

Spectral computations and Grassmannians

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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:

$$B \Delta U + c \partial_x U + DF(U_c)U = \lambda U.$$

Main solution approaches:

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

Setup

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

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

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

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

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

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 manifold:

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

- Grassmann manifold:

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

- Fibre bundle:

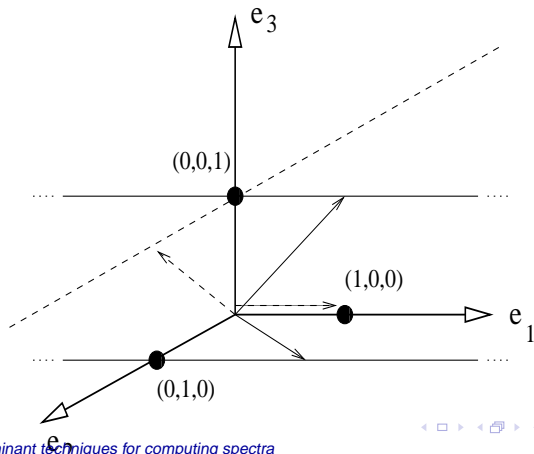
$$\pi: \mathbb{V}(n, k) \rightarrow \text{Gr}(n, k) \cong \mathbb{V}(n, k)/\text{GL}(k)$$

$$\pi: k\text{-frame} \mapsto \text{spanning } k\text{-plane}$$

Representation

Example: $\text{Gr}(3,2)$

$$\begin{pmatrix} * & 1 & 0 \\ * & 0 & 1 \end{pmatrix}; \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & * & 1 \end{pmatrix}; \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$



Representation II

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

Example coordinate patch:

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

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

Grassmannian flows

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

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

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

Project onto i° th and i th rows:

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

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

Grassmannian Gaussian elimination method (GGEM)

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

Quasi-optimal Gaussian elimination (QOGE)

GE with *free* stepwise max pivot, generates:

$$\begin{pmatrix} * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ * & * & * & * & \dots & * \\ 0 & 1 & 0 & 0 & \dots & 0 \\ * & * & * & * & \dots & * \\ * & * & * & * & \dots & * \\ 0 & 0 & 1 & 0 & \dots & 0 \\ * & * & * & * & \dots & * \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ * & * & * & * & \dots & * \\ 0 & 0 & 0 & 0 & \dots & 1 \\ * & * & * & * & \dots & * \end{pmatrix}$$

Applications (planar fronts)

- $D(\lambda) := e^{-\int_0^x \text{Tr}A(\xi; \lambda) d\xi} \det(Y^-(x; \lambda) \ Y^+(x; \lambda))$
- $\det(Y^- \ Y^+) = \det(y_{i_-}^\circ \ y_{i_+}^\circ) \cdot \det u_{i_-} \cdot \det u_{i_+}$
- $D(\lambda; \mathbf{x}_*) := \det(y_{i_-}^\circ \ y_{i_+}^\circ)$
- 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.

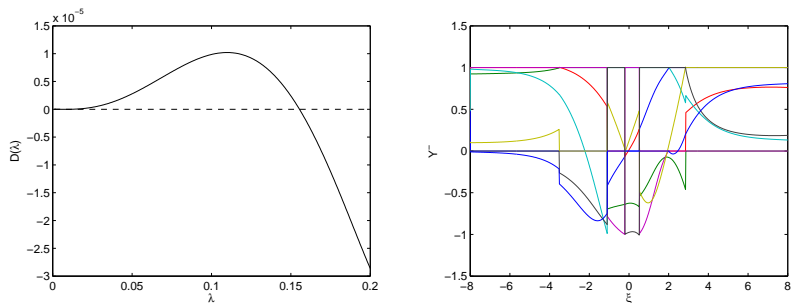


Figure: Evans function for $c = 1/4$ with GGEM-RK and $x_* = 8$ (left panel).
Entries of y_i for $\lambda = 0.15543141$ (right panel).

Boussinesq: error vs matching point

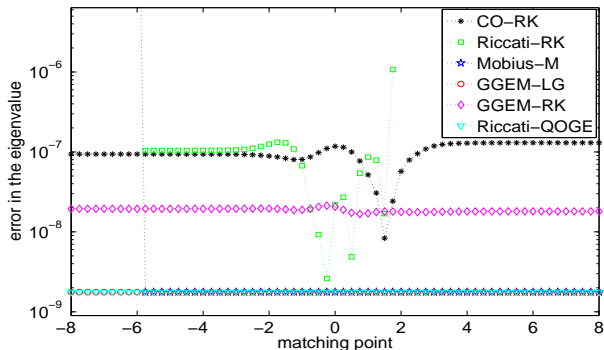


Figure: Error in the eigenvalue for different choices of the matching point: $N = 512$.

Autocatalytic fronts

$$\begin{aligned}\partial_t u &= \delta \Delta u + c \partial_x u - uv^m, \\ \partial_t v &= \Delta v + c \partial_x v + uv^m.\end{aligned}$$

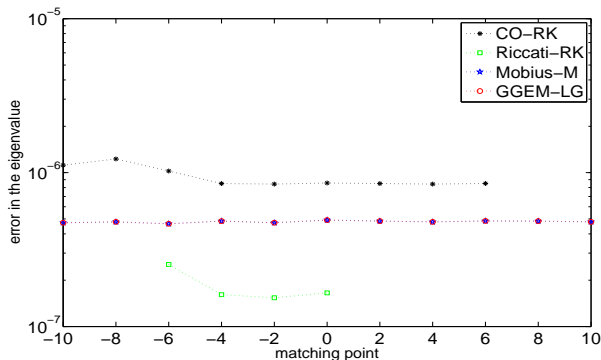


Figure: Error in the eigenvalue when $\delta = 0.1$ and $m = 9$: $N = 256$.

Transverse Fourier basis

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

$$B\Delta U + c\partial_x U + DF(U_c)U = \lambda U.$$

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

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

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

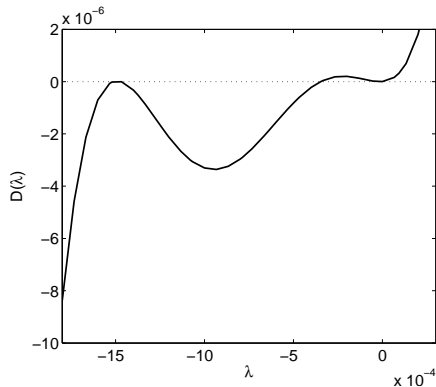
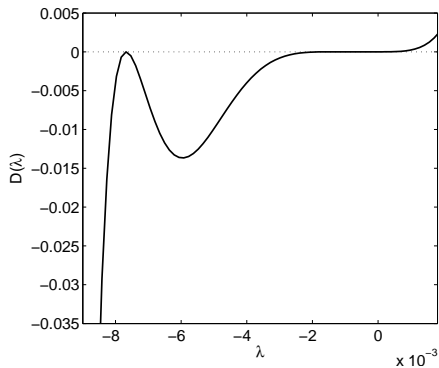
Computing travelling waves: freezing method

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

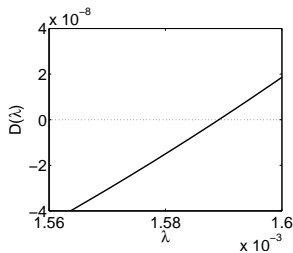
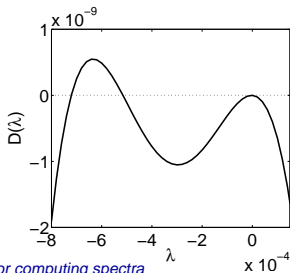
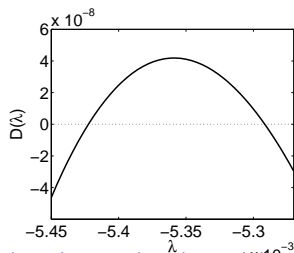
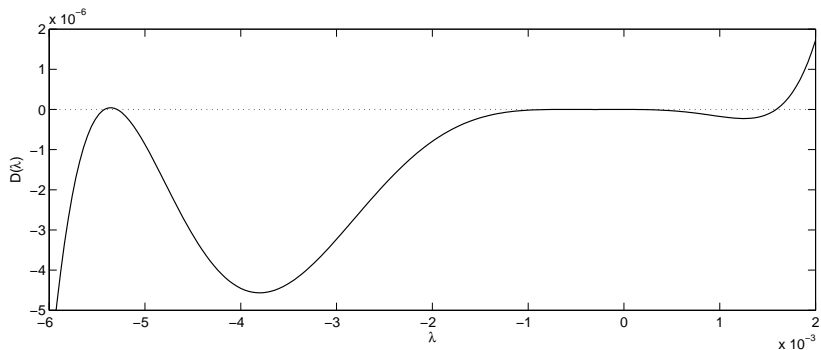
$$\begin{aligned}\partial_t V &= B \Delta V + \gamma'(t) \partial_x V + F(V), \\ 0 &= \int_{\mathbb{R} \times \mathbb{T}} (\partial_x \hat{V}(x, y, t))^T (\hat{V}(x, y, t) - V(x, y, t)) dx dy.\end{aligned}$$

(Developed by Beyn and Thümmeler.)

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
\vdots			\vdots		
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

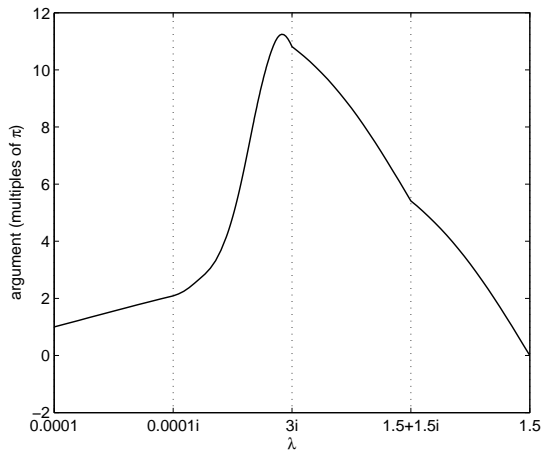
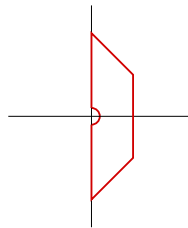
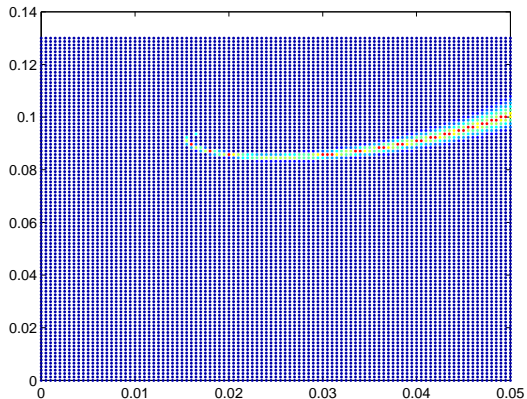


Figure: Left panel: contour. Right panel: $\arg(D(\lambda))$ when λ transverses the top half. $\delta = 3$.

Singularities and Schubert cycles



$$\begin{aligned} Y' &= (A_0(\lambda) + A_1(x)) Y \\ \Leftrightarrow (\partial_x - A_0) Y &= A_1 Y \\ \Leftrightarrow (\text{id} - (K_{A_0} \circ A_1)) Y &= 0 \end{aligned}$$

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

For Hilbert space \mathbb{H} :

$$\text{tr } K := \sum_{i \geq 1} \langle \varphi_i, K \varphi_i \rangle_{\mathbb{H}} = \int_{\mathbb{R}} \text{tr } G(x; x) dx$$

Fredholm expansion

$$\det(\text{id} + K) = \sum_{m \geq 0} \text{tr} K^{\wedge m}$$

where

$$\begin{aligned} \text{tr} K^{\wedge m} &= \sum_{i_1 < \dots < i_m} \langle \varphi_{i_1} \wedge \dots \wedge \varphi_{i_m}, K \varphi_{i_1} \wedge \dots \wedge K \varphi_{i_m} \rangle_{\mathbb{H}^{\wedge m}} \\ &= \sum_{i_1 < \dots < i_m} \det \left[\langle \varphi_{i_p}, K \varphi_{i_q} \rangle_{\mathbb{H}} \right]_{p, q \in \{1, \dots, m\}} \\ &= \frac{1}{m!} \int_{\mathbb{R}^m} \det [G(x_i, x_j)] dx_1 \dots dx_m \end{aligned}$$

Bornemann, apply quadrature to:

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

Multi-dimensional shooting

The Fredholm determinant and Evans function are related:

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

(Proved in general setting by Karambal 2011.)

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

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

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

References

- 1 J.C., Alexander, R. Gardner, and C.K.R.T. Jones, *A topological invariant arising in the stability analysis of traveling waves*, J. Reine Angew. Math. 410 (1990), pp. 167–212.
- 2 N.D. Aparicio, S.J.A. Malham and M. Oliver, *Numerical evaluation of the Evans function by Magnus integration*, BIT 45 (2005), pp. 219–258.
- 3 N.J. Balmforth, R.V. Craster and S.J.A. Malham, *Unsteady fronts in an autocatalytic system*, Proc. R. Soc. Lond A. 455 (1999), pp. 1401–1433.
- 4 J. Humpherys and K. Zumbrun, *An efficient shooting algorithm for Evans function calculations in large systems*, Physica D 220 (2006), pp. 116–126.
- 5 V. Ledoux, M. Van Daele and G. Vanden Berghe, *A numerical procedure to solve the multichannel Schrödinger eigenvalue problem*, Comp. Phys. Commun. 176 (2007). pp. 191-199.

References II

- 1 V. Ledoux, S.J.A. Malham and V. Thümmler, *Grassmannian spectral shooting*, *Mathematics of Computation* 79 (2010), pp. 1585–1619.
- 2 V. Ledoux, S.J.A. Malham, J. Niesen and V. Thümmler, *Computing stability of multi-dimensional travelling waves*, *SIADS* 8(1) (2009), pp. 480–507.
- 3 S.J.A. Malham and A. Wiese, *Stochastic Lie group integrators*, *SIAM Journal on Scientific Computing* 30(2) (2008), pp. 597–617.
- 4 G. Lord, S.J.A. Malham and A. Wiese, *Efficient strong integrators for linear stochastic systems* *SIAM Journal on Numerical Analysis* 46(6) (2008), pp. 2892–2919.
- 5 S.J.A. Malham and A. Wiese, *Stochastic expansions and Hopf algebras*, *Proceedings of the Royal Society A* 465 (2009), pp. 3729–3749.