

# Numerical evaluation of the Evans function

Simon J.A. Malham

Collaborators: Nairo Aparicio, Marcel Oliver & Jitse Niesen

Dundee: March 7th 2006

# Outline

- 1 Evans function
- 2 Numerical computation
- 3 Exterior product spaces
- 4 Numerical methods
- 5 Examples

# Outline

- 1 Evans function
- 2 Numerical computation
- 3 Exterior product spaces
- 4 Numerical methods
- 5 Examples

## Take home message:

*For non-selfadjoint stiff problems, the Evans function method, which is a shooting & matching technique, is the most accurate or even the only approach.*

## Miss distance function

Consider the **Sturm–Liouville problem** on  $[a, b]$ :

$$-u'' + q(x)u = \lambda u,$$

with boundary conditions  $u(a) = u(b) = 0$ ,

## Miss distance function

Consider the **Sturm–Liouville problem** on  $[a, b]$ :

$$-u'' + q(x)u = \lambda u,$$

with boundary conditions  $u(a) = u(b) = 0$ , i.e.

$$y' = A(x, \lambda)y, \quad \text{where } A(x, \lambda) = \begin{pmatrix} 0 & 1 \\ q(x) - \lambda & 0 \end{pmatrix}, \quad (*)$$

with boundary conditions  $y_1(a) = y_1(b) = 0$ .

## Miss distance function

Consider the **Sturm–Liouville problem** on  $[a, b]$ :

$$-u'' + q(x)u = \lambda u,$$

with boundary conditions  $u(a) = u(b) = 0$ , i.e.

$$y' = A(x, \lambda)y, \quad \text{where } A(x, \lambda) = \begin{pmatrix} 0 & 1 \\ q(x) - \lambda & 0 \end{pmatrix}, \quad (*)$$

with boundary conditions  $y_1(a) = y_1(b) = 0$ .

Denote by  $y^-(x)$  the solution of  $(*)$  with  $y^-(a) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

The **miss-distance function** is

$$D(\lambda) = y_1^-(b).$$

Eigenvalues correspond to zeros of the miss-distance function.

## The matching point $\xi$

$$y' = A(x, \lambda) y, \quad y_1(a) = y_1(b) = 0. \quad (*)$$

Denote by  $y^-(x)$  the solution of  $(*)$  with  $y^-(a) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

Denote by  $y^+(x)$  the solution of  $(*)$  with  $y^+(b) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

The SLP  $(*)$  has a solution if  $y^+$  is a multiple of  $y^-$ .

## The matching point $\xi$

$$y' = A(x, \lambda) y, \quad y_1(a) = y_1(b) = 0. \quad (*)$$

Denote by  $y^-(x)$  the solution of  $(*)$  with  $y^-(a) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

Denote by  $y^+(x)$  the solution of  $(*)$  with  $y^+(b) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

The SLP  $(*)$  has a solution if  $y^+$  is a multiple of  $y^-$ .

The miss-distance function, evaluated at  $\xi \in [a, b]$  is

$$D(\lambda) = \det \begin{pmatrix} y_1^-(\xi) & y_1^+(\xi) \\ y_2^-(\xi) & y_2^+(\xi) \end{pmatrix}.$$

For  $\xi = b$ , we get  $D(\lambda) = y_1^-(b)$ , as before.



# General spectral problems

For  $x \in \mathbb{R}$  consider

$$y' = A(x, \lambda) y,$$

with  $y(x) \in \mathbb{C}^n$ .

We assume there is a region  $\Omega \subset \mathbb{C}$  such that for all  $\lambda \in \Omega$ :

- ▶  $A(x, \lambda) \rightarrow A^\pm(\lambda)$  as  $x \rightarrow \pm\infty$ ;
- ▶  $A^\pm(\lambda)$  are hyperbolic;
- ▶  $A^-(\lambda)$  has  $k$  unstable eigenvalues  $\mu_1^-, \dots, \mu_k^-$ , with corresponding eigenvectors  $v_1^-, \dots, v_k^-$ ;
- ▶  $A^+(\lambda)$  has  $n - k$  unstable eigenvalues  $\mu_1^+, \dots, \mu_{n-k}^+$ , with corresponding eigenvectors  $v_1^+, \dots, v_{n-k}^+$ .

## General spectral problems II

Hence there exist:

- ▶  $k$  solutions:  $y_i^-(x) \sim e^{\mu_i^- x} v_i^-$  as  $x \rightarrow -\infty$ .
- ▶  $n - k$  solutions:  $y_i^+(x) \sim e^{\mu_i^+ x} v_i^+$  as  $x \rightarrow +\infty$ .

## General spectral problems II

Hence there exist:

- ▶  $k$  solutions:  $y_i^-(x) \sim e^{\mu_i^- x} v_i^-$  as  $x \rightarrow -\infty$ .
- ▶  $n - k$  solutions:  $y_i^+(x) \sim e^{\mu_i^+ x} v_i^+$  as  $x \rightarrow +\infty$ .

The **Evans function** is defined by

$$D(\lambda) = \det(y_1^-(\xi) \cdots y_k^-(\xi) y_1^+(\xi) \cdots y_{n-k}^+(\xi)).$$

It is analytic in  $\Omega$  and its zeros correspond to eigenvalues.

(Evans '75; Alexander, Gardner & Jones '90; Sandstede '02)

# Outline

- 1 Evans function
- 2 Numerical computation
- 3 Exterior product spaces
- 4 Numerical methods
- 5 Examples

## Computing the Evans function numerically

$$D(\lambda) = \det(y_1^-(\xi) \cdots y_k^-(\xi) y_1^+(\xi) \cdots y_{n-k}^+(\xi)).$$

Basic **numerical** computation:

- ▶ Compute the unstable eigenvectors  $v_1^-, \dots, v_k^-$  of  $A^-$ .
- ▶ For  $i = 1, \dots, k$ , solve  $y' = A(x, \lambda)y$  with initial condition  $y(-L) = v_i^-$  (where  $L$  is large) to get  $y_i^-(\xi)$ .
- ▶ Compute  $y_i^+(\xi)$  similarly, and calculate the determinant.

# Computing the Evans function numerically

$$D(\lambda) = \det(y_1^-(\xi) \cdots y_k^-(\xi) y_1^+(\xi) \cdots y_{n-k}^+(\xi)).$$

Basic **numerical** computation:

- ▶ Compute the unstable eigenvectors  $v_1^-, \dots, v_k^-$  of  $A^-$ .
- ▶ For  $i = 1, \dots, k$ , solve  $y' = A(x, \lambda)y$  with initial condition  $y(-L) = v_i^-$  (where  $L$  is large) to get  $y_i^-(\xi)$ .
- ▶ Compute  $y_i^+(\xi)$  similarly, and calculate the determinant.

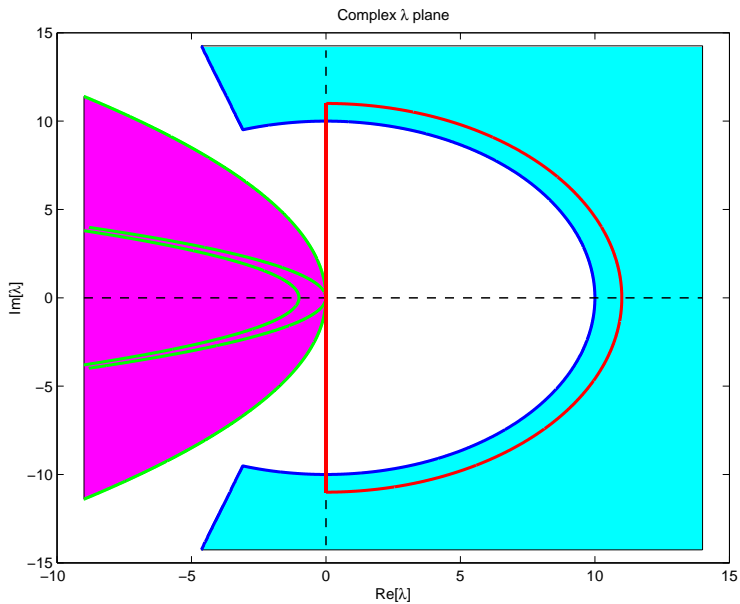
The Evans function is analytic, so we can use the **argument principle** to count the number of eigenvalues in a given region.

**(Evans & Faroe '77)**

Use **Newton's method** to solve  $D(\lambda) = 0$  and locate eigenvalues.

**(Pego, Smereka & Weinstein '93)**

# Spectrum structure



# Problems

- ▶ Unstable space  $\Rightarrow$  for example  $y_i^-$  grow with rate  $\mu_i^-$ .

**Solution:** Rescale: write  $y_i^- = e^{\mu_i^- x} u_i^-$  and solve

$$u' = (A(x, \lambda) - \mu_i^- I) u.$$

with  $u_i(x) \rightarrow v_i^-$  as  $x \rightarrow -\infty$ .

- ▶ Eigenvectors  $v_i^\pm$  must be analytic functions of  $\lambda$ .

**Solution:** Kato's algorithm.

- ▶ If  $\operatorname{Re} \mu_1^- > \operatorname{Re} \mu_2^-$ , then  $u_1^-$  can be computed accurately, but when computing  $u_2^-$  any errors in the  $u_1^-$  direction dominate the  $u_2^-$  solution.

**Solution:** Do not look at the  $y_i^-$  individually, but look at the subspace  $S = \operatorname{span}\{y_1^-, \dots, y_k^-\}$  and **lift** the equation  $y' = A(x, \lambda)y$  to  $S' = \ell(A(x, \lambda)) S$ .



# Outline

- 1 Evans function
- 2 Numerical computation
- 3 Exterior product spaces
- 4 Numerical methods
- 5 Examples

# Evans function

For  $v_j \in \mathbb{C}^n$ :

$$\det(v_1 \cdots v_n) \equiv v_1 \wedge \cdots \wedge v_n.$$

Hence Evans function

$$D(\lambda) \equiv e^{-\int_0^\xi \text{Tr} A(x, \lambda) dx} \underbrace{(y_1^- \wedge \cdots \wedge y_k^-)}_{\mathbf{w}^-(\xi, \lambda)} \wedge \underbrace{(y_1^+ \wedge \cdots \wedge y_{n-k}^+)}_{\mathbf{w}^+(\xi, \lambda)}.$$

Prefactor ensures  $\xi$ -independence, from Abel's theorem.

## Exterior product of a vector space

Let  $V$  be a vector space with basis  $e_1, \dots, e_n$ .

The **exterior product space**  $\Lambda^k(V)$  is a vector space with basis

$$\{e_{i_1} \wedge \dots \wedge e_{i_k} : 1 \leq i_1 \leq \dots \leq i_k \leq n\}.$$

For example,  $\Lambda^2(\mathbb{C}^4)$  is six dimensional with basis

$$e_1 \wedge e_2, e_1 \wedge e_3, e_1 \wedge e_4, e_2 \wedge e_3, e_2 \wedge e_4, e_3 \wedge e_4.$$

The **Grassmannian manifold**  $G_k(V)$  is the set of  $k$ -dimensional subspaces of  $V$ . We consider the identification

$$\text{span}\{v_1, \dots, v_k\} \in G_k(V) \leftrightarrow v_1 \wedge \dots \wedge v_k \in \Lambda^k(V).$$

# The Grassmannian manifold

We can embed  $G_k(V)$  in  $\Lambda^k(V)$ , or to be precise,  $\mathbb{P}(\Lambda^k(V))$ .

A form  $w \in \Lambda^k(V)$  is **decomposable** if it can be written as  $w = v_1 \wedge \dots \wedge v_k$  with  $v_i \in V$ .

Only decomposable forms correspond to subspaces.

Consider for example  $\Lambda^2(\mathbb{C}^4)$ . The form

$$S_1 e_1 \wedge e_2 + S_2 e_1 \wedge e_3 + S_3 e_1 \wedge e_4 + S_4 e_2 \wedge e_3 + S_5 e_2 \wedge e_4 + S_6 e_3 \wedge e_4$$

is decomposable iff

$$S_1 S_6 - S_2 S_5 + S_3 S_4 = 0.$$

# Lifting the differential equation

A **linear** differential equation on  $V$

$$y' = A(x)y \quad (*)$$

induces an equation on  $\Lambda^k(V)$ :

$$w' = \ell(A(x))w \quad (\dagger).$$

For example with  $k = 2$  and  $V = \mathbb{C}^n$ .

If  $y_1$  and  $y_2$  solve  $(*)$  then  $w = y_1 \wedge y_2$  solves  $(\dagger)$ .

# Outline

- 1 Evans function
- 2 Numerical computation
- 3 Exterior product spaces
- 4 Numerical methods
- 5 Examples

## Computing the Evans function II

Now basic **numerical** computation:

- ▶ Compute the unstable eigenvectors  $v_1^-, \dots, v_k^-$  of  $A^-$ .
- ▶ Lift the equation to  $\Lambda^k(\mathbb{C}^n)$ :  $w' = \ell(A(x, \lambda)) w$ ; and rescale  $w(x) = e^{(\mu_1^- + \dots + \mu_k^-)x} u(x)$  to solve

$$u' = \left( \ell(A(x, \lambda)) - (\mu_1^- + \dots + \mu_k^-) I \right) u,$$

with initial condition  $u(-L) = v_1^- \wedge \dots \wedge v_k^-$  (where  $L$  is large) to get  $w^-(\xi)$ .

- ▶ Compute  $w^+(\xi)$  similarly, and evaluate

$$D(\lambda) = w^- \wedge w^+.$$

(Bridges '99; Brin '00; Afendikov & Bridges '01)

Same as **Compound matrix method**.

(Davey '79; Ng & Reid '79)

# Magnus series

We need to solve the **linear** differential equation

$$y' = A(x) y .$$

Solution

$$y(x) = \exp(\sigma(x)) y(0) ,$$

where

$$\sigma(x) = \int_0^x A(\xi) d\xi + \frac{1}{2} \int_0^x \int_0^{\xi_1} [A(\xi_1), A(\xi_2)] d\xi_2 d\xi_1 + \dots .$$

Converges if  $\int_0^x \|A(\xi)\| d\xi < \pi$ .

**(Moan & Niesen '06)**



# Magnus numerical method

Truncate Magnus series and replace  $A(x)$  by interpolant at Gauss–Legendre points  $x_{1,2} = \left(\frac{1}{2} \pm \frac{\sqrt{3}}{6}\right)x$ :

$$y(x) \approx \exp\left(\frac{1}{2}x(A(x_1) + A(x_2)) - \frac{\sqrt{3}}{12}[A(x_1), A(x_2)]\right) y(0).$$

This is a method of **order four**.

**(Iserles & Norsett '99)**

Preserves Grassmannian invariants (decomposability conditions).

**(Niesen '05)**

## Other numerical methods

- ▶ In the case  $k = 2$  and  $n = 4$ , the Grassmannian is **attractive**, if we replace  $w' = \ell(A(x, \lambda)) w$  by  $w' = \ell(A(x, \lambda - \sigma I)) w$ , where  $\sigma$  is the largest eigenvalue, provided the spectrum of  $A$  changes not too much as  $x$  varies.  
(Bridges, Derks & Gottwald '02)
- ▶ If  $\text{tr} A = 0$ , the Grassmannian is a **strong quadratic invariant**. Gauss–Legendre methods (eg. implicit midpoint rule) conserve these.  
(Allen & Bridges '02)
- ▶ In **practice**, with proof when  $n = 2$ , fourth order Gauss–Legendre is globally most accurate.  
(Aparicio, Malham & Oliver '05; Malham & Niesen '06)

# Outline

- 1 Evans function
- 2 Numerical computation
- 3 Exterior product spaces
- 4 Numerical methods
- 5 **Examples**

# Autocatalytic model

The autocatalytic reaction  $U + mV \rightarrow (m + 1)V$  is modeled by

$$\begin{aligned}u_t &= \delta u_{xx} - uv^m, \\v_t &= v_{xx} + uv^m.\end{aligned}$$

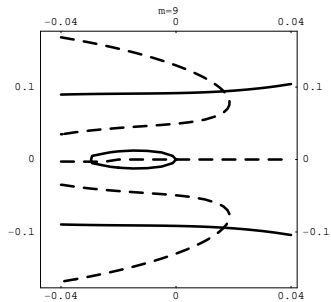
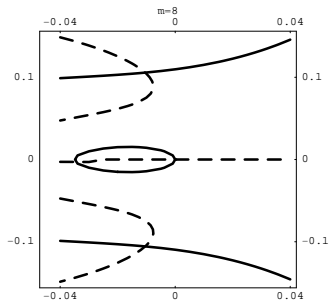
There is a unique travelling wave solution with  $(u, v) \rightarrow (0, 1)$  as  $x \rightarrow -\infty$  and  $(u, v) \rightarrow (1, 0)$  as  $x \rightarrow +\infty$  for any speed  $c \in [c_*, \infty)$ .

Evans function evaluated with the Magnus and Gauss–Legendre methods to assess the stability of travelling wave with  $c = c_*$ .

**Precomputation:**  $w' = A(x, \lambda) w$  with  $w(-L) = w_0$ .

$$A(x, \lambda) = A_0(x) + \lambda A_1(x) + \mu A_2(x).$$

# Autocatalytic model II



# Stability of rotating Ekman layer

Linearization of the 3d Navier–Stokes equation in a rotating frame about the Ekman layer coupled to a compliant surface leads to

$$\begin{aligned}\phi'''' - b(x)\phi'' - a(x)\phi + 2\psi' &= 0, \\ \psi'' + (\gamma^2 - b(x))\psi - i\gamma RV'(x)\phi - 2\phi' &= 0,\end{aligned}$$

for  $0 \leq x < \infty$  with compliant surface BCs at  $x = 0$ .

Lifting yields an ODE on  $\Lambda^3(\mathbb{C}^6)$ , which has dimension 20.

However the dimension of the Grassmannian is only 9.

(Allen & Bridges '03)

## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

- ▶ (+) simple (on finite intervals using uniform mesh);



## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

- ▶ (+) simple (on finite intervals using uniform mesh);
- ▶ (-) spurious eigenvalues (can be excised);

## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

- ▶ (+) simple (on finite intervals using uniform mesh);
- ▶ (-) spurious eigenvalues (can be excised);
- ▶ (-) mesh reduction expensive;

## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

- ▶ (+) simple (on finite intervals using uniform mesh);
- ▶ (-) spurious eigenvalues (can be excised);
- ▶ (-) mesh reduction expensive;
- ▶ (-) non-selfadjoint problems problematic.

## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

- ▶ (+) simple (on finite intervals using uniform mesh);
- ▶ (-) spurious eigenvalues (can be excised);
- ▶ (-) mesh reduction expensive;
- ▶ (-) non-selfadjoint problems problematic.

Shooting methods:

## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

- ▶ (+) simple (on finite intervals using uniform mesh);
- ▶ (-) spurious eigenvalues (can be excised);
- ▶ (-) mesh reduction expensive;
- ▶ (-) non-selfadjoint problems problematic.

Shooting methods:

- ▶ (+) Higher order approximations with uniform error bounds;

## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

- ▶ (+) simple (on finite intervals using uniform mesh);
- ▶ (-) spurious eigenvalues (can be excised);
- ▶ (-) mesh reduction expensive;
- ▶ (-) non-selfadjoint problems problematic.

Shooting methods:

- ▶ (+) Higher order approximations with uniform error bounds;
- ▶ (+) Non-selfadjoint problems natural.

## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

- ▶ (+) simple (on finite intervals using uniform mesh);
- ▶ (-) spurious eigenvalues (can be excised);
- ▶ (-) mesh reduction expensive;
- ▶ (-) non-selfadjoint problems problematic.

Shooting methods:

- ▶ (+) Higher order approximations with uniform error bounds;
- ▶ (+) Non-selfadjoint problems natural.
- ▶ (-)  $\dim(\Lambda^k(\mathbb{C}^n)) = \binom{n}{k}$ .

## Summary: shooting vs discretization

Discretization of the linearized operators via finite differences or elements generates a matrix eigenvalue problem.

Discretization methods:

- ▶ (+) simple (on finite intervals using uniform mesh);
- ▶ (-) spurious eigenvalues (can be excised);
- ▶ (-) mesh reduction expensive;
- ▶ (-) non-selfadjoint problems problematic.

Shooting methods:

- ▶ (+) Higher order approximations with uniform error bounds;
- ▶ (+) Non-selfadjoint problems natural.
- ▶ (-)  $\dim(\Lambda^k(\mathbb{C}^n)) = \binom{n}{k}$ .
- ▶ (+) Continuous orthogonalization.



# Continuous orthogonalization

(Humphreys & Zumbrun '05)

With

$$Y = (y_1^- \cdots y_k^-),$$

consider polar decomposition

$$Y = \Omega \alpha, \quad \det \alpha = \gamma.$$

Then

$$\begin{aligned}\Omega' &= (I - \Omega \Omega^*) A(x, \lambda) \Omega, \\ \gamma' &= \text{Tr}(\Omega^* A(x, \lambda) \Omega) \gamma.\end{aligned}$$

Integrate: need to preserve Stiefel manifold:  $\Omega^* \Omega = I$ .