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.

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Example : Numerov method

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

classical Numerov method :

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

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

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

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

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

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

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

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$$\lambda = \frac{1}{4\sin^2\frac{\theta}{2}} - \frac{1}{\theta^2} = \frac{1}{12} + \frac{1}{240}\theta^2 + \frac{1}{6048}\theta^4 + \dots \qquad \theta := \omega h$$

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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

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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 $y'' = f(t, y)$
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EF Runge-Kutta methods of collocation type (Gauss, LobattoIIIA, . . .)

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

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 $n \to \infty$?
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The linear stability properties for both classical methods and EF methods are studied by means of linear test equations

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Explicit Euler method

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

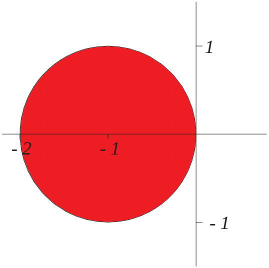
$$y_{n+1} = y_n + h\, f(x_n, y_n)$$

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 $|R(z)| < 1$



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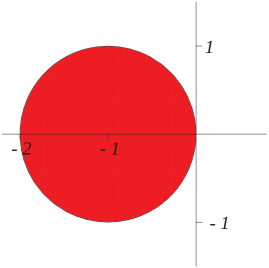


EF explicit Euler method fitted to $\mathcal{S} = \langle \exp(\omega_1 x), \exp(\omega_2 x) \rangle$

Let ω_1 and ω_2 be both real or complex conjugate.

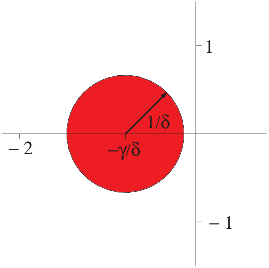
$$y_{n+1} = \gamma(\omega_1 h, \omega_2 h)\, y_n + h\, \delta(\omega_1 h, \omega_2 h)\, f(x_n, y_n)$$

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

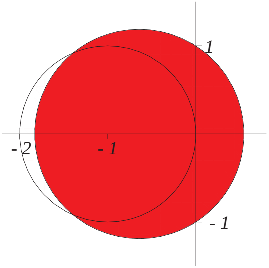
$$\omega_1\, h = i\, \omega\, h = i\, \beta \qquad \omega_2\, h = -i\, \omega\, h = -i\, \beta$$

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

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

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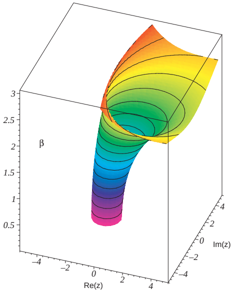

$\mathcal{R}_{(i\beta,-i\beta)}$

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

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

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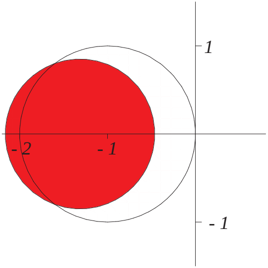

$\mathcal{R}_{(1,-1)}$

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

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

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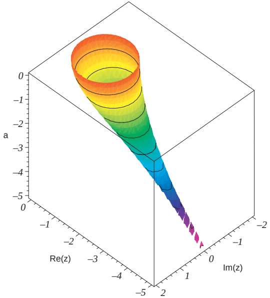

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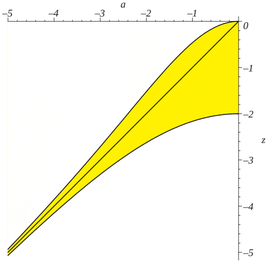


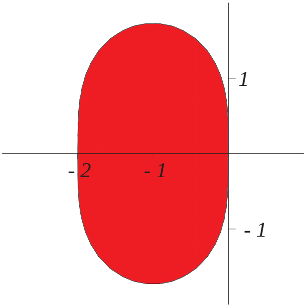
$\mathcal{R}_{(a,-a)} \cap \mathbb{R}^-$

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

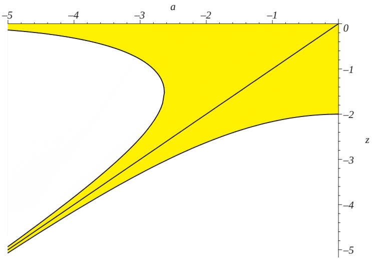


Figure: Interval along the negative real axis for the $(a, -a)$-EF variant of the 2-stage RK method.

The 2-step Adams-Bashforth method

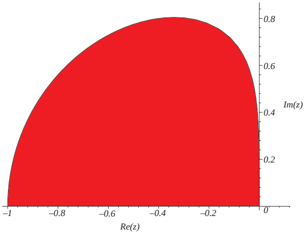
$$\mathcal{S} = \langle 1, x, x^2 \rangle$$

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

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 $\langle 1, \exp(\omega x), \exp(-\omega x)\rangle$

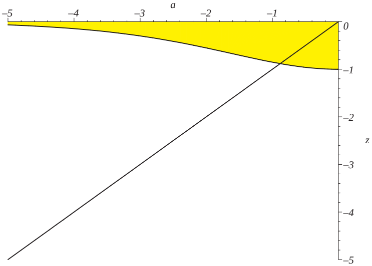


Figure: Interval along the negative real axis for the $(a, -a)$-EF variant of the 2-step Adams-Bashforth method.

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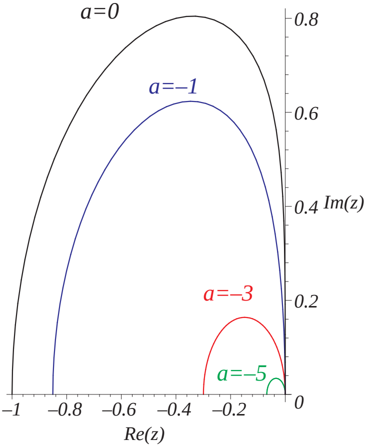

Figure: Boundary of stability regions of the $(a, -a)$-EF two-step Adams-Bashforth method whereby $a = -5, -3, -1$ and 0.

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.

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Why does the stability region shrink?

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

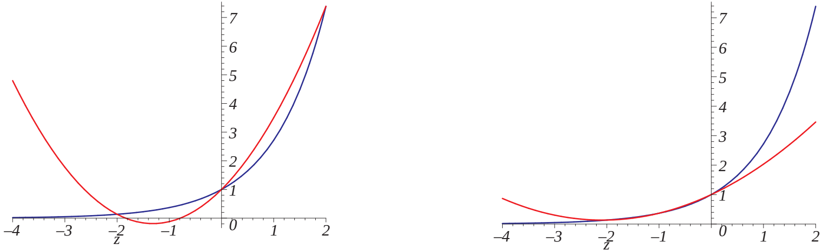

Figure: $\exp(z)$ and $R(z)$ with $(a,b) = (-2,2)$ (left) and $(a,b) = (-2,-1)$ (right)

$R(z)$ 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 :

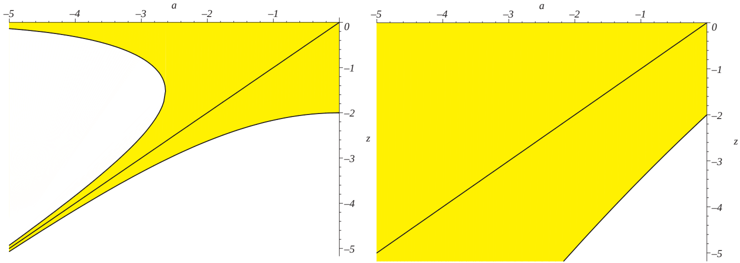

Figure: Interval along the negative real axis for the $(a, -a)$-EF variant (left) and (a, a)-EF variant (right) of the 2-stage RK method.

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.