Shooting and operator determinant techniques for computing spectra

Simon J.A. Malham
Issa Karambal (NAIS),
Veerle Ledoux (Ghent),
Robert Marangell (UNC),
Jitse Niesen (Leeds),
Vera Thümmler (D-fine)

Heriot–Watt University, Edinburgh, UK

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Spectral problems

Parabolic nonlinear systems on $\mathbb{R} \times \mathbb{T}$:

$$\partial_t U = B\,\Delta U + c\,\partial_x U + F(U).$$

Travelling wave U_c. Small perturbations U satisfy:

$$B\,\Delta U + c\,\partial_x U + \mathrm{D}F(U_c)U = \lambda U.$$

Main solution approaches:

- *Projection and iteration.*
- *Shooting and matching.*
- *Operator determinants.*

Setup

On $\mathbb{R}$: $B\,\partial_{xx}U + c\,\partial_x U + \mathrm{D}F(U_c)U = \lambda U$

$$\Leftrightarrow \qquad \begin{aligned} \partial_x U &= P, \\ \partial_x P &= B^{-1}\big(\lambda - \mathrm{D}F(U_c)\big)U - cB^{-1}P. \end{aligned}$$

$$\Leftrightarrow \qquad Y' = A(x;\lambda)\,Y.$$

For $\lambda \in \mathbb{C}$: matching condition

$$\begin{aligned} D(\lambda) &:= \mathrm{e}^{\int_0^x \mathrm{Tr} A(\xi;\lambda)\,\mathrm{d}\xi} \det\big(Y_1^- \cdots Y_k^- \, Y_{k+1}^+ \cdots Y_n^+\big) \\ &= \mathrm{e}^{\int_0^x \mathrm{Tr} A(\xi;\lambda)\,\mathrm{d}\xi} \det\big(Y^- \;\; Y^+\big) \end{aligned}$$

Synonyms

Carrying the same information are:

- In one dimension $d = 1$:
  - Evans determinant function;
  - Miss-distance function;
  - Fredholm determinant;
  - Titchmarsh–Weyl matrix-function;
  - Grassmannian Riccati flow.
- In multi-dimensions $d > 1$:
  - Fredholm determinant;
  - Dirichlet-to-Neumann map;
  - Fredholm Grassmannian flow.

Numerical issues

- Computational domain.
- Different exponential growth rates.
- Polynomial complexity.
- Flow singularities?!
- Where to match?
- Retaining analyticity?
- How to project transversely.
- How to approximate the Fredholm Grassmannian flow.

Stiefel and Grassmann manifolds

- Stiefel manifold:

$$\mathbb{V}(n,k) = \{k\text{-frames centred at the origin}\}.$$

- Grassmann manifold:

$$\mathrm{Gr}(n,k) = \{k\text{-dimensional subspaces of } \mathbb{C}^n\}.$$

- Fibre bundle:

$$\pi\colon \mathbb{V}(n,k) \to \mathrm{Gr}(n,k) \cong \mathbb{V}(n,k)/\mathrm{GL}(k)$$
$$\pi\colon k\text{-frame} \mapsto \text{spanning } k\text{-plane}$$

Representation

$\pi\colon Y = y_{\mathfrak{i}^\circ} u \mapsto y_{\mathfrak{i}^\circ}$

Example coordinate patch:

$$y_{\mathfrak{i}^\circ} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ \hat{y}_{k+1,1} & \hat{y}_{k+1,2} & \cdots & \hat{y}_{k+1,k} \\ \hat{y}_{k+2,1} & \hat{y}_{k+2,2} & \cdots & \hat{y}_{k+2,k} \\ \vdots & \vdots & \ddots & \vdots \\ \hat{y}_{n,1} & \hat{y}_{n,2} & \cdots & \hat{y}_{n,k} \end{pmatrix}.$$

Local chart $\mathbb{U}_{\mathfrak{i}} \to \mathbb{C}^{(n-k)k}$ given by $y_{\mathfrak{i}^\circ} \mapsto \hat{y}$.

Grassmannian flows

$$Y' = A(x, Y)\, Y$$

Substitute decomposition $Y = y_{\mathfrak{i}^\circ} u$:

$$y_{\mathfrak{i}^\circ}' u + y_{\mathfrak{i}^\circ} u' = (A_{\mathfrak{i}} + A_{\mathfrak{i}^\circ} \hat{y})\, u$$

Project onto $\mathfrak{i}^\circ$th and $\mathfrak{i}$th rows:

$$\hat{y}' = c + d\,\hat{y} - \hat{y}(a + b\,\hat{y}) \qquad \text{and} \qquad u' = (a + b\,\hat{y})\, u$$

where $a = A_{\mathfrak{i}\times\mathfrak{i}}$, $b = A_{\mathfrak{i}\times\mathfrak{i}^\circ}$, $c = A_{\mathfrak{i}^\circ\times\mathfrak{i}}$ and $d = A_{\mathfrak{i}^\circ\times\mathfrak{i}^\circ}$.

Grassmannian Gaussian elimination method (GGEM)

$$
\begin{array}{ccccc}
\mathbb{C}^{(n-k)k} & \xrightarrow{\text{chartmap}^{-1}} & \mathbb{U}_{\mathfrak{i}} & \xrightarrow{\text{id}} & \mathbb{V}(n,k) \\
\Big\downarrow \textit{Riccati} & & \Big\downarrow \textit{GGEM} & & \Big\downarrow \textit{RK} \\
\mathbb{C}^{(n-k)k} & \xleftarrow[\text{newchart}]{} & \mathbb{U}_{\mathfrak{i}'} & \xleftarrow[\text{QOGE}]{} & \mathbb{V}(n,k)
\end{array}
$$

Quasi-optimal Gaussian elimination (QOGE)

GE with *free* stepwise max pivot, generates:

$$\begin{pmatrix} * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ * & * & * & * & \cdots & * \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ * & * & * & * & \cdots & * \\ * & * & * & * & \cdots & * \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ * & * & * & * & \cdots & * \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ * & * & * & * & \cdots & * \\ 0 & 0 & 0 & 0 & \cdots & 1 \\ * & * & * & * & \cdots & * \end{pmatrix}$$

Applications (planar fronts)

- $D(\lambda) := \mathrm{e}^{-\int_0^x \mathrm{Tr} A(\xi;\lambda)\,\mathrm{d}\xi} \det\big(Y^-(x;\lambda)\ \ Y^+(x;\lambda)\big)$
- $\det\big(Y^-\ Y^+\big) = \det\big(y_{\mathfrak{i}_-^\circ}\quad y_{\mathfrak{i}_+^\circ}\big) \cdot \det\, u_{\mathfrak{i}_-} \cdot \det\, u_{\mathfrak{i}_+}$
- $D(\lambda; x_*) := \det\big(y_{\mathfrak{i}_-^\circ}\quad y_{\mathfrak{i}_+^\circ}\big)$
- Record any patch change to retain analyticity.

Boussinesq system

PDE: $u_{tt} = (1 - c^2)\, u_{xx} + 2c\, u_{xt} - u_{xxxx} - (u^2)_{xx}$.

Solitary waves with sech^2 profile.

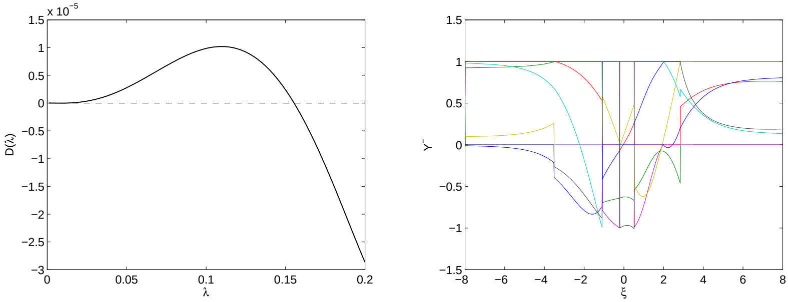


Figure: Evans function for $c = 1/4$ with GGEM-RK and $x_* = 8$ (left panel). Entries of $y_\imath$ for $\lambda = 0.15543141$ (right panel).

Boussinesq: error vs matching point

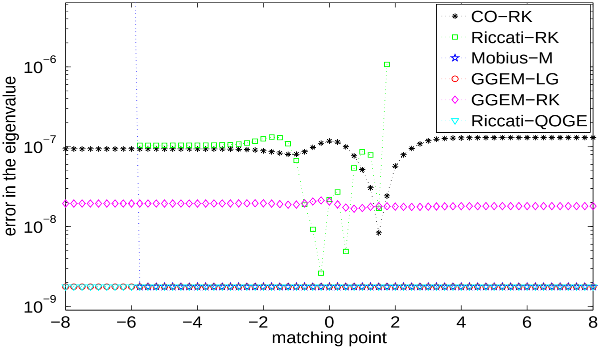


Figure: Error in the eigenvalue for different choices of the matching point: $N = 512$.

Autocatalytic fronts

$$\partial_t u = \delta \Delta u + c \partial_x u - uv^m,$$
$$\partial_t v = \Delta v + c \partial_x v + uv^m.$$

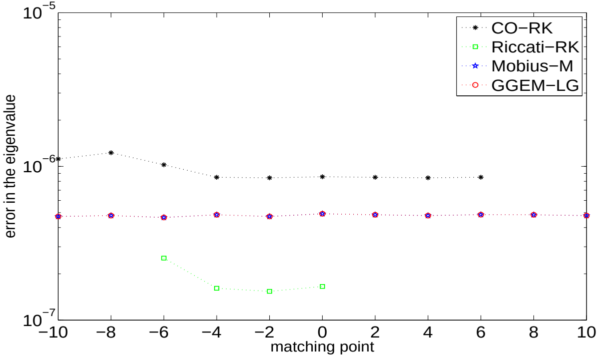


Figure: Error in the eigenvalue when $\delta = 0.1$ and $m = 9$: $N = 256$.

Transverse Fourier basis

On $\mathbb{R} \times \mathbb{T}$ we have:

$$B\Delta U + c\,\partial_x U + \mathrm{D}F(U_c)U = \lambda U.$$

On the Fourier modes $k = -K, -K+1, \ldots, K$:

$$\partial_x \hat{U}_k = \hat{P}_k,$$

$$\partial_x \hat{P}_k = \lambda B^{-1}\hat{U}_k + (k/\tilde{L})^2 \hat{U}_k - \sum_{\nu=-K}^{K} B^{-1}\hat{D}_{k-\nu}\hat{U}_\nu - c\,B^{-1}\hat{P}_k.$$

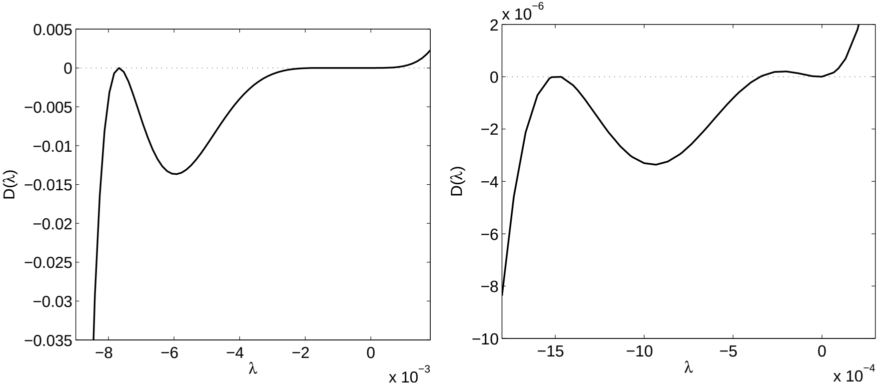
Computing travelling waves: freezing method

Substitute $U(x,y,t) = V(x - \gamma(t), y, t)$ into original PDE:

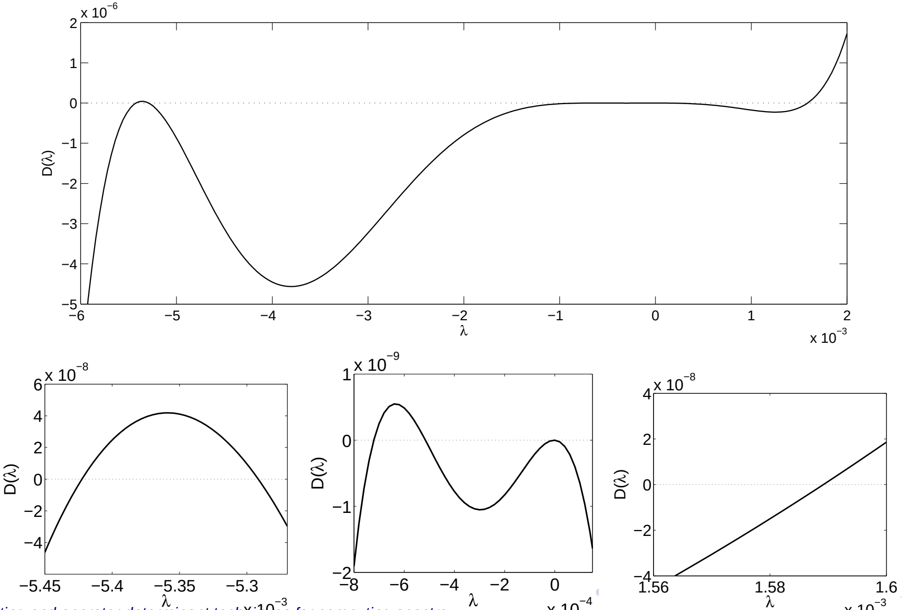
$$\partial_t V = B\,\Delta V + \gamma'(t)\partial_x V + F(V),$$
$$0 = \int_{\mathbb{R}\times\mathbb{T}} \left(\partial_x \hat{V}(x,y,t)\right)^{\mathrm{T}} \left(\hat{V}(x,y,t) - V(x,y,t)\right) \mathrm{d}x\,\mathrm{d}y.$$

(Developed by Beyn and Thümmler.)

Wrinkled front: Evans function for $\delta = 2.5$



Wrinkled front: Evans function for $\delta = 3$



Wrinkled front: Eigenvalues for $\delta = 3$

K	Eigenvalues (Evans function)				
3	0.001609	−0.000026	−0.000781	−0.001296	−0.000670
4	0.001609	0.000002	−0.000001	−0.000519	−0.000670
5	0.001589	0.000002	−0.000001	−0.000519	−0.000720
6	0.001589	−0.000002	−0.000003	−0.000515	−0.000720
7	0.001589	−0.000002	−0.000003	−0.000515	−0.000721
8	0.001589	−0.000002	−0.000003	−0.000515	−0.000721
9	0.001589	−0.000002	−0.000003	−0.000515	−0.000721
⋮			⋮		
24	0.001589	−0.000002	−0.000003	−0.000515	−0.000721
	Eigenvalues (ARPACK)				
	0.001592	0.000000	0.000000	−0.000514	−0.000719

Wrinkled front: contour integration

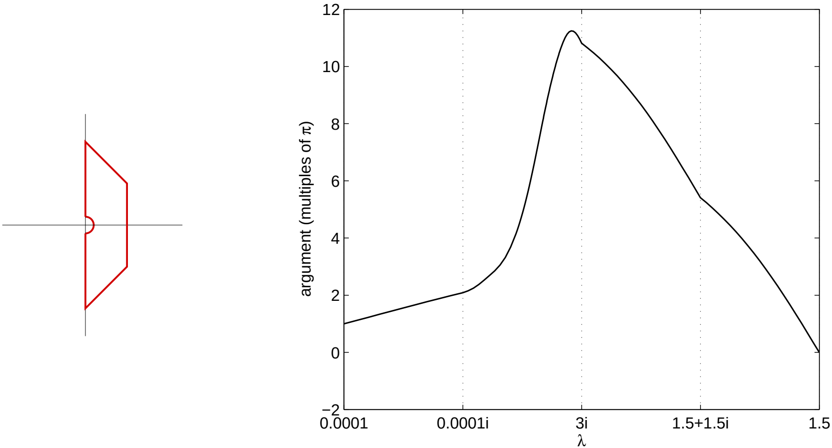
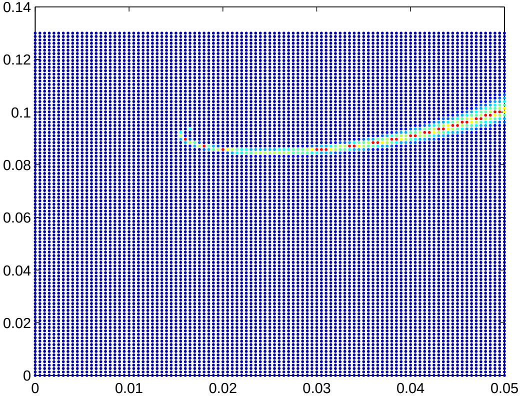


Figure: Left panel: contour. Right panel: $\arg\big(D(\lambda)\big)$ when λ transverses the top half. $\delta = 3$.

Singularities and Schubert cycles



Fredholm determinant

$$
\begin{aligned}
& Y' = \big(A_0(\lambda) + A_1(x)\big)\,Y \\
\Leftrightarrow \quad & \big(\partial_x - A_0\big)Y = A_1 Y \\
\Leftrightarrow \quad & \big(\mathrm{id} - (K_{A_0} \circ A_1)\big)\,Y = O
\end{aligned}
$$

Compute $\det_{\mathrm{F}}(\mathrm{id} + K)$ for $K = -K_{A_0} \circ A_1$.

For Hilbert space $\mathbb{H}$:

$$
\operatorname{tr} K := \sum_{i \geqslant 1} \langle \varphi_i, K\varphi_i \rangle_{\mathbb{H}} = \int_{\mathbb{R}} \operatorname{tr} G(x; x)\,\mathrm{d}x
$$

Fredholm expansion

$$\det(\mathrm{id} + K) = \sum_{m \geqslant 0} \mathrm{tr}\, K^{\wedge m}$$

where

$$\begin{aligned}
\mathrm{tr}\, K^{\wedge m} &= \sum_{i_1 < \cdots < i_m} \left\langle \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_m}, K\varphi_{i_1} \wedge \ldots \wedge K\varphi_{i_m} \right\rangle_{\mathbb{H}^{\wedge m}} \\
&= \sum_{i_1 < \cdots < i_m} \det\left[\langle \varphi_{i_p}, K\varphi_{i_q} \rangle_{\mathbb{H}} \right]_{p,q \in \{1,\ldots,m\}} \\
&= \frac{1}{m!} \int_{\mathbb{R}^m} \det\left[G(x_i, x_j) \right] \mathrm{d}x_1 \ldots \mathrm{d}x_m
\end{aligned}$$

Bornemann, apply quadrature to:

$$(\mathrm{id} + K)\, Y = f$$

Multi-dimensional shooting

The Fredholm determinant and Evans function are related:

$$\det(\mathrm{id}+K) = \frac{\det(Y^- \;\; Y^+)}{\det(Y_0^- \;\; Y_0^+)}$$

(yet to be proved in general)

Suppose $\mathbb{H} = \mathbb{H}_1 \oplus \mathbb{H}_2$: say $\mathbb{H}_1 = H^{\frac{1}{2}}(\partial\Omega)$ and $\mathbb{H}_2 = H^{-\frac{1}{2}}(\partial\Omega)$:

$$\mathrm{Gr}(\mathbb{H}) := \begin{cases} W & : \pi_1 : W \to \mathbb{H}_1 \text{ is Fredholm} \\ W & : \pi_2 : W \to \mathbb{H}_2 \text{ is Hilbert–Schmidt} \end{cases}$$

i.e. it is a Hilbert manifold modelled on $\mathbb{J}_2(\mathbb{H}_1, \mathbb{H}_2)$.