Applying this method to $y' = \lambda\,y$ gives

$$y_{n+1} = R(i\,\beta, -i\,\beta; \lambda\,h)\,y_n$$

$$R(i\,\beta, -i\,\beta; z) = \cos(\beta) + z\,\frac{\sin(\beta)}{\beta}$$



$\mathcal{R}_{(i,-i)}$

EF explicit Euler method fitted to $\mathcal{S} = \langle \sin(\omega x), \cos(\omega x) \rangle$

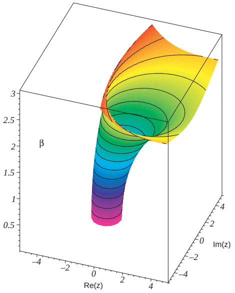
$$\omega_1 h = i\,\omega\,h = i\,\beta \qquad \omega_2 h = -i\,\omega\,h = -i\,\beta$$

$$y_{n+1} = \cos(\beta)\,y_n + h\,\frac{\sin(\beta)}{\beta}\,f(x_n, y_n)$$

Applying this method to $y' = \lambda\,y$ gives

$$y_{n+1} = R(i\,\beta, -i\,\beta; \lambda\,h)\,y_n$$

$$R(i\,\beta, -i\,\beta; z) = \cos(\beta) + z\,\frac{\sin(\beta)}{\beta}$$



$\mathcal{R}_{(i\beta, -i\beta)}$

EF explicit Euler method fitted to $\mathcal{S} = \langle \exp(\omega x), \exp(-\omega x) \rangle$

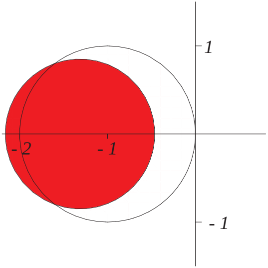
$$\omega_1 h = \omega h = a \qquad \omega_2 h = -\omega h = -a$$

$$y_{n+1} = \cosh(\omega h)\, y_n + h\, \frac{\sinh(\omega h)}{\omega h}\, f(x_n, y_n)$$

Applying this method to $y' = \lambda y$ gives

$$y_{n+1} = R(\omega h, -\omega h, \lambda h)\, y_n$$

$$R(a, -a; z) = \cosh(a) + z\, \frac{\sinh(a)}{a}$$



$\mathcal{R}_{(1,-1)}$

EF explicit Euler method fitted to $\mathcal{S} = \langle \exp(\omega x), \exp(-\omega x) \rangle$

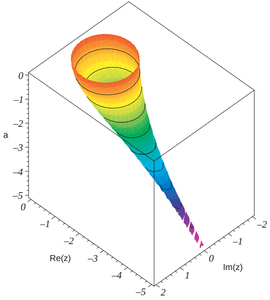
$$\omega_1 h = \omega h = a \qquad \omega_2 h = -\omega h = -a$$

$$y_{n+1} = \cosh(\omega h)\, y_n + h\, \frac{\sinh(\omega h)}{\omega h}\, f(x_n, y_n)$$

Applying this method to $y' = \lambda y$ gives

$$y_{n+1} = R(\omega h, -\omega h, \lambda h)\, y_n$$

$$R(a, -a; z) = \cosh(a) + z\, \frac{\sinh(a)}{a}$$



$\mathcal{R}_{(a,-a)}$

EF explicit Euler method fitted to $\mathcal{S} = \langle \exp(\omega x), \exp(-\omega x) \rangle$

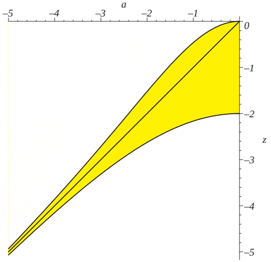
$$\omega_1 h = \omega h = a \qquad \omega_2 h = -\omega h = -a$$

$$y_{n+1} = \cosh(\omega h)\, y_n + h \, \frac{\sinh(\omega h)}{\omega h} \, f(x_n, y_n)$$

Applying this method to $y' = \lambda y$ gives

$$y_{n+1} = R(\omega h, -\omega h, \lambda h)\, y_n$$

$$R(a, -a; z) = \cosh(a) + z \, \frac{\sinh(a)}{a} \, .$$



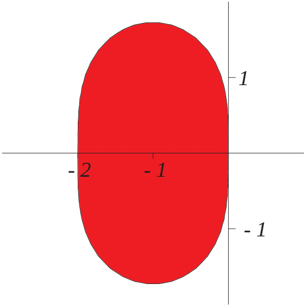
$\mathcal{R}_{(a,-a)} \cap \mathbb{R}^-$

An explicit 2-stage RK method

We consider the Runge-Kutta method

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array}$$

This method has stability function
$R(z) = 1 + z + z^2/2$
and the interval of stability is $[-2, 0]$



An EF explicit 2-stage RK method

We consider the EF Runge-Kutta method with modified tableau

$$\begin{array}{c|c|cc} 0 & 0 & 0 & 0 \\ 1/2 & \gamma_2 & a_{21} & 0 \\ \hline & \gamma & b_1 & b_2 \end{array}$$

- the second stage is fitted to $\langle \exp(\omega x), \exp(-\omega x) \rangle$
- the outer stage is fitted to $\langle 1, \exp(\omega x), \exp(-\omega x) \rangle$.

An EF explicit 2-stage RK method

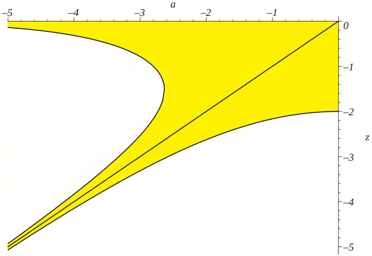


Figure: Interval along the negative real axis for the $(a, -a)$-EF variant of the 2-stage RK method.

The 2-step Adams-Bashforth method

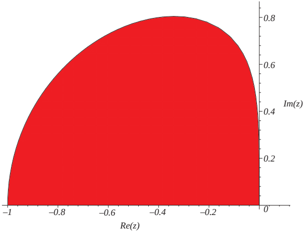
$$\mathcal{S} = \langle 1,\, x,\, x^2 \rangle$$

$$y_{n+2} - y_{n+1} = h\, \left(\frac{3}{2} f(x_{n+1}, y_{n+1}) - \frac{1}{2} f(x_n, y_n) \right)$$

Applying the method to $y' = \lambda y$ we obtain (with $z = \lambda h$)

$$y_{n+2} - \left(1 + \frac{3}{2} z\right) y_{n+1} + \frac{1}{2} z\, y_n = 0$$

$\mathcal{R}$: region of z-values such that $y_n \to 0$ as $n \to \infty$.



The EF 2-step Adams-Bashforth method fitted to $\langle 1, \exp(\omega x), \exp(-\omega x)\rangle$

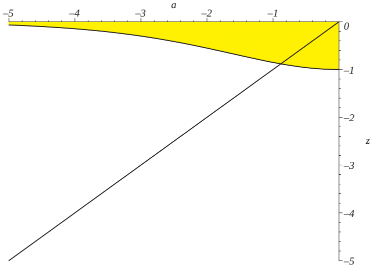


Figure: Interval along the negative real axis for the $(a, -a)$-EF variant of the 2-step Adams-Bashforth method.

The EF 2-step Adams-Bashforth method

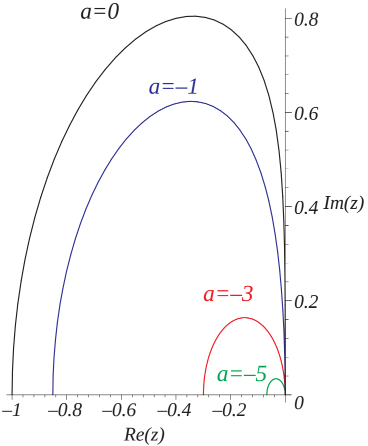


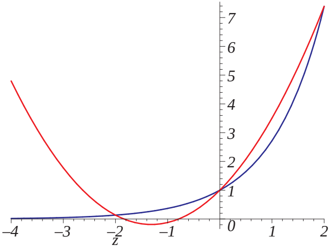
Figure: Boundary of stability regions of the $(a, -a)$-EF two-step Adams-Bashforth method whereby $a = -5$, -3, -1 and 0.

Conclusions

- The choice of the fitting space $\mathcal{S}$ greatly influences the size of the stability region
- We have illustrated that the traditional choice to fit to $\langle \exp(\omega x), \exp(-\omega x)\rangle$ with $\omega \in \mathbb{R}$ can be a very bad choice, as far as stability is concerned.
- In general, fitting to an increasing exponential function may cause the stability region to schrink compared to the stability region of the underlying polynomial method.

Why does the stability region shrink?

Interpolate $\exp(z)$ by a quadratic function $R(z)$ in 3 points $(0, 1)$, $(a, \exp(a))$ and $(b, \exp(b))$



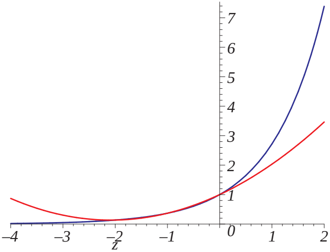


Figure: $\exp(z)$ and $R(z)$ with $(a, b) = (-2, 2)$ (left) and $(a, b) = (-2, -1)$ (right)

$R(z)$ will be a better approximation of $\exp(z)$ for small $z < 0$ when both a and b are negative!

Conclusions

- A much better alternative, leading to increased stability, is to fit to two decreasing exponentials $\exp(\omega x)$, $\exp(\theta x)$. In particular, when $\theta \to \omega$, good results are found.
- Example :

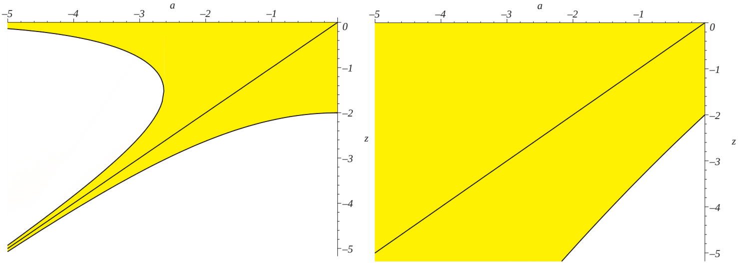


Figure: Interval along the negative real axis for the $(a, -a)$-EF variant (left) and (a, a)-EF variant (right) of the 2-stage RK method.

Conclusions

- To be able to cope with both the exponential and the trigonometric case, we therefore advocate the use of $\langle \exp(\omega x), \exp(\theta x) \rangle$, where ω and θ can both be real or complex conjugate, rather than of opposite sign.