On the global error committed when evaluating the Evans function numerically*

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1 Introduction

The Evans function is a tool for assessing the stability of travelling waves solutions for partial differential equations.

A recent paper [2] analyzes the order reduction experienced when evaluating the Evans function numerically. The details of some lengthy calculations were excluded from that paper for clarity. The purpose of this technical report is to make these details publicly available. This report is not intended to be read on its own; the reader is referred to [2] for background and references.

2 Setting

We consider scalar reaction–diffusion equations of the form

\[ u_t = u_{xx} + f(u). \]

Let \( u(x, t) = \hat{u}(\xi) \) with \( \xi = x - ct \) be a travelling wave solution of this equation. A linear stability analysis of this travelling wave leads to the eigenvalue problem

\[ \frac{dy}{d\xi} = A(\xi; \lambda) y, \quad (1a) \]

where

\[ A(\xi; \lambda) = \begin{bmatrix} 0 & 1 \\ \lambda - f'(\hat{u}(\xi)) & -c \end{bmatrix}. \quad (1b) \]

The limits of \( A \) as \( \xi \to \pm \infty \) are given by

\[ A_{\pm}(\lambda) = \begin{bmatrix} 0 & 1 \\ \lambda - f'(\hat{u}_\pm) & -c \end{bmatrix}. \]

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Furthermore, the eigenvalues of $A_-(\lambda)$ are

$$
\mu_{-1} = \frac{1}{2} \left( -c + \sqrt{c^2 + 4(\lambda - f'(\hat{u}_-))} \right) \quad \text{and} \\
\mu_{-2} = \frac{1}{2} \left( -c - \sqrt{c^2 + 4(\lambda - f'(\hat{u}_-))} \right),
$$

where $\hat{u}_- = \lim_{\xi \to -\infty} \hat{u}(\xi)$. Similarly, the eigenvalues of $A_+(\lambda)$ are

$$
\mu_{+1} = \frac{1}{2} \left( -c + \sqrt{c^2 + 4(\lambda - f'(\hat{u}_+))} \right) \quad \text{and} \\
\mu_{+2} = \frac{1}{2} \left( -c - \sqrt{c^2 + 4(\lambda - f'(\hat{u}_+))} \right),
$$

where $\hat{u}_+ = \lim_{\xi \to +\infty} \hat{u}(\xi)$. The corresponding eigenvectors are $(1, \mu_{-1}^{-1})^T$ and $(1, \mu_{-2}^{-1})^T$, respectively.

To define the Evans function, assume that

$$
\text{Re} \lambda > \max \left( f'(\hat{u}_-), f'(\hat{u}_+) \right) - \left( \frac{c}{\text{Im} \lambda} \right)^2. \tag{2}
$$

This condition ensures that $\mu_{-1}$ and $\mu_{+1}$ have positive real part, while $\mu_{-2}$ and $\mu_{+2}$ have negative real part.

The differential equation (1) is linear, and hence its solutions form a linear space. Let $y_-$ be the solution which satisfies

$$
y_-(\xi) \sim \exp \left( \mu_{-1}^{-1} \xi \right) \left[ \begin{array}{c} 1 \\ \mu_{-1}^{-1} \end{array} \right] \quad \text{as} \quad \xi \to -\infty. \tag{3}
$$

Condition (2) implies that this defines $y_-$ uniquely, so that $y_-$ satisfies the boundary condition $y(\xi) \to 0$ as $\xi \to -\infty$, and that any solutions satisfying this boundary condition is a multiple of $y_-$. Similarly, we define $y_+$ as the solution satisfying

$$
y_+(\xi) \sim \exp \left( \mu_{+1}^{-1} \xi \right) \left[ \begin{array}{c} 1 \\ \mu_{+1}^{-1} \end{array} \right] \quad \text{as} \quad \xi \to \infty. \tag{4}
$$

The Evans function is then the function $D$ defined by

$$
D(\lambda) = \det \left[ \begin{array}{c} y_-(0) \\ y_+(0) \end{array} \right].
$$

We are interested in computing this function.

### 3 Asymptotics near infinity

In this section, we study the behaviour of $D(\lambda)$ as $|\lambda| \to \infty$. 
3.1 The solution satisfying the left boundary condition

Define a transformation $y_\rightarrow \bar{y}_\rightarrow$ by

$$y_\rightarrow(\xi) = \exp(\mu^{[1]}\xi) \left( \frac{1}{\mu^{[1]}} \bar{u}_\rightarrow(\xi) + \bar{v}_\rightarrow(\xi) \left[ \frac{1}{\mu^{[2]}} \right] \right) = \exp(\mu^{[1]}\xi) B_\rightarrow \bar{y}_\rightarrow(\xi),$$  \hfill (5)

where

$$\bar{y}_\rightarrow = \left[ \frac{\bar{u}_\rightarrow}{\bar{v}_\rightarrow} \right] \quad \text{and} \quad B_\rightarrow = \left[ \frac{1}{\mu^{[1]}} \frac{1}{\mu^{[2]}} \right].$$  \hfill (6)

The differential equation (1) transforms to

$$\frac{d}{d\xi} \bar{u}_\rightarrow(\xi) = -\frac{1}{\kappa_\rightarrow} \varphi_\rightarrow(\xi) \bar{u}_\rightarrow(\xi) - \frac{1}{\kappa_\rightarrow} \varphi_\rightarrow(\xi) \bar{v}_\rightarrow(\xi),$$

$$\frac{d}{d\xi} \bar{v}_\rightarrow(\xi) = \frac{1}{\kappa_\rightarrow} \varphi_\rightarrow(\xi) \bar{u}_\rightarrow(\xi) - \left( \kappa_\rightarrow - \frac{1}{\kappa_\rightarrow} \varphi_\rightarrow(\xi) \right) \bar{v}_\rightarrow(\xi),$$  \hfill (7)

where

$$\varphi_\rightarrow(\xi) = f'(\hat{u}(\xi)) - f'(\hat{u}_\rightarrow) \quad \text{and} \quad \kappa_\rightarrow = \sqrt{\kappa^2 + 4(\lambda - f''(\hat{u}_\rightarrow))},$$

and the boundary condition (3) becomes

$$\bar{u}_\rightarrow(\xi) \rightarrow 1 \quad \text{and} \quad \bar{v}_\rightarrow(\xi) \rightarrow 0 \quad \text{as} \quad \xi \rightarrow -\infty.$$  \hfill (9)

Now, suppose that $\bar{u}_\rightarrow$ and $\bar{v}_\rightarrow$ can be expanded in inverse powers of $\kappa_\rightarrow$:

$$\bar{u}_\rightarrow(\xi; \kappa_\rightarrow) = \bar{u}_0(\xi) + \kappa_\rightarrow^{-1} \bar{u}_1(\xi) + \kappa_\rightarrow^{-2} \bar{u}_2(\xi) + \kappa_\rightarrow^{-3} \bar{u}_3(\xi) + O(\kappa_\rightarrow^{-4}),$$

$$\bar{v}_\rightarrow(\xi; \kappa_\rightarrow) = \bar{v}_0(\xi) + \kappa_\rightarrow^{-1} \bar{v}_1(\xi) + \kappa_\rightarrow^{-2} \bar{v}_2(\xi) + \kappa_\rightarrow^{-3} \bar{v}_3(\xi) + O(\kappa_\rightarrow^{-4}).$$

We now substitute these expansions in (7) and equate the coefficients of the powers of $\kappa_\rightarrow$.

- At $O(\kappa_\rightarrow)$, we get $0 = \bar{v}_0$, so $\bar{v}_0$ is identically zero.
- At $O(1)$, we get $(\bar{u}_0)' = 0$ and $(\bar{v}_0)' = -\bar{v}_1$. The first equation, together with the boundary condition (9), implies that $\bar{u}_0 = 1$. It follows from the second equation that $\bar{v}_1$ is identically zero.
- At $O(\kappa_\rightarrow^{-1})$, we get

$$\left( \bar{u}_1 \right)' = -\varphi_\rightarrow(\xi) (\bar{u}_0 + \bar{v}_0) \quad \text{and} \quad \left( \bar{v}_1 \right)' = \varphi_\rightarrow(\xi) (\bar{u}_0 + \bar{v}_0) - \bar{v}_2.$$  \hfill (8)

Substituting what we found before yields

$$\left( \bar{u}_1 \right)' = -\varphi_\rightarrow(\xi) \quad \text{and} \quad 0 = \varphi_\rightarrow(\xi) - \bar{v}_2.$$

Hence, $\bar{u}_1(\xi) = -\Phi_\rightarrow(\xi)$ and $\bar{v}_2(\xi) = \varphi_\rightarrow(\xi)$, where

$$\Phi_\rightarrow(\xi) = \int_{-\infty}^{\xi} \varphi_\rightarrow(x) \, dx.$$ 

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At $O(\kappa^{-2})$, we get

$$(\tilde{u}_-') = -\varphi_-(\xi) (\tilde{u}_- + \tilde{v}_-)$$

and

$$(\tilde{v}_-') = \varphi_-(\xi) (\tilde{u}_- + \tilde{v}_-) - \tilde{v}_-.$$ 

Substituting $\tilde{u}_-$ and $\tilde{v}_-$ in the first equation yields $(\tilde{u}_-') = \varphi_-(\xi) \Phi_-(\xi)$, and hence,

$$\tilde{u}_-(\xi) = \int_{-\infty}^{\xi} \varphi_-(x) \int_{-\infty}^{x} \varphi_-(y) \, dy \, dx = \frac{1}{2} \int_{-\infty}^{\xi} \int_{-\infty}^{x} \varphi_-(x) \varphi_-(y) \, dy \, dx = \frac{1}{2} (\Phi_-(\xi))^2.$$ 

Summarizing, we have the following series expansions for the transformed solution:

$$\tilde{u}_-(\xi; \kappa_-) = 1 - \kappa^{-1}_- \Phi_-(\xi) + \frac{1}{2} \kappa^{-2}_- (\Phi_-(\xi))^2 + O(\kappa^{-3})_-, \quad \tilde{v}_-(\xi; \kappa_-) = \kappa^{-2}_- \varphi_-(\xi) + O(\kappa^{-3}).$$ (10)

### 3.2 The solution satisfying the right boundary condition

The computation for the solution $y_+$ satisfying the right boundary condition (4) is analogous. Define the transformation $y_+ \to \tilde{y}_+$ by

$$y_+(\xi) = \exp(\mu_+^{[2]} \xi) \left( \tilde{u}_+(\xi) \begin{bmatrix} 1 \\ \mu_+^{[1]} \end{bmatrix} + \tilde{v}_+(\xi) \begin{bmatrix} 1 \\ \mu_+^{[2]} \end{bmatrix} \right) = \exp(\mu_+^{[2]} \xi) B_+ \tilde{y}_+(\xi)$$

where

$$\tilde{y}_+ = \begin{bmatrix} \tilde{u}_+ \\ \tilde{v}_+ \end{bmatrix} \quad \text{and} \quad B_+ = \begin{bmatrix} 1 & 1 \\ \mu_+^{[1]} & \mu_+^{[2]} \end{bmatrix}.$$ 

The differential equation (1) transforms to

$$\frac{d}{d\xi} \tilde{u}_+(\xi) = \left( \kappa_+ - \frac{1}{\kappa_+} \varphi_+(\xi) \right) \tilde{u}_+(\xi) - \frac{1}{\kappa_+} \varphi_+(\xi) \tilde{v}_+(\xi),$$

$$\frac{d}{d\xi} \tilde{v}_+(\xi) = \frac{1}{\kappa_+} \varphi_+(\xi) \tilde{u}_+(\xi) + \frac{1}{\kappa_+} \varphi_+(\xi) \tilde{v}_+(\xi),$$ (11)

where

$$\varphi_+(\xi) = f'(\tilde{u}(\xi)) - f'(\tilde{u}_+) \quad \text{and} \quad \kappa_+ = \sqrt{\epsilon^2 + 4(\lambda - f'(\tilde{u}_+))},$$ (12)

and the boundary condition (4) becomes

$$\tilde{u}_+(\xi) \to 0 \quad \text{and} \quad \tilde{v}_+(\xi) \to 1 \quad \text{as} \quad \xi \to \infty.$$ 

Expand $\tilde{u}_+$ and $\tilde{v}_+$ in inverse powers of $\kappa_+$:

$$\tilde{u}_+(\xi; \kappa_+) = \tilde{u}_0^+ (\xi) + \kappa_+^{-1} \tilde{u}_1^+ (\xi) + \kappa_+^{-2} \tilde{u}_2^+ (\xi) + \kappa_+^{-3} \tilde{u}_3^+ (\xi) + O(\kappa_+^{-4}),$$

$$\tilde{v}_+(\xi; \kappa_-) = \tilde{v}_0^+ (\xi) + \kappa_+^{-1} \tilde{v}_1^+ (\xi) + \kappa_+^{-2} \tilde{v}_2^+ (\xi) + \kappa_+^{-3} \tilde{v}_3^+ (\xi) + O(\kappa_+^{-4}).$$
Substituting these expansions in the transformed differential equation (11) and equating the coefficients of the powers of $\kappa_+$ yields the following equations:

\[
\begin{align*}
0 &= \tilde{u}_0^+, \\
(\tilde{u}_0^+)' &= -\tilde{u}_0^+, \\
(\tilde{u}_1^+)' &= -\varphi_+(\xi)(\tilde{u}_0^+ + \tilde{v}_1^+) + \tilde{u}_2^+, \\
(\tilde{v}_1^+)' &= \varphi_+(\xi)(\tilde{u}_0^+ + \tilde{v}_1^+), \\
(\tilde{u}_2^+)' &= -\varphi_+(\xi)(\tilde{u}_1^+ + \tilde{v}_2^+) + \tilde{u}_3^+, \\
(\tilde{v}_2^+)' &= \varphi_+(\xi)(\tilde{u}_1^+ + \tilde{v}_2^+).
\end{align*}
\]

Solving these equations in the same way as in the previous case yields the following series expansions for the transformed solution:

\[
\begin{align*}
\tilde{u}_+^+(\xi; \kappa_+) &= \kappa_-^2 \varphi_+(\xi) + \mathcal{O}(\kappa_-^3), \\
\tilde{v}_+^+(\xi; \kappa_+) &= 1 - \kappa_-^2 \Phi_+(\xi) + \frac{1}{2} \kappa_-^2 (\Phi_+(\xi))^2 + \mathcal{O}(\kappa_-^3),
\end{align*}
\]

where

\[
\Phi_+(\xi) = \int_\xi^\infty \varphi_+(x) \, dx.
\]

### 3.3 Asymptotics for the Evans function

The Evans function is obtained by evaluating both $y_-$ and $y_+$ at $\xi = 0$ and taking the wedge product (which equals the determinant of the 2-by-2 matrix having these vectors as its columns). This yields

\[
D(\lambda) = y_-(0) \wedge y_+(0) = (B_- \tilde{y}_-(0)) \wedge (B_+ \tilde{y}_+(0))
\]

\[
= \left[ \begin{array}{cc} 1 & 1 \\
\frac{1}{2}(\kappa_- - c) & -\frac{1}{2}(\kappa_- + c) \end{array} \right] \left[ \begin{array}{c} \tilde{u}_-(0) \\
\tilde{v}_-(0) \end{array} \right] \wedge \left[ \begin{array}{cc} \frac{1}{2}(\kappa_+ - c) & -1 \\
\frac{1}{2}(\kappa_+ + c) & 1 \end{array} \right] \left[ \begin{array}{c} \tilde{u}_+(0) \\
\tilde{v}_+(0) \end{array} \right]
\]

\[
= \frac{1}{2}(\kappa_- - \kappa_+) (\tilde{v}_-(0) \tilde{v}_+(0) - \tilde{u}_-(0) \tilde{u}_+(0)) + \frac{1}{2}(\kappa_- + \kappa_+) (\tilde{v}_-(0) \tilde{u}_+(0) - \tilde{u}_-(0) \tilde{v}_+(0))
\]

It follows from (10) and (13) that, as $|\lambda| \to \infty$,

\[
\tilde{u}_- = \mathcal{O}(1), \quad \tilde{u}_+ = \mathcal{O}(\kappa_-^2) = \mathcal{O}(\lambda^{-1}),
\]

\[
\tilde{v}_- = \mathcal{O}(\kappa_-^2) = \mathcal{O}(\lambda^{-1}), \quad \tilde{v}_+ = \mathcal{O}(1).
\]

Furthermore, we have $\kappa_- - \kappa_+ = \mathcal{O}(\lambda^{-1/2})$. Hence,

\[
D(\lambda) = -\frac{1}{2}(\kappa_- + \kappa_+) \tilde{u}_-(0) \tilde{v}_+(0) + \mathcal{O}(\lambda^{-1}).
\]

Finally,

\[
D(\lambda) = -2\lambda^{1/2} + \Phi - \frac{1}{2}\lambda^{-1/2} \left( \Phi^2 - 2f'(\tilde{u}_-) - 2f'(\tilde{u}_+) + c^2 \right) + \mathcal{O}(\lambda^{-1}),
\]

where

\[
\Phi = \Phi_-(0) + \Phi_+(0) = \int_{-\infty}^0 \varphi_-(x) \, dx + \int_0^\infty \varphi_+(x) \, dx.
\]
4 The exponential midpoint rule

The exponential midpoint rule (or second-order Magnus method) for solving the differential equation
\[ y' = A(\xi) y \]
is
\[ y_{k+1} = \exp \left( hA(\xi_k + \frac{1}{2}h) \right) y_k. \]

We assume that the step size \( h \) is fixed, so that \( \xi_k = \xi_0 + nh \).

The transformation (5) changes the recursion for the exponential midpoint rule to
\[ \bar{y}_{k+1} = \exp \left( -\mu^1_\xi \left( \xi_{k+1} - \frac{1}{2}h \right) \right) \bar{y}_k \]
where
\[ \bar{A}_- (\xi) = B^{-1} A(\xi) B - \mu^1_\xi I. \]

Using (1b), we find that
\[ \bar{A}_- (\xi) = \begin{bmatrix} -\frac{1}{\kappa_-} \varphi_- (\xi) & -\frac{1}{\kappa_-} \varphi_- (\xi) \\ \frac{1}{\kappa_-} \varphi_- (\xi) & -\kappa_- + \frac{1}{\kappa_-} \varphi_- (\xi) \end{bmatrix}, \]
with \( \varphi_- \) and \( \kappa_- \) as defined in (8).

The transformed recursion for the exponential midpoint rule is the same as the exponential midpoint rule applied to the transformed equation \( \bar{y}' = \bar{A}(\xi) \bar{y} \), cf. (7). The reason for this is that the Magnus method is equivariant under transformations such as (5).

4.1 The local error

The local error for the exponential midpoint rule is defined by
\[ L^-_k = \exp \left( hA(\xi_k + \frac{1}{2}h) \right) y(\xi_k) - y(\xi_{k+1}), \]
or, in transformed coordinates,
\[ \bar{L}^-_k = \exp \left( h\bar{A}_-(\xi_k + \frac{1}{2}h) \right) \bar{y}(\xi_k) - \bar{y}(\xi_{k+1}), \]

We compute the matrix exponential of \( h\bar{A}_- \) by diagonalization. The eigenvalues of \( h\bar{A}_- (\xi) \) are
\[ \lambda_1 = -\frac{1}{2} h \left( \kappa_- \sqrt{\kappa_-^2 - 4 \varphi_- (\xi)} \right) \]
\[ = -h \left( \kappa_-^{-1} \varphi_- (\xi) + \kappa_-^{-3} (\varphi_- (\xi))^2 + O(\kappa_-^{-5}) \right) \]
and
\[
\lambda_2 = -\frac{1}{2} h \left( \kappa_- + \sqrt{\kappa_-^2 - 4 \varphi_- (\xi)} \right)
= -h \left( \kappa_- - \kappa_-^{-1} \varphi_- (\xi) - \kappa_-^{-3} (\varphi_- (\xi))^2 + O(\kappa_-^{-5}) \right).
\]

The corresponding eigenvector matrix is
\[
V = \begin{bmatrix} 1 & 1 \\ v_1 & v_2 \end{bmatrix}
\]
with
\[
v_1 = \frac{1}{2 \varphi} \left( \kappa^2 - \kappa \sqrt{\kappa^2 - 4 \varphi} \right) - 1,
\]
\[
v_2 = \frac{1}{2 \varphi} \left( \kappa^2 + \kappa \sqrt{\kappa^2 - 4 \varphi} \right) - 1,
\]
where we are writing \( \kappa \) for \( \kappa_- \) and \( \varphi \) for \( \varphi_- (\xi) \). Its inverse is
\[
V^{-1} = \frac{1}{v_2 - v_1} \begin{bmatrix} v_2 & -1 \\ -v_1 & 1 \end{bmatrix}.
\]

We have \( h \tilde{A} = V \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} V^{-1} \), and thus \( \exp(h \tilde{A}) = V \begin{bmatrix} \exp \lambda_1 & 0 \\ 0 & \exp \lambda_2 \end{bmatrix} V^{-1} \). However, \( \lambda_2 \sim -h \kappa \) so that \( \exp \lambda_2 \) is exponentially small as \( |\kappa| \to \infty \) if \( \kappa \) is restricted to lie in a sector of the form \( |\arg \kappa| < \frac{1}{2} \pi - \epsilon \). Under this assumption,
\[
\exp(h \tilde{A}) = V \left[ \begin{array}{c} \exp \lambda_1 \\ 0 \end{array} \right] V^{-1}
= \frac{\exp \lambda_1}{v_2 - v_1} \begin{bmatrix} v_2 & -1 \\ v_1 & v_2 - v_1 \end{bmatrix} + \text{e.s.t.}
= \exp \left( -\frac{1}{2} h \left( \kappa - \sqrt{\kappa^2 - 4 \varphi} \right) \right)
\times \left[ \begin{array}{c} 1 - \frac{h^2 \varphi}{\kappa^2} + \frac{O(\kappa^{-3})}{2 \kappa^2} + \frac{\varphi}{\kappa^2} + O(\kappa^{-3}) \\ \frac{\varphi}{\kappa^2} + O(\kappa^{-3}) \end{array} \right],
\]
where \( \text{e.s.t.} \) stands for exponentially small terms.

Hence, using the exact solution (10), we find that
\[
\exp \left( h \tilde{A} (\xi_k + \frac{1}{2} h) \right) \hat{y}(\xi_k)
= \left[ 1 - \frac{\Phi(\xi_k) + h \varphi (\xi_k + \frac{1}{2} h)}{\kappa} + \frac{\Phi(\xi_k) + h \varphi (\xi_k + \frac{1}{2} h)}{2 \kappa^2} + O(\kappa^{-3}) \right] \frac{\varphi (\xi_k + \frac{1}{2} h)}{\kappa^2} + O(\kappa^{-3})
\]

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We thus arrive at the following expression for the local error:

\[
\bar{L}_k^- = \exp\left(h\bar{A}(\xi_k + \frac{1}{2}h)\right) \bar{y}(\xi_k) - \bar{y}(\xi_{k+1}) \\
= \left[ \frac{\Phi(\xi_k+h) - \Phi(\xi_k) + h\varphi(\xi_k + \frac{1}{2}h)}{\kappa^2} \right] + \frac{(\Phi(\xi_1+h) - \Phi(\xi_1))}{2\kappa^2} + O(\kappa^{-3}) + O(\kappa^{-3}) \\
= \left[ \frac{1}{\kappa^2}\kappa^{-1} h^3 \varphi''(\xi_k + \frac{1}{2}h) + O(\kappa^{-1} h^5, \kappa^{-2} h^3) \right] \\
\]

We need to assume that \(|\kappa| \gg h^{-1}\) for the last equality.

### 4.2 The global error

We write the local error as

\[
\bar{L}_k^- = \left[ \kappa^{-1} \gamma_k + O(\kappa^{-2} h^3) \right] \\
\]

where

\[
\gamma_k = \int_{\xi_k}^{\xi_k+h} \varphi_-(x) dx - h\varphi_-(\xi_k + \frac{1}{2}h) = O(h^3), \\
\delta_k = \varphi_-(\xi_k + \frac{1}{2}h) - \varphi_-(\xi_k + h) = O(h). \\
\]

The global error satisfies the recurrence relation

\[
\bar{E}_{k+1}^- = \exp\left(h\bar{A}(\xi_k + \frac{1}{2}h)\right) \bar{E}_k^- + \bar{L}_k^- , \\
\bar{E}_0^- = 0, \\
\]

or, in transformed coordinates,

\[
\bar{E}_{k+1}^- = \exp\left(h\bar{A}_-(\xi_k + \frac{1}{2}h)\right) \bar{E}_k^- + \bar{L}_k^- , \\
\bar{E}_0^- = 0. \\
\]

The solution of this recursion is

\[
\bar{E}_k^- = \left[ \kappa^{-1} \sum_{j=0}^{k-1} \gamma_j + O(\kappa^{-2} h^2) \right] \\
\]

This can easily be proved by induction. The case \(k = 1\) is trivial. Assuming that (16) holds for a particular value of \(k\), we have, using (14) and (15),

\[
\bar{E}_{k+1}^- = \exp\left(h\bar{A}_-(\xi_k + \frac{1}{2}h)\right) \bar{E}_k^- + \bar{L}_k^- \\
= \left[ \begin{array}{c}
1 + O(\kappa^{-1}) \\
O(\kappa^{-2}) \\
O(\kappa^{-4})
\end{array} \right] \left[ \begin{array}{c}
\kappa^{-1} \sum_{j=0}^{k-1} \gamma_j + O(\kappa^{-2} h^2) \\
\kappa^{-2} \delta_{k-1} + O(\kappa^{-3} h) \\
O(\kappa^{-4})
\end{array} \right] \\
+ \left[ \begin{array}{c}
\kappa^{-1} \gamma_k + O(\kappa^{-2} h^3) \\
\kappa^{-2} \delta_k + O(\kappa^{-3} h)
\end{array} \right] \\
= \left[ \begin{array}{c}
\kappa^{-1} \sum_{j=0}^{k} \gamma_j + O(\kappa^{-2} h^2) \\
\kappa^{-2} \delta_k + O(\kappa^{-3} h)
\end{array} \right] ,
\]

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which concludes the induction.

Substituting $\gamma_k$ and $\delta_k$ back in (16), we find that

$$
\bar{E}_k = \begin{bmatrix}
\kappa^{-1} \left( \int_{\xi_0}^{\xi_k} \varphi-(x) \, dx - h \sum_{j=0}^{k-1} \varphi-(\xi_j + \frac{1}{2}h) \right) + O(\kappa^{-2}h^2) \\
\kappa^{-2} \left( \varphi-(\xi_k + \frac{1}{2}h) - \varphi-(\xi_k + h) \right) + O(\kappa^{-3}h)
\end{bmatrix}
$$

and

$$
\bar{E}_k = \begin{bmatrix}
\kappa^{-1} \left( \int_{\xi_0}^{\xi_k} \varphi(x) \, dx - h \sum_{j=0}^{k-1} \varphi(\xi_j + \frac{1}{2}h) \right) + O(\kappa^{-2}h^2) \\
\kappa^{-2} \left( \varphi(\xi_k + \frac{1}{2}h) - \varphi(\xi_k + h) \right) + O(\kappa^{-3}h)
\end{bmatrix}
$$

where $\varphi(\xi) = f'(\hat{u}(\xi))$ differs from $\varphi-\xi$ by a constant.

### 4.3 The solution on $[0, \infty)$

To compute the solution $y_+$ satisfying the right boundary condition, we run the exponential midpoint rule backwards:

$$
\bar{y}_{k+1} = \exp\left(-h\bar{A}_+(\xi_k - \frac{1}{2}h)\right) \bar{y}_k,
$$

where $\xi_k = \xi_0 - kh$ and

$$
\bar{A}_+(\xi) = B_+^{-1} A(\xi) B_+ - \mu_2[I = \begin{bmatrix} \kappa_+ - \frac{1}{\kappa_+} \varphi_+(\xi) & -\frac{1}{\kappa_+} \varphi_+(\xi) \\ \frac{1}{\kappa_+} \varphi_+(\xi) & \frac{1}{\kappa_+} \varphi_+(\xi) \end{bmatrix}, \text{ (17)}
$$

with $\kappa_+$ and $\varphi_+$ as defined in (12). A similar computation as before yields

$$
\exp(-h\bar{A}_+) = \begin{bmatrix}
\frac{\varphi_+}{\kappa_+} + O(\kappa_+^{-5}) & \frac{\varphi_+}{\kappa_+} + O(\kappa_+^{-3}) \\
-\frac{\varphi_+}{\kappa_+} + O(\kappa_+^{-3}) & 1 - \frac{h\varphi_+}{\kappa_+} + \frac{h^2\varphi_+^2}{2\kappa_+} + O(\kappa_+^{-3})
\end{bmatrix}
$$

and

$$
\exp(h\bar{A}_+(\xi_k - \frac{1}{2}h)) \bar{y}(\xi_k)
$$

where $\varphi_+ (\ldots)$ stands for $\varphi_+(\xi_k - \frac{1}{2}h)$. When we use this to determine the local error, we find

$$
\bar{L}_k = \begin{bmatrix}
\frac{\varphi_+ (\xi_k - \frac{1}{2}h) - \varphi_+ (\xi_{k+1})}{\kappa_+^2} + O(\kappa_+^{-3}) \\
\frac{\Phi_+ (\xi_{k+1}) - \Phi_+ (\xi_k) - h\varphi_+ (\xi_k + \frac{1}{2}h)}{\kappa_+} + O(\kappa_+^{-2})
\end{bmatrix}.
$$
A standard induction argument shows that the global error is
\[
\tilde{E}_k^+ = \left[ \kappa_+^{-2} (\varphi(\xi_k + \frac{1}{2}h) - \varphi(\xi_k + h)) + \mathcal{O}(\kappa_+^{-3}h) \right. \\
\left. \kappa_+^{-1} \left( \int_{\xi_k}^{\xi_0} \varphi(x) \, dx - h \sum_{j=0}^{k-1} \varphi(\xi_j - \frac{1}{2}h) \right) + \mathcal{O}(\kappa_+^{-2}h^2) \right].
\]

### 4.4 The error in the Evans function

The numerically computed value for the Evans function is the wedge product of the numerical solutions:
\[
D_{\text{num}}(\lambda) = \bar{y}_k^+ \wedge E_k^+ = (y_-(0) + E^{-}_k) \wedge (y_+(0) + E^{+}_k),
\]

with \( k \) chosen such that \( 0 = 0 \). Hence the error in the Evans function is
\[
E_D(\lambda) = D(\lambda) - D_{\text{num}}(\lambda) = y_-(0) \wedge E^+_k + E^-_k \wedge y_+(0) + E^-_k \wedge E^+_k.
\]

Substituting \( B_- \) and \( B_+ \), we find
\[
E_D = \frac{1}{2} (\kappa_- - \kappa_+) \left( \bar{u}_-(0) [\tilde{E}^+_k]_2 - \bar{u}_-(0) [\tilde{E}^-_k]_1 + [\tilde{E}^-_k]_2 \bar{v}_+(0) \\
- [\tilde{E}^-_k]_1 \bar{v}_+(0) + [\tilde{E}^-_k]_2 [\tilde{E}^+_k]_1 - [\tilde{E}^+_k]_1 \tilde{E}^+_k \right) + \mathcal{O}(h)
\]

\[
+ \frac{1}{2} (\kappa_- + \kappa_+) \left( \bar{v}_-(0) [\tilde{E}^+_k]_1 - \bar{v}_-(0) [\tilde{E}^-_k]_2 + [\tilde{E}^-_k]_2 \bar{u}_+(0) \\
- [\tilde{E}^-_k]_1 \bar{u}_+(0) + [\tilde{E}^-_k]_2 [\tilde{E}^+_k]_1 - [\tilde{E}^+_k]_1 \tilde{E}^+_k \right). \tag{18}
\]

We now estimate all the terms in this expression and drop the ones of lower order:
\[
E_D = -\frac{1}{2} (\kappa_- + \kappa_+) \left( \bar{u}_-(0) [\tilde{E}^+_k]_2 + [\tilde{E}^-_k]_1 \bar{v}_+(0) + [\tilde{E}^-_k]_2 [\tilde{E}^+_k]_1 \right) + \mathcal{O}(\lambda^{-1}h)
\]

\[
= h \sum_{j=-N}^{N-1} \varphi(jh + \frac{1}{2}h) - \int_{-L}^{L} \varphi(x) \, dx + \mathcal{O}(\lambda^{-1/2}h^2),
\]

assuming that the differential equations are solved on the intervals \([-L, 0]\) and \([0, L]\) with \( L = Nh \). The final step is to apply the Euler–MacLaurin summation formula (see e.g. [1]), which states that
\[
h \sum_{j=0}^{n} f(jh) = \int_{0}^{nh} f(x) \, dx + \frac{h}{2} f(0) + f(nh) \\
+ \sum_{i=1}^{m} \frac{B_{2i}h^{2i}}{(2i)!} \left( f^{(2i-1)}(nh) - f^{(2i-1)}(0) \right) \\
+ \frac{nB_{2m+2}h^{2m+3}}{(2m+2)!} f^{(2m+2)}(\xi)
\]

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for some $\xi \in [0, nh]$, where $B_k$ denote the Bernoulli numbers. This yields

$$
E_D = \int_{-L}^{-L+\frac{1}{2}h} \varphi(x) \, dx + \int_{L-\frac{1}{2}h}^{L} \varphi(x) \, dx + \frac{1}{2}h(\varphi(-L) + \varphi(L))
+ \sum_{i=1}^{m} \frac{B_{2i}}{(2i)!} (f^{(2i-1)}(L) - f^{(2i-1)}(-L)) + O(h^{2m+2}, \lambda^{-1/2} h^2).
$$

Now, $\varphi(\xi)$ decays exponentially fast to zero as $|\xi| \to \infty$. So if we assume that $L$ is sufficiently large, we can ignore all terms in this equation but the last one. We thus arrive at the final result, which is that the error in the Evans function is of order $\lambda^{-1/2} h^2$.

### 5 The fourth-order Magnus method

We repeat the computation in the previous section for the fourth-order Magnus method. This method is given by

$$
y_{k+1} = \exp \left( \frac{1}{2}h \left( A(\xi_k^1) + A(\xi_k^2) \right) - \frac{\sqrt{3}}{12} h^2 \left[ A(\xi_k^1), A(\xi_k^2) \right] \right) y_k,
$$

where $[\cdot, \cdot]$ denotes the matrix commutator defined by $[X, Y] = XY - YX$ and $\xi_k^1, \xi_k^2$ are the Gauss–Legendre points

$$
\xi_k^1 = \xi_k + \left( \frac{1}{2} - \frac{1}{6} \sqrt{3} \right) h \quad \text{and} \quad \xi_k^2 = \xi_k + \left( \frac{1}{2} + \frac{1}{6} \sqrt{3} \right) h.
$$

After the transformation (5), the method reads

$$
\tilde{y}_{k+1} = \exp(\tilde{\Omega}_k) \tilde{y}_k
$$

with

$$
\tilde{\Omega}_k = \frac{1}{2} h \left( A_- (\xi_k^1) + A_- (\xi_k^2) \right) - \frac{\sqrt{3}}{12} h^2 \left[ A_- (\xi_k^1), A_- (\xi_k^2) \right]
= h \begin{bmatrix}
-\alpha_k & \beta_k - \frac{\alpha_k}{\kappa_-} \\
\beta_k - \frac{\alpha_k}{\kappa_-} & -\kappa_- + \frac{\alpha_k}{\kappa_-}
\end{bmatrix},
$$

where $\alpha_k$ and $\beta_k$ are given by

$$
\alpha_k = \frac{1}{2} (\varphi_-(\xi_k^1) + \varphi_-(\xi_k^2)) \quad \text{and} \quad \beta_k = -\frac{\sqrt{3}}{12} h (\varphi_-(\xi_k^1) - \varphi_-(\xi_k^2)).
$$

#### 5.1 The local error

The eigenvalues of $\tilde{\Omega}_k$ are

$$
\lambda_1 = -\frac{1}{2} h (\kappa_- - \tilde{\chi}_k) = -h \left( \kappa_-^2 \chi_k + \kappa_-^3 \chi_k^2 + O(\kappa^{-5}) \right)
$$
and
\[ \lambda_2 = -\frac{1}{2} h (\kappa_+ + \bar{\chi}_k) = -h \left( \kappa_+ - \kappa_-^3 \bar{\chi}_k + O(\kappa_-^3) \right), \]

where \( \chi_k = \alpha_k - \beta_k^2 \) and
\[ \bar{\chi}_k = \sqrt{\kappa_-^2 - 4(\alpha_k - \beta_k^2)}. \]

The corresponding eigenvector matrix is
\[ V = \begin{bmatrix} 1 & 1 \\ v_1 & v_2 \end{bmatrix} \]

with
\[ v_1 = \frac{2\alpha_k - \kappa_-^2 + \kappa_- \bar{\chi}_k}{2(\kappa_- \beta_k + \alpha_k)} \quad \text{and} \quad v_2 = \frac{2\alpha_k - \kappa_-^2 - \kappa_- \bar{\chi}_k}{2(\kappa_- \beta_k + \alpha_k)}. \]

Its inverse is
\[ V^{-1} = \frac{1}{v_2 - v_1} \begin{bmatrix} v_2 & -1 \\ -v_1 & 1 \end{bmatrix}. \]

As in the previous section, where we were considering the exponential midpoint rule, we have \( \lambda_1 \sim -h \kappa \) so that \( \exp \lambda_1 \) is exponentially small (under the same assumption as before). Hence,
\[ \exp(\bar{\Omega}_k) \bar{y}(\xi_k) = \begin{bmatrix} 1 - \frac{\Phi_- (\xi_k) + h \chi_k}{\kappa_-} + O(\kappa_-^3) \\ \beta_k \kappa_- + O(\kappa_-^2) \end{bmatrix}, \]

where e.s.t. stands for exponentially small terms.

Hence, using the exact solution (10), we find that
\[ \exp(\bar{\Omega}_k) \bar{y}(\xi_k) = \begin{bmatrix} 1 - \frac{\Phi_- (\xi_k) + h \chi_k}{\kappa_-} + O(\kappa_-^3) \\ \beta_k \kappa_- + O(\kappa_-^2) \end{bmatrix}. \]
We thus arrive at the following expression for the local error:

$$L_k^- = \exp(\bar{\Omega}_k) \bar{y}(\xi_k) - \bar{y}(\xi_{k+1}) = \begin{bmatrix} \kappa^{-1} \gamma_k + O(\kappa^{-2} h^4) \\ \kappa^{-1} \beta_k + O(\kappa^{-2} h) \end{bmatrix},$$

where

$$\gamma_k = \int_{\xi_k}^{\xi_{k+1}} \varphi_-(x) \, dx - h(\alpha_k - \beta_k^2)$$

$$= h^5 \left( \frac{1}{4320} \varphi'''(\xi_k + \frac{1}{2} h) + \frac{1}{144} (\varphi'(\xi_k + \frac{1}{2} h))^2 \right) + O(h^7)$$

and

$$\beta_k = \frac{1}{2} h^2 \varphi'(\xi_k + \frac{1}{2} h) + O(h^4).$$

5.2 The global error

The global error satisfies the recurrence relation

$$\bar{E}_{k+1}^- = \exp(\bar{\Omega}_k) \bar{E}_k^- + L_k^-,$$

$$\bar{E}_0^- = 0.$$

The solution of this recursion is

$$\bar{E}_k^- = \begin{bmatrix} \kappa^{-1} \sum_{j=0}^{k-1} \gamma_j + O(\kappa^{-2} h^4) \\ \kappa^{-1} \beta_{k-1} + O(\kappa^{-2} h) \end{bmatrix}.$$

This can easily be proved by induction. The key step in the proof is the following computation:

$$\bar{E}_{k+1}^- = \exp(\bar{\Omega}_k A) \bar{E}_k^- + L_k^-$$

$$= \begin{bmatrix} 1 + O(\kappa^{-1}) & O(\kappa^{-1}) \\ O(\kappa^{-1}) & O(\kappa^{-2}) \end{bmatrix} \begin{bmatrix} \kappa^{-1} \sum_{j=0}^{k-1} \gamma_j + O(\kappa^{-2} h^4) \\ \kappa^{-1} \beta_{k-1} + O(\kappa^{-2} h) \end{bmatrix}$$

$$+ \begin{bmatrix} \kappa^{-1} \gamma_k + O(\kappa^{-2} h^4) \\ \kappa^{-1} \beta_k + O(\kappa^{-2} h) \end{bmatrix}$$

$$= \begin{bmatrix} \kappa^{-1} \sum_{j=0}^{k} \gamma_j + O(\kappa^{-2} h^4) \\ \kappa^{-1} \beta_k + O(\kappa^{-2} h) \end{bmatrix}.$$

Substituting $\gamma_j$ back in the formula for $\bar{E}_k^-$, we find that

$$\bar{E}_k^- = \begin{bmatrix} \kappa^{-1} \left( \int_{\xi_0}^{\xi_k} \varphi_-(x) \, dx - h \sum_{j=0}^{k-1} (\alpha_k - \beta_k^2) \right) + O(\kappa^{-2} h^4) \\ \kappa^{-1} \beta_k + O(\kappa^{-2} h) \end{bmatrix}.$$

We now approximate

$$\beta_k = -\frac{\sqrt{3}}{12} h(\varphi_-(\xi_k) - \varphi_-(\xi_{k+1})) = \frac{1}{144} h^2 \varphi'(\xi_k - \frac{1}{2} h) + O(h^4).$$
Thus,
\[ h \sum_{j=0}^{k-1} \beta_k^2 = \frac{1}{12} h^4 \int_{\xi_0}^{\xi_k} (\varphi'(x))^2 \, dx + O(h^6), \]
and therefore,
\[ \bar{E}_k^- = \left[ \kappa^{-1} \left( \int_{\xi_0}^{\xi_k} \varphi(x) + \frac{1}{144} h^4 (\varphi'(x))^2 \, dx - \frac{1}{2} h \sum_{j=0}^{k-1} (\varphi(\xi_k^j) + \varphi(\xi_k^2)) \right) \right. \\
\left. + O(\kappa^{-1} h^6, \kappa^{-2} h^4) \right]. \]

5.3 The solution on \([0, \infty)\)

To compute the solution \(y_+\) satisfying the right boundary condition, we run the same method backwards:
\[ \bar{y}_{k+1} = \exp(\bar{\Omega}_k^+ \bar{y}_k) \]
with
\[ \bar{\Omega}_k^+ = -\frac{1}{2} h (\bar{A}_+(\xi_k^1) + \bar{A}_+(\xi_k^2)) - \frac{\sqrt{3}}{12} h^2 [\bar{A}_+(\xi_k^1), \bar{A}_+(\xi_k^2)], \]
where
\[ \xi_k = \xi_0 - kh, \quad \xi_k^1 = \xi_k - (\frac{1}{2} - \frac{1}{6} \sqrt{3}) h \quad \text{and} \quad \xi_k^2 = \xi_k - (\frac{1}{2} + \frac{1}{6} \sqrt{3}) h. \] (22)

We can write the matrix \(\bar{\Omega}_k^+\) as
\[ \bar{\Omega}_k^+ = h \begin{bmatrix} \kappa_+ - \frac{\alpha_k}{\kappa_+} & \beta_k + \frac{\alpha_k}{\kappa_+} \\
\beta_k - \frac{\alpha_k}{\kappa_+} & -\frac{\alpha_k}{\kappa_+} \end{bmatrix}, \]
where
\[ \alpha_k = \frac{1}{2} (\varphi_+(\xi_k^1) + \varphi_+(\xi_k^2)) \quad \text{and} \quad \beta_k = -\frac{\sqrt{3}}{12} h (\varphi_+(\xi_k^1) - \varphi_+(\xi_k^2)). \]

A similar computation as before yields
\[ \exp(-\bar{\Omega}_+^+) = \begin{bmatrix} \frac{\beta_k^2}{\kappa_+^2} + O(\kappa_-^3) \\
\frac{\beta_k}{\kappa_+} + O(\kappa_-^2) \end{bmatrix} \left[ 1 - \frac{h(\alpha_k - \beta_k^2)}{\kappa_+} + \frac{h^2(\alpha_k - \beta_k^2)^2 - 2\beta_k^2}{2\kappa_+^2} + O(\kappa_-^3) \right] \]
and
\[ \exp(-\bar{\Omega}_+^+) \bar{y}(\xi_k) = \begin{bmatrix} \frac{\beta_k}{\kappa_+} + O(\kappa_-^2) \\
1 - \frac{\Phi_+(\xi_k) + h(\alpha_k - \beta_k^2)}{\kappa_+} + O(\kappa_-^2) \end{bmatrix}. \]
When we use this to determine the local error, we find
\[ \bar{L}_k^+ = \left[ \frac{1}{\kappa_+} \left( \int_{\xi_{k+1}}^{\xi_k} \varphi_+(x) \, dx \right) + \mathcal{O}(\kappa_+^{-2} h^4) \right]. \]

As in the previous section, we conclude that the global error is given by
\[ \bar{E}_k^+ = \left[ \frac{1}{12} \kappa_+^{-1} h^2 \varphi'(\xi_k) + \mathcal{O}(\kappa_+^{-1} h^4, \kappa_+^{-2} h^4) \right]. \]

### 5.4 The error in the Evans function

Substituting the results for the global error in (18), we find that the error in evaluating the Evans function is
\[ \bar{E}_D = \frac{1}{12} h^2 \sum_{j=-N}^{-1} \left( \varphi(jh + \left( \frac{1}{2} - \frac{1}{6} \sqrt{3} \right) h) + \varphi(jh + \left( \frac{1}{2} + \frac{1}{6} \sqrt{3} \right) h) \right) \]
\[ - \int_{-L}^{L} \varphi(x) + \frac{1}{144} h^4 (\varphi'(x))^2 \, dx + \mathcal{O}(\lambda^{-1/2} h^2), \]

As with the exponential midpoint rule, the Euler–MacLaurin summation formula can be applied to show that the term
\[ \frac{1}{h} \sum_{j=-N}^{-1} \left( \varphi(jh + \left( \frac{1}{2} - \frac{1}{6} \sqrt{3} \right) h) + \varphi(jh + \left( \frac{1}{2} + \frac{1}{6} \sqrt{3} \right) h) \right) - \int_{-L}^{L} \varphi(x) \, dx \] (23)

is negligible if \( L \) is sufficiently large. So, we find that the error in the Evans function is given by
\[ \bar{E}_D = -\frac{1}{144} h^4 \int_{-\infty}^{\infty} (\varphi'(x))^2 \, dx + \mathcal{O}(\lambda^{-1/2} h^2). \]

### 6 The fourth-order Gauss–Legendre method

The two-stage Gauss–Legendre method for solving the equation \( y' = A(\xi) y \) is given by
\[ s_1 = A(\xi_k^1) \left( y_k + \frac{1}{4} h s_1 + \left( \frac{1}{4} - \frac{\sqrt{3}}{6} \right) h s_2 \right), \]
\[ s_2 = A(\xi_k^2) \left( y_k + \left( \frac{1}{4} + \frac{\sqrt{3}}{6} \right) h s_1 + \frac{1}{4} h s_2 \right), \]
\[ y_{k+1} = y_k + \frac{1}{2} h (s_1 + s_2), \]
where $\xi^k_1$ and $\xi^k_2$ are the Gauss–Legendre points, given in (19). As usual, we transform this to

$$
\bar{s}_1 = \bar{A}_- (\xi^k_1) (\bar{y}_k + \frac{1}{4} h \bar{s}_1 + (\frac{1}{4} - \frac{\sqrt{3}}{6}) h \bar{s}_2),
$$

$$
\bar{s}_2 = \bar{A}_- (\xi^k_2) (\bar{y}_k + (\frac{1}{4} + \frac{\sqrt{3}}{6}) h \bar{s}_1 + \frac{1}{4} h \bar{s}_2),
$$

$$
\bar{y}_{k+1} = \bar{y}_k + \frac{1}{4} h (\bar{s}_1 + \bar{s}_2).
$$

### 6.1 The local error

Substituting $\bar{A}_-$ and $\bar{y}_k = \bar{y}(\xi_k)$ in the above formula and rearranging yields

$$
\left(1 + \frac{h \varphi_1}{4 \kappa}\right) \bar{s}_{11} + \frac{h \varphi_1}{4 \kappa} \bar{s}_{12} + \frac{h \sigma_1 \varphi_1}{\kappa} \bar{s}_{21} + \frac{h \sigma_1 \varphi_1}{\kappa} \bar{s}_{22} = -\frac{\varphi_1}{\kappa} \bar{y}_{k1} - \frac{\varphi_1}{\kappa} \bar{y}_{k2},
$$

$$
- \frac{h \varphi_1}{4 \kappa} \bar{s}_{11} + \left(\frac{h \kappa}{4} + 1 - \frac{h \varphi_1}{4 \kappa}\right) \bar{s}_{12} - \frac{h \sigma_1 \varphi_1}{\kappa} \bar{s}_{21} + h \sigma_1 \left(\kappa - \frac{\varphi_1}{\kappa}\right) \bar{s}_{22}
$$

$$
= \frac{\varphi_1}{\kappa} \bar{y}_{k1} - \left(\kappa - \frac{\varphi_1}{\kappa}\right) \bar{y}_{k2},
$$

$$
\frac{h \sigma_2 \varphi_2}{\kappa} \bar{s}_{11} + \frac{h \sigma_2 \varphi_2}{\kappa} \bar{s}_{12} + \left(1 + \frac{h \varphi_2}{4 \kappa}\right) \bar{s}_{21} + \frac{h \varphi_2}{4 \kappa} \bar{s}_{22} = \bar{y}_{k1} = -\frac{\varphi_2}{\kappa} \bar{y}_{k1} - \frac{\varphi_2}{\kappa} \bar{y}_{k2},
$$

$$
- \frac{h \sigma_2 \varphi_2}{\kappa} \bar{s}_{11} + h \sigma_2 \left(\kappa - \frac{\varphi_2}{\kappa}\right) \bar{s}_{12} - \frac{h \varphi_2}{4 \kappa} \bar{s}_{21} + \left(\frac{h \kappa}{4} + 1 - \frac{h \varphi_2}{4 \kappa}\right) \bar{s}_{22}
$$

$$
= \frac{\varphi_2}{\kappa} \bar{y}_{k1} - \left(\kappa - \frac{\varphi_2}{\kappa}\right) \bar{y}_{k2},
$$

where

$$
\sigma_1 = \frac{1}{4} - \frac{1}{6} \sqrt{3}, \quad \sigma_2 = \frac{1}{4} + \frac{1}{6} \sqrt{3}, \quad \varphi_1 = \varphi_- (\xi^k_1), \quad \text{and} \quad \varphi_2 = \varphi_- (\xi^k_2).
$$

We assume that the unknowns $\bar{s}_{ij}$ can be expanded in powers of $\kappa$ like

$$
\bar{s}_{ij} = \bar{s}^0_{ij} + \frac{\bar{s}^1_{ij}}{\kappa} + \frac{\bar{s}^2_{ij}}{\kappa^2} + \mathcal{O}(\kappa^{-3}).
$$

Substitute this into the set of four equations above and collect like powers of $\kappa$.

- At order $\kappa$, we find

$$
\bar{h} s^0_{12} + h \sigma_1 \bar{s}^0_{22} = -\bar{y}_{k2},
$$

$$
\bar{h} \sigma_2 \bar{s}^0_{12} + h \bar{s}^0_{22} = -\bar{y}_{k2}.
$$

Solving these equations yields

$$
\bar{s}^0_{12} = -\frac{2 \sqrt{3}}{h} \bar{y}_{k2} \quad \text{and} \quad \bar{s}^0_{22} = \frac{2 \sqrt{3}}{h} \bar{y}_{k2}.
$$
At order $\kappa^0$, we find
\begin{align*}
\bar{s}^0_{11} &= 0, \\
\frac{1}{4}h\bar{s}^0_{12} + \bar{s}^0_{12} + h\sigma_1 \bar{s}^0_{22} &= 0, \\
\bar{s}^0_{21} &= 0, \\
h\sigma_2 \bar{s}^0_{12} + \frac{1}{2}h\bar{s}^0_{22} + \bar{s}^0_{22} &= 0.
\end{align*}
Substituting $\bar{s}^0_{12}$ and $\bar{s}^0_{22}$ and solving the resulting set of equations yields
\begin{align*}
\bar{s}^0_{11} &= \bar{s}^0_{21} = 0, \\
\bar{s}^0_{12} &= \frac{12(\sqrt{3} - 1)}{h^2} y_{k2} \quad \text{and} \quad \bar{s}^0_{22} = -\frac{12(\sqrt{3} + 1)}{h^2} y_{k2}.
\end{align*}

At order $\kappa^{-1}$, we find
\begin{align*}
\bar{s}^1_{11} + \frac{1}{4}h\varphi_1 \bar{s}^1_{11} + \frac{1}{4}h\varphi_1 \bar{s}^0_{11} + h\sigma_1 \varphi_1 \bar{s}^0_{21} + h\sigma_1 \varphi_1 \bar{s}^0_{22} &= -\varphi_1 \bar{y}_{k1} - \varphi_1 \bar{y}_{k2}, \\
-\frac{1}{4}h\varphi_1 \bar{s}^1_{11} + \frac{1}{4}h\bar{s}^1_{12} + \bar{s}^1_{12} - \frac{1}{4}h\varphi_1 \bar{s}^0_{12} - h\sigma_1 \varphi_1 \bar{s}^0_{21} + h\sigma_1 \bar{s}^2_{22} - h\sigma_1 \varphi_1 \bar{s}^0_{22} &= \varphi_1 \bar{y}_{k1} + \varphi_1 \bar{y}_{k2}, \\
h\sigma_2 \varphi_2 \bar{s}^0_{11} + h\sigma_2 \varphi_2 \bar{s}^0_{11} + \bar{s}^0_{22} + \frac{1}{4}h\varphi_2 \bar{s}^0_{22} + \frac{1}{4}h\varphi_2 \bar{s}^0_{22} &= -\varphi_2 \bar{y}_{k1} - \varphi_2 \bar{y}_{k2}, \\
-h\sigma_1 \varphi_2 \bar{s}^0_{11} + h\sigma_2 \varphi_2 \bar{s}^0_{11} - \bar{s}^0_{12} - \frac{1}{4}h\varphi_2 \bar{s}^0_{21} + \frac{1}{4}h\bar{s}^2_{12} + \bar{s}^0_{12} - \frac{1}{4}h\varphi_2 \bar{s}^0_{22} &= \varphi_1 \bar{y}_{k1} + \varphi_1 \bar{y}_{k2}.
\end{align*}
We substitute all the known quantities in these equation. The values of $\bar{s}^1_{11}$ and $\bar{s}^1_{21}$ can then be found from the first and third equation, respectively:
\begin{align*}
\bar{s}^1_{11} &= -\varphi_1 \bar{y}_{k1} \quad \text{and} \quad \bar{s}^1_{21} = -\varphi_2 \bar{y}_{k1}.
\end{align*}
The second and fourth equation become
\begin{align*}
\frac{1}{4}h\bar{s}^2_{12} + h\sigma_1 \bar{s}^2_{22} &= \varphi_1 \bar{y}_{k1} - 12(\sqrt{3} - 1)h^{-2} y_{k2}, \\
h\sigma_2 \bar{s}^2_{12} + \frac{1}{4}h\bar{s}^2_{22} &= \varphi_2 \bar{y}_{k1} + 12(\sqrt{3} + 1)h^{-2} y_{k2}.
\end{align*}
The solution of this system is
\begin{align*}
\bar{s}^2_{12} &= -\frac{1}{h} \left(3\varphi_1 + (2\sqrt{3} - 3)\varphi_2\right) \bar{y}_{k1} - \frac{24}{h^3} (2\sqrt{3} - 3) \bar{y}_{k2}, \\
\bar{s}^2_{22} &= \frac{1}{h} \left((2\sqrt{3} + 3)\varphi_1 - 3\varphi_2\right) \bar{y}_{k1} + \frac{24}{h^3} (2\sqrt{3} + 3) \bar{y}_{k2}.
\end{align*}

At order $\kappa^{-2}$, the first and third equations are
\begin{align*}
\bar{s}^3_{11} + \frac{1}{4}h\varphi_1 \bar{s}^1_{11} + \frac{1}{4}h\varphi_1 \bar{s}^1_{12} + h\sigma_1 \varphi_1 \bar{s}^1_{21} + h\sigma_1 \varphi_1 \bar{s}^1_{22} &= 0, \\
h\sigma_2 \varphi_2 \bar{s}^1_{11} + h\sigma_2 \varphi_2 \bar{s}^1_{12} + \bar{s}^1_{21} + \frac{1}{4}h\varphi_2 \bar{s}^1_{21} + \frac{1}{4}h\varphi_2 \bar{s}^1_{22} &= 0.
\end{align*}
The values of $\bar{s}^3_{11}$ and $\bar{s}^3_{21}$ follow immediately:
\begin{align*}
\bar{s}^3_{11} &= h \left(\frac{3}{2} \varphi_1^2 + \left(\frac{1}{12} - \frac{1}{10} \sqrt{3}\right) \varphi_1 \varphi_2\right) \bar{y}_{k1} - \frac{2\sqrt{3}}{h} \varphi_1 \bar{y}_{k2}, \\
\bar{s}^3_{21} &= h \left(\left(\frac{1}{4} + \frac{1}{6} \sqrt{3}\right) \varphi_1 \varphi_2 + \frac{1}{4} \varphi_2^2\right) \bar{y}_{k1} + \frac{2\sqrt{3}}{h} \varphi_2 \bar{y}_{k2}.
\end{align*}
Collecting the results, we find that the stage values for the Gauss–Legendre method are

\[
\begin{align*}
\bar{s}_{11} &= -\frac{\varphi_1}{\kappa} \bar{y}_{k1} + \frac{h(3\varphi_1^2 + (3 - 2\sqrt{3})\varphi_1\varphi_2)}{6\kappa^2} \bar{y}_{k1} - \frac{2\sqrt{3} \varphi_1}{h\kappa^2} \bar{y}_{k2} + O(\kappa^{-3}), \\
\bar{s}_{12} &= -\frac{2\sqrt{3}}{h} \bar{y}_{k2} + \frac{12(\sqrt{3} - 1)}{h^2\kappa} \bar{y}_{k2} + \frac{3\varphi_1 + (2\sqrt{3} - 3)\varphi_2}{h\kappa^2} \bar{y}_{k1} - \frac{24(2\sqrt{3} - 3)}{h^3\kappa^2} \bar{y}_{k2} + O(\kappa^{-3}), \\
\bar{s}_{21} &= -\frac{\varphi_2}{\kappa} \bar{y}_{k1} + \frac{h(3 + 2\sqrt{3})\varphi_1\varphi_2 + 3\varphi_2^2}{6\kappa^2} \bar{y}_{k1} + \frac{2\sqrt{3} \varphi_2}{h\kappa^2} \bar{y}_{k2} + O(\kappa^{-3}), \\
\bar{s}_{22} &= \frac{2\sqrt{3}}{h} \bar{y}_{k2} - \frac{12(\sqrt{3} + 1)}{h^2\kappa} \bar{y}_{k2} - \frac{(2\sqrt{3} + 3)\varphi_1 - 3\varphi_2}{h\kappa^2} \bar{y}_{k1} + \frac{24(2\sqrt{3} + 3)}{h^3\kappa^2} \bar{y}_{k2} + O(\kappa^{-3}).
\end{align*}
\]

The result of doing one step is therefore

\[
\bar{y}_{k+1,1} = \bar{y}_{k1} + \frac{1}{2} h(\bar{s}_{11} + \bar{s}_{21}) = \bar{y}_{k1} - \frac{h(\varphi_1 + \varphi_2)}{2\kappa} \bar{y}_{k1} + \frac{h^2(\varphi_1 + \varphi_2)^2}{4\kappa^2} \bar{y}_{k1} + \frac{\sqrt{3}(\varphi_2 - \varphi_1)}{\kappa^2} \bar{y}_{k2} + O(\kappa^{-3})
\]

and

\[
\bar{y}_{k+1,2} = \bar{y}_{k2} + \frac{1}{2} h(\bar{s}_{12} + \bar{s}_{22}) = \bar{y}_{k2} - \frac{12}{h\kappa} \bar{y}_{k2} + \frac{\sqrt{3}(\varphi_2 - \varphi_1)}{\kappa^2} \bar{y}_{k1} + \frac{72}{h^2\kappa^2} \bar{y}_{k2} + O(\kappa^{-3}).
\]

We can write this as \(\bar{y}_{k+1} = \Psi^{-\bar{y}}_{k} \bar{y}_{k}\) with

\[
\Psi^{-\bar{y}}_{k} = \begin{bmatrix}
1 - \frac{h\alpha_k}{\kappa} + \frac{h^2\alpha_k^2}{2\kappa^2} & \frac{12\beta_k}{h\kappa^2} \\
\frac{12\beta_k}{h\kappa^2} & 1 - \frac{12\beta_k}{h\kappa} + \frac{72}{h^2\kappa^2}
\end{bmatrix} + O(\kappa^{-3}),
\]

where \(\alpha_k\) and \(\beta_k\) are defined by (20). It follows that

\[
\Psi^{-\bar{y}}(\xi_k) = \begin{bmatrix}
1 - \frac{\Phi^{-\bar{y}}(\xi_k) + h\alpha_k}{\kappa} + \frac{(\Phi^{-\bar{y}}(\xi_k) + h\alpha_k)^2}{2\kappa^2} \\
\frac{h\varphi^{-\bar{y}}(\xi_k) + 12\beta_k}{h\kappa^2}
\end{bmatrix} + O(\kappa^{-3}).
\]

Finally, the local error is given by

\[
\tilde{L}_k = \Psi^{-\bar{y}}(\xi_k) - \bar{y}(\xi_{k+1}) = \begin{bmatrix}
k^{-1}L^a_{k^{-1}} + k^{-2}L^b_{k^{-1}} + O(\kappa^{-3}h^5) \\
k^{-2}L^a_{k^{-2}} + O(\kappa^{-3}h^2)
\end{bmatrix}
\]
Indeed, assuming that the result holds for some value of \( k \) and \( \xi \), the solution of this recursion relation is

The global error is given by the recursion

The solution of this recursion relation is

where

and

and

Indeed, assuming that the result holds for some value of \( k \), we have

and the formula for the global error follows by induction.
6.3 The error on \([0, \infty)\)

The solution on the interval \([0, \infty)\) can be computed by running the Gauss–Legendre method backwards:

\[
\begin{align*}
\bar{s}_1 &= \bar{A}_+ (\xi^1_k) \left( \bar{y}_k - \frac{1}{4} h \bar{s}_1 - \left( \frac{1}{4} - \frac{\sqrt{3}}{6} \right) h \bar{s}_2 \right), \\
\bar{s}_2 &= \bar{A}_+ (\xi^2_k) \left( \bar{y}_k - \left( \frac{1}{4} + \frac{\sqrt{3}}{6} \right) h \bar{s}_1 - \frac{1}{4} h \bar{s}_2 \right), \\
\bar{y}_{k+1} &= \bar{y}_k - \frac{1}{h} (\bar{s}_1 + \bar{s}_2),
\end{align*}
\]

with \(\bar{A}_+\) as given in (17) and \(\xi_k, \xi^1_k\) and \(\xi^2_k\) as given in (22). The global error can be computed as before, but here we will take a short-cut. If we comparing the matrix \(\bar{A}_+\) with \(\bar{A}_-\) and the exact solution on the interval \((-\infty, 0]\) with the exact solution on \([0, \infty)\), we find that they can be related by swapping the components 1 and 2, replacing \(\xi\) by \(-\xi\), and replacing the \(-\) subscript with a + subscript. Hence, the global error of the Gauss–Legendre method run backwards is

\[
\tilde{E}_k^+ = \left[ \begin{array}{c}
\frac{1}{\kappa_+} \sum_{j=0}^{k-1} \tilde{L}^a_{k+j} + \mathcal{O}(\kappa_-^{-3} h^2) \\
\frac{1}{\kappa_+} \sum_{j=0}^{k-1} \tilde{L}^b_{k+j} - \hbar \alpha_j \sum_{i=0}^{j-1} \tilde{L}^a_i + \mathcal{O}(\kappa_-^{-3} h^4)
\end{array} \right]
\]

where

\[
\begin{align*}
\tilde{L}^a_{k+j} &= \int_{\xi_k}^{\xi_{k+j}} \varphi(x) \, dx - \frac{1}{2} h \left( \varphi(\xi^1_k) + \varphi(\xi^2_k) \right) \\
\tilde{L}^b_{k+j} &= -\tilde{L}^a_{k+j} + \frac{1}{2} \left( \tilde{L}^c_{k+j} + \Phi_-(\xi_k) + \frac{1}{2} h \left( \varphi(\xi^1_k) + \varphi(\xi^2_k) \right) \right) \\
\tilde{L}^c_{k+j} &= \varphi(\xi_k) - \varphi(\xi_{k+j}) + \sqrt{3} \left( \varphi(\xi^1_k) - \varphi(\xi^2_k) \right).
\end{align*}
\]

6.4 The error in the Evans function

The error in the Evans function is given by (18):

\[
E_D = \frac{1}{2} (\kappa_- - \kappa_+) \left( \tilde{v}_-(0) \left[ \bar{E}^+ \right]_2 - \tilde{u}_-(0) \left[ \bar{E}^+ \right]_1 + \left[ \bar{E}^- \right]_2 \bar{v}_+(0) - \left[ \bar{E}^- \right]_1 \bar{u}_+(0) \right) \\
+ \frac{1}{2} (\kappa_- + \kappa_+) \left( \tilde{v}_-(0) \left[ \bar{E}^+ \right]_1 - \tilde{u}_-(0) \left[ \bar{E}^+ \right]_2 + \left[ \bar{E}^- \right]_2 \bar{v}_+(0) - \left[ \bar{E}^- \right]_1 \bar{u}_+(0) \right).
\]

Estimating all the terms, we find that

\[
E_D = -\frac{1}{2} (\kappa_- + \kappa_+) \left( \tilde{v}_-(0) \left[ \bar{E}^+ \right]_2 + \left[ \bar{E}^- \right]_1 \bar{v}_+(0) \right) + \mathcal{O}(\lambda^{-1/2} h^{8}, \lambda^{-3/2} h^{2}).
\]
Let $\mathcal{X}$ denote the expression between the big parentheses. We need to evaluate this expression:

$$
\mathcal{X} = \bar{u}_-(0) \left[ \bar{L}_k^+ \right]_2 + \left[ \bar{E}_k^- \right]_1 \bar{v}_+(0)
$$

$$
= \left( 1 - \frac{\Phi_-(0)}{\kappa_-} \right) \left( \frac{1}{\kappa_+} \sum_{j=0}^{N-1} \bar{L}_j^{a,+} + \frac{1}{\kappa_+} \sum_{j=0}^{N-1} \left( \bar{L}_j^{b,+} - h\alpha_j^+ \sum_{i=0}^{j-1} \bar{L}_i^{a,+} \right) \right)
$$

$$
+ \left( \frac{1}{\kappa_-} \sum_{j=0}^{N-1} \bar{L}_j^{a,-} + \frac{1}{\kappa_-} \sum_{j=0}^{N-1} \left( \bar{L}_j^{b,-} - h\alpha_j^- \sum_{i=0}^{j-1} \bar{L}_i^{a,-} \right) \right) \left( 1 - \frac{\Phi_+(0)}{\kappa_+} \right)
$$

$$
+ O(\lambda^{-3/2} h^4)
$$

$$
= \frac{1}{\lambda} \sum_{j=0}^{N-1} \left( \bar{L}_j^{a,-} + \bar{L}_j^{a,+} \right)
$$

$$
+ \frac{1}{\lambda} \sum_{j=0}^{N-1} \left( \bar{L}_j^{b,-} + \bar{L}_j^{b,+} - h\alpha_j^- \sum_{i=0}^{j-1} \bar{L}_i^{a,-} - h\alpha_j^+ \sum_{i=0}^{j-1} \bar{L}_i^{a,+} \right)
$$

$$
- \Phi_-(0) \bar{L}_j^{a,+} - \Phi_+(0) \bar{L}_j^{a,-} + O(\lambda^{-3/2} h^4).
$$

The sum $\sum_j (\bar{L}_j^{a,-} + \bar{L}_j^{a,+})$ is the same as expression (23), which appeared in the fourth-order Magnus method. As we discussed there, this expression is negligible. Substituting the values of $\bar{L}_j^{b,-}$ and $\bar{L}_j^{b,+}$, we find that

$$
\mathcal{X} = -\frac{1}{\lambda} \sum_{j=0}^{N-1} \left( L_j^{a,-} \left( \frac{1}{2} \bar{L}_j^{a,-} + \Phi_-(-L + jh) + \alpha_j^- + \Phi_+(0) \right) + h\alpha_j^- \sum_{i=0}^{j-1} \bar{L}_i^{a,-} \right)
$$

$$
+ \bar{L}_j^{a,+} \left( \frac{1}{2} \bar{L}_j^{a,+} + \Phi_+(L - jh) + \alpha_j^+ + \Phi_-(0) \right) + h\alpha_j^+ \sum_{i=0}^{j-1} \bar{L}_i^{a,+}
$$

Exchanging the double sums yields

$$
\mathcal{X} = -\frac{1}{\lambda} \left( \sum_{j=0}^{N-1} \left( \frac{1}{2} \bar{L}_j^{a,-} + \Phi_-(-L + jh) + \Phi_+(0) + h \sum_{i=j}^{N-1} \alpha_i^- \right) \right)
$$

$$
+ \bar{L}_j^{a,+} \left( \frac{1}{2} \bar{L}_j^{a,+} + \Phi_+(L - jh) + \Phi_-(0) + h \sum_{i=j}^{N-1} \alpha_i^+ \right) \right).
$$

Now, $\bar{L}_j^{a,-}$ was defined as

$$
\bar{L}_j^{a,-} = \Phi_-(-L + jh + h) - \Phi_-(L + jh) - h\alpha_j^-,
$$

and thus we have

$$
h \sum_{i=j}^{N-1} \alpha_i^- = \Phi_-(0) - \Phi_-(L + jh) + \sum_{i=j}^{N-1} \bar{L}_j^{a,-}.
$$
Using this expression, and its equivalent for \( \sum_i \alpha_i \), we find that

\[
\mathcal{X} = -\frac{1}{\lambda} \left( \sum_{j=0}^{N-1} L_j^{a,-} \left( \Phi_-(0) + \Phi_+(0) + \frac{1}{2} L_j^{a,-} + \sum_{i=j}^{N-1} L_i^{a,-} \right) + L_j^{a,+} \left( \Phi_-(0) + \Phi_+(0) + \frac{1}{2} L_j^{a,+} + \sum_{i=j}^{N-1} L_i^{a,+} \right) \right).
\]

We know that \( L_i^{a,\pm} = \mathcal{O}(h^5) \), which yields

\[
\mathcal{X} = -\frac{1}{\lambda} \left( \Phi_-(0) + \Phi_+(0) \right) \sum_{j=0}^{N-1} \left( L_j^{a,-} + L_j^{a,+} \right) + \mathcal{O}(\lambda^{-1}h^8).
\]

The last step is to recall that the sum \( \sum_j \left( L_j^{a,-} + L_j^{a,+} \right) \) is negligible, and thus, \( \mathcal{X} = \mathcal{O}(\lambda^{-1}h^8) \). We finally conclude that the error in evaluating the Evans function with the Gauss–Legendre method is

\[
E_D = \mathcal{O}(\lambda^{-1/2}h^8, \lambda^{-1}h^4, \lambda^{-3/2}h^2).
\]

References

[1] K. E. Atkinson. *An Introduction to Numerical Analysis*. John Wiley & Sons, New York, second edition, 1989.

[2] S. J. A. Malham and J. Niesen. Evaluating the Evans function: Order reduction in numerical methods. Accepted for publication in Math. Comp., 2006, math.NA/0605581.