Pollution-free methods for finding eigenvalues in the gaps of the continuous spectrum

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$(\mathcal{L}_k)_{k\in\mathbb{N}}$ — a sequence of closed linear subspaces of $\mathrm{Dom}(A)$ (usually finite-dimensional, we can take $\mathcal{L}_k = \mathrm{span}\{e_1, \dots, e_k\}$), projectors $P_k : \mathcal{H} \to \mathcal{L}_k$ converge to I strongly

$\Lambda(A)$ — the set of all such sequences of subspaces

$\mathrm{Spec}(A, \mathcal{L}_k)$ is the spectrum of $P_k A : \mathcal{L}_k \to \mathcal{L}_k (= M_k = [\langle Ae_i, e_j\rangle]_{i,j=1}^k)$

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Question: whether or not $\boxed{\lim_{k\to\infty} \mathrm{Spec}(A, \mathcal{L}_k) = \mathrm{Spec}(A)}$?

Answer

not necessarily, we may have either

- *lack of approximation:* $\mathrm{Spec}(A) \setminus (\lim_{k\to\infty} \mathrm{Spec}(A, \mathcal{L}_k)) \neq \varnothing$

or

- *spectral pollution:* $\underbrace{\left(\lim_{k\to\infty} \mathrm{Spec}(A, \mathcal{L}_k)\right) \setminus \mathrm{Spec}(A)}_{\text{spurious eigenvalues}} \neq \varnothing$

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Reminder: $R(A) := \{\lambda : \exists (A-\lambda)^{-1}\}$ — resolvent set of A

$\mathrm{Spec}(A) := \mathbb{R} \setminus R(A)$ — spectrum of A

$\{\lambda : \exists u \in \mathcal{H} \setminus \{0\} \text{ such that } Au = \lambda u\} \subseteq \mathrm{Spec}(A)$ —eigenvalues of A

$\mathrm{Spec}_{\mathrm{d}}(A) := \{\text{isolated eigenvalues of finite multiplicity}\} \subseteq \mathrm{Spec}(A)$ — discrete spectrum of A

$\mathrm{Spec}_{\mathrm{ess}}(A) := \mathrm{Spec}(A) \setminus \mathrm{Spec}_{\mathrm{d}}(A)$ — essential spectrum of A

Limit of the spectrum

What is "$\lim\limits_{k\to\infty} M_k$" for a sequence of sets $M_k \subset \mathbb{C}$?
We may use both

$$\lim_{k\to\infty}{}_{*} M_k = \left\{ z \in \mathbb{C} : \exists z_k \in M_k \text{ s.t. } \lim_{k\to\infty} z_k = z \right\};$$

and

$$\lim_{k\to\infty}{}^{*} M_k = \left\{ z \in \mathbb{C} : \exists k_m \in \mathbb{N}, \exists z_{k_m} \in M_{k_m} \text{ s.t. } k_m \to \infty \text{ and } z_{k_m} \to z \text{ as } m \to \infty \right\}$$

Remark: If A is bounded, then
$\lim\limits_{k\to\infty}{}^{*} \operatorname{Spec}(A, \mathcal{L}_k) \supseteq \lim\limits_{k\to\infty}{}_{*} \operatorname{Spec}(A, \mathcal{L}_k) \supseteq \operatorname{Spec}(A)$. If, in addition, the essential spectrum of A is either empty or connected, then the equalities hold [see e.g. Shargorosky 2000; well known for compact operators]

Trivial example I

Example I: $A = aI : L_2([-\pi,\pi]) \to L_2([-\pi,\pi])$ with

$$a(x) = \begin{cases} -\frac{3}{2} + \frac{1}{2}\cos\sqrt{5}\,x\,, & \text{for} \quad -\pi \le x < 0\,, \\ 2 + \cos\sqrt{2}\,x\,, & \text{for} \quad 0 \le x < \pi\,. \end{cases}$$

Obviously, $\mathrm{Spec}(A) = \mathrm{Spec}_{\mathrm{ess}}(A) = a([-\pi,\pi]) = [-2,-1] \cup [1,3]$.
Fourier basis $e_k(x) := (2\pi)^{-1/2}\exp(ikx)$, $k \in \mathbb{Z}$.
A is represented as a (doubly) infinite Toeplitz matrix.
Take $\mathcal{L}_N := \mathrm{span}(\{e_k\}_{k=-n}^{n})$, where $N = \dim\mathcal{L}_N = 2n+1$.

Trivial example I — numerics

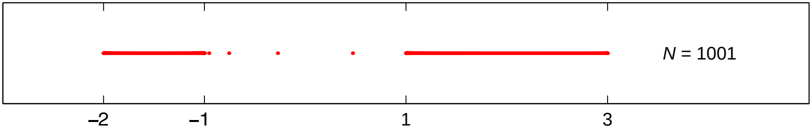

Figure: $\text{Spec}(A, \mathcal{L}_{1001})$.

N	101	401	701	1001
$\text{Spec}(A, \mathcal{L}_N) \cap (-1, 1)$			-0.9997	-0.9985
		-0.9834	-0.9673	-0.9550
	-0.9264	-0.8250	-0.7823	-0.7553
	-0.4866	-0.3478	-0.3002	-0.2721
	0.4362	0.4597	0.4673	0.4717

Table: Eigenvalues lying in the gap of the essential spectrum of A for some values of N.

Why spurious eigenvalues?

Presence of **spurious eigenvalues** is not surprising:

$$P_{\mathcal{L}_N} A P_{\mathcal{L}_N} \equiv P_{\mathcal{M}_N} T_a P_{\mathcal{M}_N}$$

where $T_a : \mathtt{H}^2 \to \mathtt{H}^2$ (Hardy space) and $\mathcal{M}_N = \{e_k\}_{k=0}^{N-1}$.
But

$$\mathrm{Spec}(T_a) = \mathrm{conv}\,(a\,([-\pi, \pi])) = [-2, 3]$$

[Hartman & Wintner; Szegö].
The interval $(-1, 1)$ is in $\mathrm{Spec}(T_a)$ because of the discontinuities of $a(x)$ at $x = 0$ and $x = -\pi \sim \pi$.

Trivial example II

$H = \begin{pmatrix} -\frac{d^2}{dx^2} & -\frac{d}{dx} \\ \frac{d}{dx} & 2 \end{pmatrix}$ subject to periodic boundary conditions, acting in $L_2([-\pi,\pi])$.

H is Agmon–Douglis–Nirenberg elliptic, so the essential spectrum, by Grubb–Geymonat, is

$$\mathrm{Spec}_{\mathrm{ess}}(H) = \left\{ \lambda \in \mathbb{C} \middle| \; \exists \xi \in \mathbb{R} \setminus \{0\} : \; \det \begin{pmatrix} \xi^2 & i\xi \\ -i\xi & 2-\lambda \end{pmatrix} = 0 \right\} = \{1\}.$$

The discrete spectrum is easy to find analytically:

$$\lambda \in \mathrm{Spec}_{\mathrm{d}}(H) \quad \text{iff} \quad \frac{\lambda(\lambda-2)}{\lambda-1} \in \mathrm{Spec}\left(-\frac{d^2}{dx^2}\right) = \{k^2 : k \in \mathbb{Z}\}. \qquad (1)$$

Trivial example II — numerics

There are two series of eigenvalues

$$\lambda_k^\pm = \frac{k^2 + 2 \pm \sqrt{(k^2+2)^2 - 4k^2}}{2}, \qquad k = 0, 1, 2, \dots$$

(each is a double eigenvalue for $k \neq 0$).

Numerics: Use the finite element method (FEM) - a projection method - and the space $\mathbf{L}_N \times \mathbf{L}_N$ of Lagrange elements.

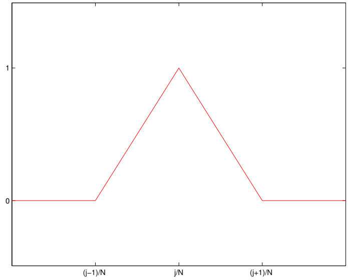

Figure: Element of the space $\mathbf{L}_N$

Trivial example II — numerics (contd.)

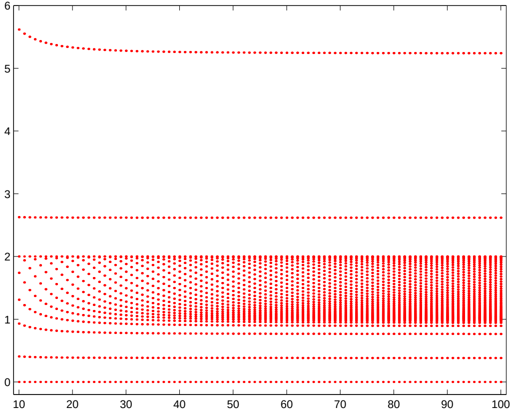

Figure: FEM calculated $\mathrm{Spec}(H, \mathbf{L}_N \times \mathbf{L}_N)$ plotted against N. All eigenvalues in the interval $(1, 2)$ are spurious!

Plan

So far:

. . . spectral pollution does happen. . .

What now?

. . . general theory. . .

. . . how to cure spectral pollution using the second order relative spectra — theory. . .

. . . does it work in practice? — Examples I and II, perturbed periodic Schrödinger operator. . .

Why pollution?

Spectral pollution does not happen if A is bounded and its essential spectrum has no gaps. In other situations, however, it may occur at any point in the gap of the extended essential spectrum

$$\widehat{\mathrm{Spec}}_{\mathrm{ess}}(A) := \widehat{\mathrm{Spec}}(A) \setminus \{\text{isolated eigenvalues of finite multiplicity}\}$$

(here $\widehat{\mathrm{Spec}}(A)$ is the set obtained from $\mathrm{Spec}(A)$ by adding to it $-\infty$, $+\infty$, or both, if A is unbounded below, above, or from both sides, respectively).

Theorem

For any $\lambda \in \mathrm{conv}\left(\widehat{\mathrm{Spec}}_{\mathrm{ess}}(A)\right) \setminus \widehat{\mathrm{Spec}}_{\mathrm{ess}}(A)$ *there exists an increasing sequence* $(\mathcal{L}_k)_{k\in\mathbb{N}} \in \Lambda(A)$ *such that*

$$\lambda \in \mathrm{Spec}(A, \mathcal{L}_k), \qquad \forall k \in \mathbb{N}.$$

Why pollution (more)?

Relative spectral distance

$$\tilde{F}_k(x) := \min_{0 \neq u \in \mathcal{L}_k} \frac{\|P_k(x - A)u\|}{\|u\|}$$

$$\mu \in \operatorname{Spec} M_k \iff \tilde{F}_k(\mu) = 0$$

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$\mu \in \operatorname{Spec} M_k \iff \tilde{F}_k(\mu) = 0 \iff \exists\, v \in \mathcal{L}_k$ s.t. $(\mu - A)v \perp \mathcal{L}_k$.

As $\|(\mu - A)v\|/\|v\|$ is not guaranteed to be small, we have no indication whether μ is close to Spec A or not.

Second order spectra (quadratic projection method)

Definition

Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and let $\mathcal{L}$ be a finite dimensional subspace of $\mathrm{Dom}(A)$. A number $z \in \mathbb{C}$ is said to belong to the *second order spectrum* $\mathrm{Spec}_2(A, \mathcal{L})$ *of* A *relative to* $\mathcal{L}$ if there exists $u \in \mathcal{L} \setminus \{0\}$ such that

$$((A - zI)u, (A - \overline{z}I)v) = 0, \quad \forall v \in \mathcal{L}, \tag{2}$$

where $(\cdot, \cdot)$ is the scalar product in $\mathcal{H}$.

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Remark. Suppose $\mathcal{L} \subset \mathrm{Dom}(A^2)$ and let P be the orthogonal projection onto $\mathcal{L}$. Then $z \in \mathrm{Spec}_2(A, \mathcal{L})$

- iff there exists $u \in \mathcal{L} \setminus \{0\}$ such that $((A - zI)^2 u, v) = 0$, $\forall v \in \mathcal{L}$,
- i.e. iff there exists $u \in \mathcal{L} \setminus \{0\}$ such that $u \in \mathrm{Ker}(P(A - zI)^2)$,
- i.e. iff the operator $Q(z) := P(A - zI)^2 : \mathcal{L} \to \mathcal{L}$ is not invertible.

The last is the definition of the second order relative spectrum introduced by Brian Davies.

Quadratic method does not pollute and approximate!

Theorem (Shargorodsky, Sh./L.)

Suppose that $(a, b) \cap \operatorname{Spec} A = \varnothing$. *If* $z \in D(a, b) := \{w \in \mathbb{C} : |w - (a+b)/2| < (b-a)/2\}$, *then* $Q(z)$ *is non-singular.*

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Theorem (Boulton)

If $\lambda \in \operatorname{Spec}_{\mathrm{d}}(A)$, *then under some natural additional conditions of* $\mathcal{L}_\backslash$

$$\exists \lambda_n \in \operatorname{Spec} Q_n(z) : \lim_{n \to \infty} = \lambda \,.$$

Non-pollution

Corollary

If $z \in \mathrm{Spec}_2(A, \mathcal{L})$ *then*

$$\mathrm{Spec}(A) \cap [\mathrm{Re}\, z - |\mathrm{Im}\, z|, \mathrm{Re}\, z + |\mathrm{Im}\, z|] \neq \varnothing.$$

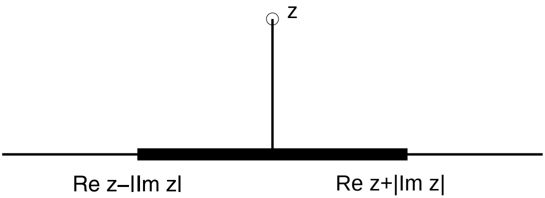

Figure: If z belongs to a second order relative spectrum of A, and $\mathrm{Im}\, z$ is small, then there is a point of the spectrum of A close to $\mathrm{Re}\, z$.

Second order relative spectra in Example I

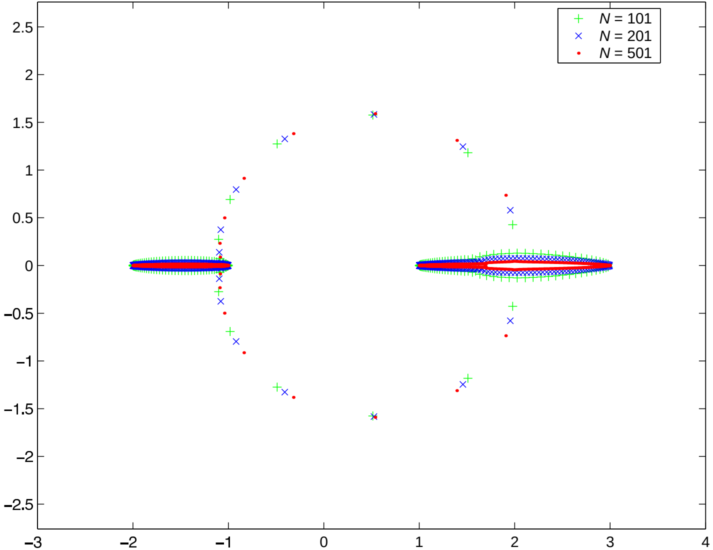

Figure: $\mathrm{Spec}_2(A, \mathcal{L}_N)$

Second order relative spectra in Example I (contd.)

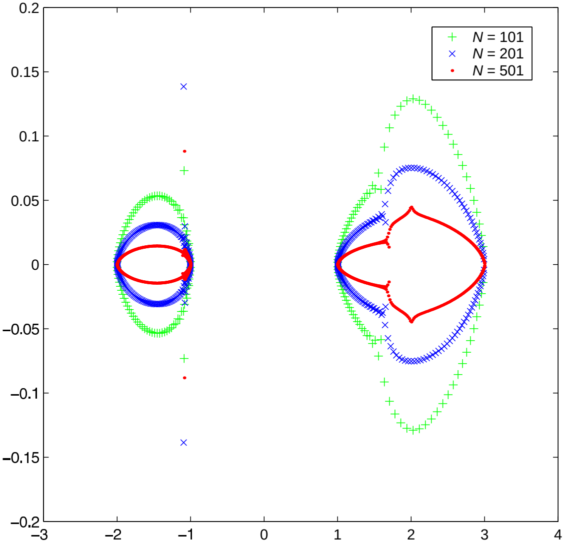

Figure: Detailed view of Figure 5 near the real axis

Finite rank perturbation of Example I

A finite-dimensional perturbation of $A = aI$ with non-empty discrete spectrum:

$$Bu(x) := a(x)u(x) - \frac{3\exp(-ix)}{2\pi}\int_{-\pi}^{\pi} u(t)\exp(it)dt + \frac{\exp(2ix)}{2\pi}\int_{-\pi}^{\pi} f(t)\exp(-2it)dt\,, \qquad x \in [-\pi,\pi]. \tag{3}$$

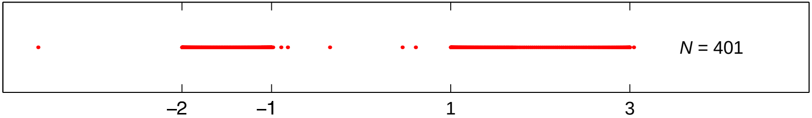

Figure: $\mathrm{Spec}(B, \mathcal{L}_{401})$.

Second order relative spectra of B

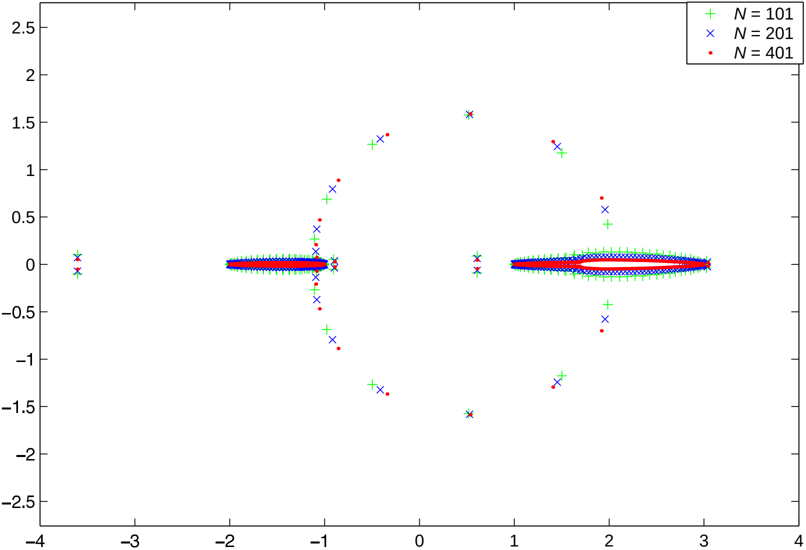

Figure: $\mathrm{Spec}_2(B, \mathcal{L}_N)$

Second order relative spectra of B (contd.)

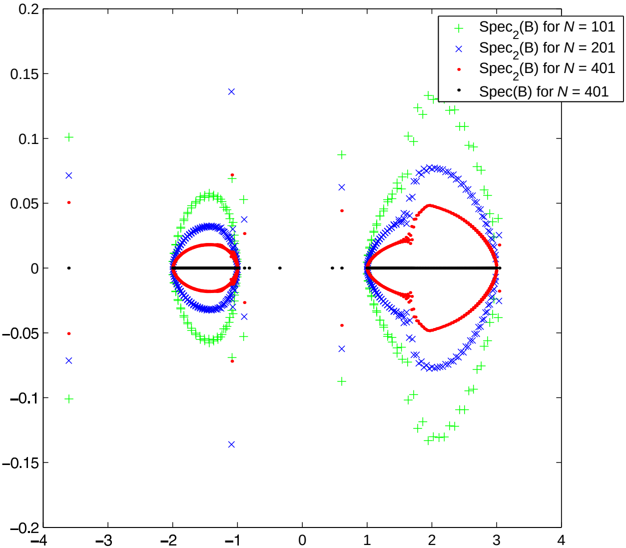

Figure: Detailed view of Figure 8 near the real axis and, for comparison.

Perturbed periodic Schrödinger

$$Hf = -\Delta f + [\cos(x) + \cos(y) - ce^{-(x^2+y^2)}]f \qquad c = 5.5$$

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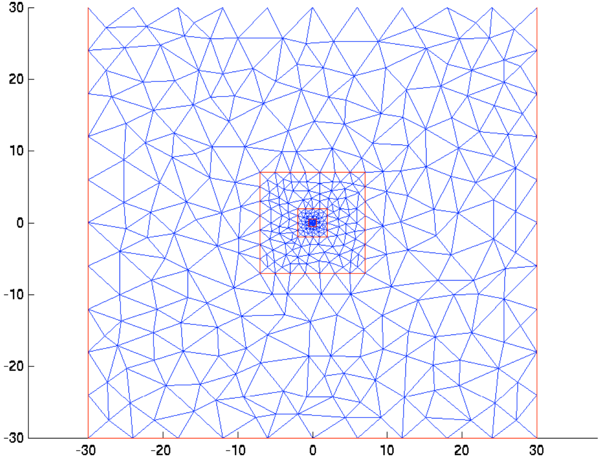
$$\text{Spec } H \approx [-.75, -.69] \cup [.21, .57] \cup [.91, \infty) \cup \{\text{possibly isolated evs}\}$$

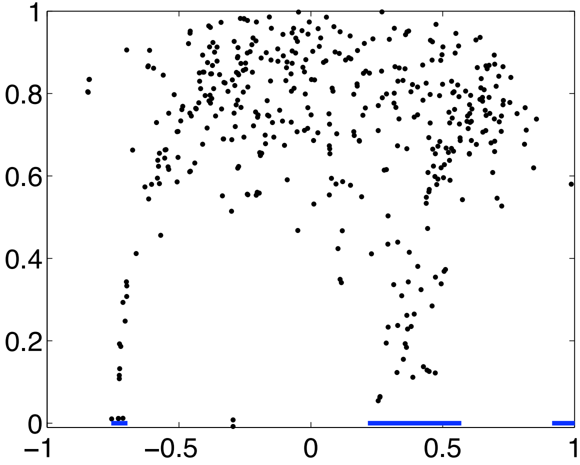
$\mathcal{L}_{s,h}$ — FEs in a mesh of max element size $h > 0$ with support in $[-s, s]^2$ and C^1 in $\mathbb{R}^2$. Mesh adapted around the origin.

Standard projection methods (without Floquet) would pollute/

A typical mesh



Results for $H = -\Delta + \cos x + \cos y - 5.5e^{-(x^2+y^2)}$



eigenvalue at $\approx -0.295247 \pm 10^{-5}$

More on Example I:
Consider

$$a(x) = a_y(x) = \begin{cases} -\frac{3}{2} + \frac{1}{2}\cos\sqrt{5}\,x\,, & \text{for} \quad -\pi \le x < y\,, \\ 2 + \cos\sqrt{2}\,x\,, & \text{for} \quad y \le x < \pi\,. \end{cases} \tag{4}$$

and denote the operator of multiplication

$$A_y := a_y I$$

Start with the original example $A = A_0$.

We know already that $\mathrm{Spec}(A, \mathcal{L}_N)$ stays very stable as $N = 2n + 1$ increases. Compare the results with those for $\mathrm{Spec}(A, \mathcal{L}_N)$ for $N = 2n$ (non-symmetric truncation):

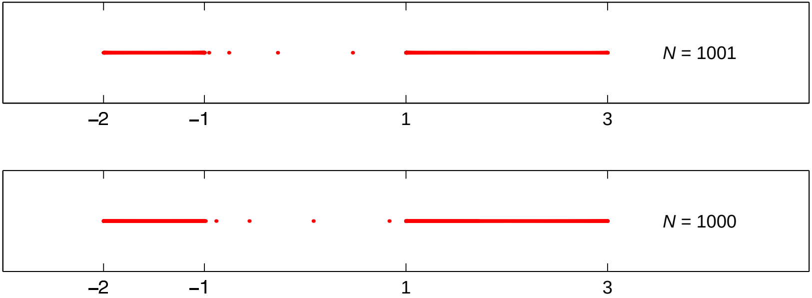


Figure: $\mathrm{Spec}(A, \mathcal{L}_{1001})$ compared with $\mathrm{Spec}(A, \mathcal{L}_{1000})$.

N	301	302	303	304	...	307	308
$\mathrm{Spec}(A, \mathcal{L}_N) \cap (-1, 1)$	-0.9899	-0.9470	-0.9898	-0.9467	...	-0.9895	-0.9461
	-0.8468	-0.6622	-0.8463	-0.6616	...	-0.8453	-0.6603
	-0.3740	0.0143	-0.3734	0.0147	...	-0.3721	0.0155
	0.4554	0.8604	0.4555	0.8603	...	0.4557	0.8600

Table: Eigenvalues lying in the gap of the essential spectrum of A for some consecutive values of N. 2-periodicity in N is clearly visible.

We shall show that the "period" depends on the location y of the discontinuity of a_y.
Let $y = -\pi/3$.

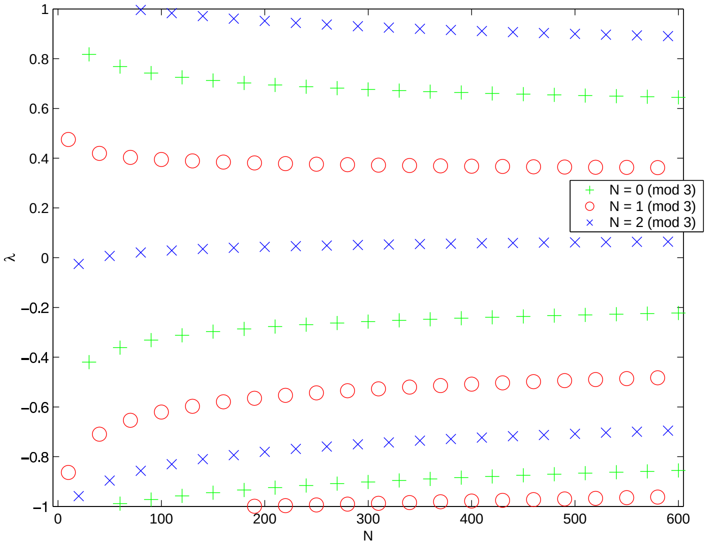


Figure: Points of $\mathrm{Spec}(A_y, \mathcal{L}_N)$, $y = -\pi/3$, in the interval $(-1, 1)$ as functions of N.

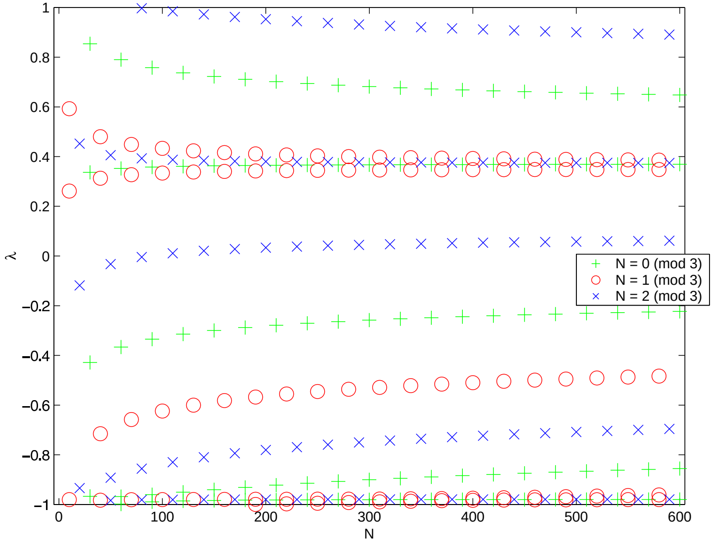


Figure: Points of Spec$(B_y, \mathcal{L}_N)$, $y = -\pi/3$, in the interval $(-1, 1)$ as functions of N. Note the presence of both "genuine" and "spurious" eigenvalues.

Similar calculations for $y = -\pi/(p/q) = -\pi q/p$ for the following values $p/q = 2$, 4, 5, 6, 7, 21, 21/10, 21/5, 7/3, 8/3, and 5/2. In all cases the spurious eigenvalues of A_y are "periodic" in N with the minimal "period"

$$\omega(p/q) := \begin{cases} 2, & \text{if} \quad p/q = 0, \\ p, & \text{if} \quad p \text{ and } q \text{ are both odd}, \\ 2p, & \text{if} \quad p \neq 0 \text{ and either } p \text{ or } q \text{ is even}. \end{cases}$$

In fact, $\omega(p/q)$ is the smallest natural number such that $\omega\times$ (length of $[-\pi, -\pi q/p]$) and $\omega\times$ (length of $[-\pi q/p, \pi]$) are integer multiples of 2π

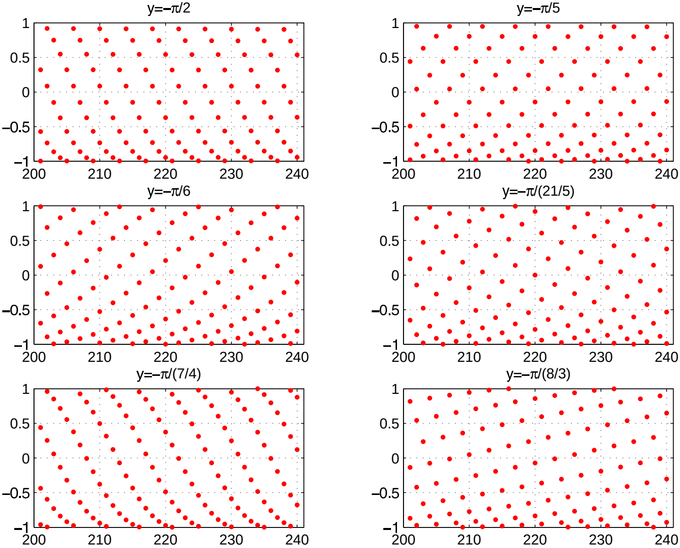


Figure: Points of $\mathrm{Spec}(A_y, \mathcal{L}_N)$, in the interval $(-1, 1)$ as functions of N, plotted for various values of y.

More on Example II:

We used different spaces so far for calculations of the spectrum and the second order relative spectra, namely we've computed $\text{Spec}(H, \mathbf{L}_N \times \mathbf{L}_N)$ (which is polluted in $(1, 2)$) and $\text{Spec}_2(H, \mathbf{M}_N \times \mathbf{L}_N)$ (works very well).

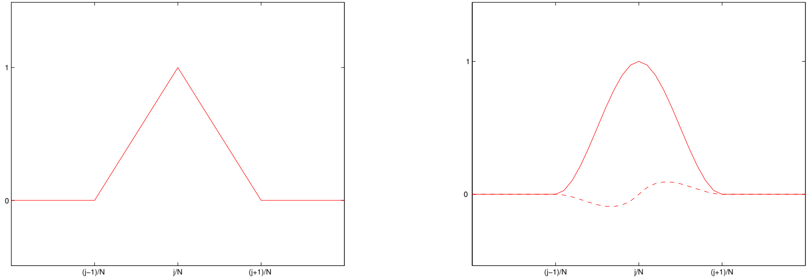


Figure: Elements of the spaces $\mathbf{L}_N$ and $\mathbf{M}_N$

What happens if we use the same space $\mathbf{M}_N \times \mathbf{L}_N$ for the first order spectrum?

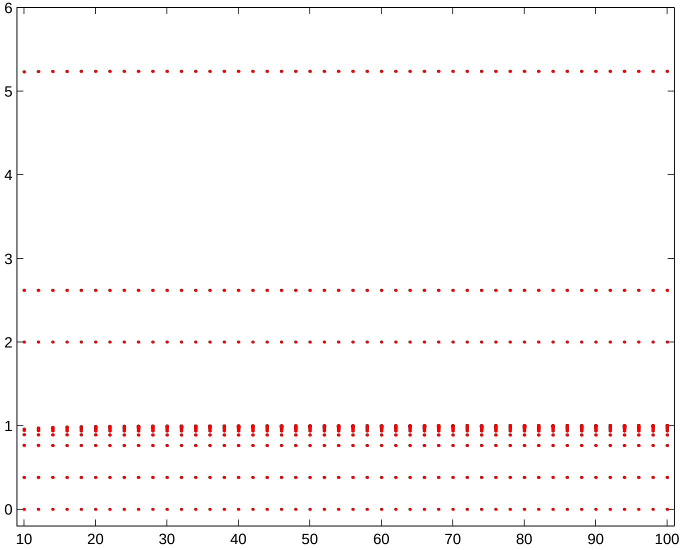


Figure: FEM calculated $\mathrm{Spec}(H, \mathbf{M}_N \times \mathbf{L}_N)$ plotted against N. There are no spurious eigenvalues!

But what about even higher smoothness, e.g. the space $\mathbf{M}_N \times \mathbf{M}_N$? Does not work for the first order spectra — we again have heavy spectral pollution, but works reasonably well for the second order relative spectra.

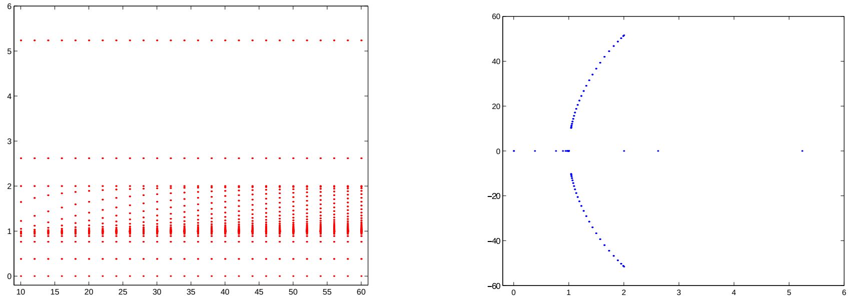


Figure: $\mathrm{Spec}(H, \mathbf{M}_N \times \mathbf{M}_N)$ plotted against N, and $\mathrm{Spec}_2(H, \mathbf{M}_{50} \times \mathbf{M}_{50})$

So, use mixed order elements in mixed order problems!

Some concluding remarks :

"Real life" problems:

The vibration of an elastic **shell** in vacuum is described by the system of three partial differential equations on a surface Γ:

$$h \sum_{i=1}^{3} \mathcal{L}_{ij} u_i = h\omega^2 u_j + g_j \,, \qquad j = 1, 2, 3 \,.$$

The $\mathcal{L}_{ij}$ are the linear differential operators of shell theory which have the form

$$\mathcal{L}_{ij} = \frac{h^2}{12} n_{ij} + \ell_{ij} \,, \qquad i, j = 1, 2, 3 \,.$$

Here n_{ij} and ℓ_{ij} are the moment and membrane operators respectively.

Explicit expressions for ℓ_{ij} from the book of GOLDENVEIZER–LIDSKIĬ–TOVSTIK:

$$\ell_{ii} = -\frac{1}{1-\nu^2}\frac{1}{A_i}\frac{\partial}{\partial\alpha_i}\frac{1}{A_iA_j}\frac{\partial}{\partial\alpha_i}A_j - \frac{1}{2(1+\nu)}\frac{1}{A_j}\frac{\partial}{\partial\alpha_j}\frac{1}{A_iA_j}\frac{\partial}{\partial\alpha_j}A_i$$
$$-\frac{1}{1+\nu}R_i{}^{-1}R_j{}^{-1}, \qquad i = 1,2,3,$$
$$\ell_{ij} = -\frac{1}{1-\nu^2}\frac{1}{A_i}\frac{\partial}{\partial\alpha_i}\frac{1}{A_iA_j}\frac{\partial}{\partial\alpha_j}A_i + \frac{1}{2(1+\nu)}\frac{1}{A_j}\frac{\partial}{\partial\alpha_j}\frac{1}{A_jA_i}\frac{\partial}{\partial\alpha_i}A_j,$$
$$\ell_{i3} = -\frac{1}{1-\nu^2}\frac{1}{A_i}\frac{\partial}{\partial\alpha_i}\left(R_i{}^{-1}+R_j{}^{-1}\right) + \frac{1}{1+\nu}\frac{1}{A_iR_j}\frac{\partial}{\partial\alpha_i},$$
$$\ell_{3i} = \frac{1}{1-\nu^2}\frac{1}{A_iA_j}\left(R_i{}^{-1}+R_j{}^{-1}\right)\frac{\partial}{\partial\alpha_i}A_j - \frac{1}{1+\nu}\frac{1}{A_iA_j}\frac{\partial}{\partial\alpha_i}\frac{A_j}{R_j},$$
$$\ell_{33} = \frac{1}{1-\nu^2}\left(R_1{}^{-2}+2\nu R_1{}^{-1}R_2{}^{-1}+R_2{}^{-2}\right), \qquad i,j = 1,2.$$

The operators n_{ij} depend on the choice of the particular variant of shell theory.

When $h = 0$, $\mathrm{Spec}_{\mathrm{ess}}(\mathcal{L})$ is rather complicated, spectral polution often occur and is very difficult to eliminate - see papers by RAPPAZ, SANCHEZ-HUBERT, SANCHEZ-PALENCIA, VASSILIEV.

Questions: Would the second order method work and what are the difficulties in its implementation?

Cosserat spectral problem

$$\Delta \mathbf{u} + \lambda\, \mathbf{grad}\, \mathrm{div}\, \mathbf{u} = \mathbf{0}$$

with appropriate boundary conditions (say $\mathbf{u} = \mathbf{0}$) and its generalizations. Pollution happens, see work by DAUGE, SÜRI.

Also, **Dirac** spectral problem in 2D — a lot of work by mathematical physicists/analysts recently (ESTEBAN, SÉRÉ ET AL.).