Infinite dimensional spectral computations & linear algebra: Extending the QR algorithm to infinite dimensions

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Outline

- Background
- Introducing IQR
- Non Normal Operators
- How To Compute
- Numerical Examples
- Conclusion

Background

Background

- Hilbert space $l^2(\mathbb{N})$ with $\|x\|_2 = \sqrt{\sum_{j=1}^{\infty} |x_j|^2}$, $\langle x, y \rangle = \sum_{j=1}^{\infty} x_j \bar{y}_j$
- Bounded linear operator $T : l^2(\mathbb{N}) \to l^2(\mathbb{N})$ realised as matrix

$$\begin{pmatrix} t_{11} & t_{12} & t_{13} & \cdots \\ t_{21} & t_{22} & t_{23} & \cdots \\ t_{31} & t_{32} & t_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

  Denote these by $\mathcal{B}(l^2(\mathbb{N}))$.
- Want to compute spectrum (generalistion of eigenvalues)

$$\sigma(T) := \{z \in \mathbb{C} : T - zI \text{ not invertible}\}.$$

  from the matrix elements. What about eigenvectors etc.?

Well Studied

- Quantum mechanics, quasicrystals


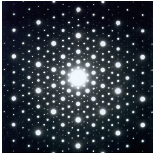

Figure: Left: Dan Shechtman, Nobel Prize in Chemistry 2011. Right: Electron diffraction pattern of quasicrystal.

- Intensely investigated since the 1950s, still very active today.

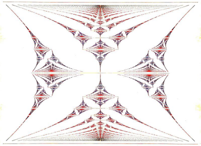

Figure: Left: Artur Avila, Fields Medal 2014. Right: Hofstadter butterfly.

Hierarchy of complexity

Definition (Tower of Algorithms)

A tower of algorithms of height k is a family of sequences of functions

$$\Gamma_{n_k,\ldots,n_1} : \Omega \to \mathcal{M},$$

where $n_k, \ldots, n_1 \in \mathbb{N}$ and $\Gamma_{n_k,\ldots,n_1}$ are "algorithms". Moreover,

$$\sigma(T) = \lim_{n_k \to \infty} \ldots \lim_{n_1 \to \infty} \Gamma_{n_k,\ldots,n_1}(T).$$

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Definition (Solvability Complexity Index (SCI))

Solvability Complexity Index, $\mathrm{SCI}(\sigma, \Omega)$ is the smallest integer k for which there exists a tower of algorithms of height k. If no such tower exists then $\mathrm{SCI}(\sigma, \Omega) = \infty$.

Example Results

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Methods based on approximating pseudospectrum:

$$\sigma_\epsilon(T) = \{z : \left\|(T - zI)^{-1}\right\| \geq \epsilon^{-1}\},$$

where we interpret $\left\|S^{-1}\right\|$ as $+\infty$ if S does not have a bounded inverse.

Motivation

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2. Due to taking square root, above method can only gain precision $\sqrt{\epsilon_{\text{mach}}}$.
3. Can we generalise staple finite matrix algorithms to infinite dimensions?
4. Can we gain error control and classification results in the hierarchy?

Classical QR

$$T = Q_1 R_1$$

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&\vdots \\
T_n &= Q_n^* ... Q_1^* T Q_1 ... Q_n
\end{aligned}
$$

Classical Result

Theorem

Let $T \in \mathbb{C}^{N \times N}$ be a normal matrix with eigenvalues satisfying $|\lambda_1| > \ldots > |\lambda_N|$. Let $\{Q_m\}$ be a Q-sequence of unitary operators. Then (up to re-ordering of the basis)

$$Q_m^* T Q_m \longrightarrow \bigoplus_{j=1}^{N} \lambda_j e_j \otimes e_j, \qquad m \to \infty.$$

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Numerical Example ...

Introducing IQR

The Main Idea

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\begin{pmatrix} t_{11} & t_{12} & t_{13} & \cdots \\ t_{21} & t_{22} & t_{23} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \overset{\text{Truncate}}{\Rightarrow} \begin{pmatrix} t_{11} & t_{12} & t_{13} & \cdots & t_{1n} \\ t_{21} & t_{22} & t_{23} & \cdots & t_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{n1} & t_{n2} & t_{n3} & \cdots & t_{nn} \end{pmatrix} \overset{\text{Iterate QR}}{\Rightarrow} \begin{pmatrix} d_{11} & 0 & \cdots & 0 \\ 0 & d_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_{nn} \end{pmatrix}
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The QR Decomposition

Definition

A Householder reflection is an operator $S \in \mathcal{B}(\mathcal{H})$ of the form

$$S = I - \frac{2}{\|\psi\|^2}\psi \otimes \bar{\psi}, \qquad \psi \in \mathcal{H},$$

where $\bar{\psi}$ denotes the associated functional in $\mathcal{H}^*$ given by $x \to \langle x, \psi \rangle$.

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where $\bar{\psi}$ denotes the associated functional in $\mathcal{H}^*$ given by $x \to \langle x, \psi \rangle$.In the case where $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ and I_i is the identity on $\mathcal{H}_i$ then

$$U = I_1 \oplus \left(I_2 - \frac{2}{\|\psi\|^2} \psi \otimes \bar{\psi} \right) \qquad \psi \in \mathcal{H}_2,$$

is called a Householder transformation.

The QR Decomposition

Theorem (Hansen 2008)

Let T be a bounded operator on a separable Hilbert space $\mathcal{H}$ and let $\{e_j\}_{j\in\mathbb{N}}$ be an orthonormal basis for $\mathcal{H} \cong l^2(\mathbb{N})$. Then there exist an isometry Q such that $T = QR$ where R is upper triangular with respect to $\{e_j\}$. Moreover,

$$Q = \operatorname*{SOT-lim}_{n\to\infty} V_n$$

where $V_n = U_1 \cdots U_n$ are unitary and each U_j is a Householder transformation.

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Good for numerics - more stable than Gram-Schmidt...

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Assume T invertible...

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$$T^m = \hat{Q}_m \hat{R}_m.$$

$\hat{R}_m$ upper triangular since R_j, $j \leq m$ are. By invertibility of T, $\langle Re_i, e_i \rangle \neq 0$. Hence

$$\mathrm{span}\{T^m e_j\}_{j=1}^{J} = \mathrm{span}\{\hat{Q}_m e_j\}_{j=1}^{J}, \quad J \in \mathbb{N}.$$

Questions

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2. When do we gain convergence to a diagonal operator and in what sense?
3. Can we prove anything for non normal operators in infinite dimensions?
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A Result for Normal Operators

Assume the following:

(A1) $T \in \mathcal{B}(\mathcal{H})$ is an invertible normal operator and $\{e_j\}_{j\in\mathbb{N}}$ an orthonormal basis for $\mathcal{H}$. $\{Q_k\}$ and $\{R_k\}$ are Q- and R-sequences of T with respect to the basis $\{e_j\}_{j\in\mathbb{N}}$.

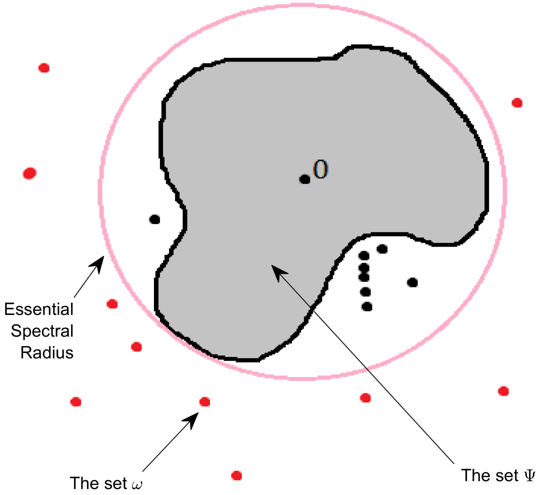
(A2) $\sigma(T) = \omega \cup \Psi$ such that $\omega \cap \Psi = \emptyset$ and $\omega = \{\lambda_i\}_{i=1}^{N}$, where the λ_is are isolated eigenvalues with (possibly infinite) multiplicity m_i. Let $M = m_1 + ... + m_N = \dim(\mathrm{ran}\chi_\omega(T))$ and suppose that $|\lambda_1| > \ldots > |\lambda_N|$. Suppose further that $\sup\{|\theta| : \theta \in \Psi\} < |\lambda_N|$.

Define

$$\rho = \sup\{|z| : z \in \Psi\}, \quad r = \max\{|\lambda_2/\lambda_1|, ..., |\lambda_N/\lambda_{N-1}|, \rho/|\lambda_N|\}$$

then $r < 1$.

What This Really Means!



A Result for Normal Operators

Theorem

There exists $\{\hat{e}_j\}_{j=1}^M \subset \{e_j\}_{j\in\mathbb{N}}$, where $M = m_1 + \ldots + m_N$, so that $\operatorname{span}\{Q_k \hat{e}_j\} \to \operatorname{span}\{\hat{q}_j\}$ where $\{\hat{q}_j\}_{j=1}^M \subset \operatorname{ran}\chi_\omega(T)$ is a collection of orthonormal eigenvectors of T and if $e_j \notin \{\hat{e}_j\}_{j=1}^M$, then $\chi_\omega(T) Q_k e_j \to 0$. Also:

(i) Every subsequence of $\{Q_n^* T Q_n\}_{n\in\mathbb{N}}$ has a convergent subsequence $\{Q_{n_k}^* T Q_{n_k}\}_{k\in\mathbb{N}}$ such that

$$Q_{n_k}^* T Q_{n_k} \xrightarrow{\text{WOT}} \left(\bigoplus_{j=1}^M \langle T\hat{q}_j, \hat{q}_j\rangle \hat{e}_j \otimes \hat{e}_j\right) \oplus \sum_{j\in\Theta} \xi_j \otimes e_j,$$

as $k \to \infty$, where

$$\Theta = \{j : e_j \notin \{\hat{e}_j\}_{j=1}^M\}, \quad \xi_j \in \overline{\operatorname{span}\{e_i\}_{i\in\Theta}}$$

and only $\sum_{j\in\Theta} \xi_j \otimes e_j$ depends on the choice of subsequence.

(ii)

$$\widehat{P}_M Q_n^* T Q_n \widehat{P}_M \xrightarrow{\text{SOT}} \left(\bigoplus_{j=1}^M \langle T\hat{q}_j, \hat{q}_j\rangle \hat{e}_j \otimes \hat{e}_j\right), \qquad \text{as } n \to \infty,$$

where $\widehat{P}_M$ denotes the orthogonal projection onto $\overline{\operatorname{span}\{\hat{e}_j\}_{j=1}^M}$. For any fixed $x \in \operatorname{span}\{\hat{e}_j\}_{j=1}^M$ we have the following rate of convergence

$$\left\|\widehat{P}_M Q_n^* T Q_n \widehat{P}_M x - \left(\bigoplus_{j=1}^M \langle T\hat{q}_j, \hat{q}_j\rangle \hat{e}_j \otimes \hat{e}_j\right) x\right\| \le \mathcal{O}(r^n).$$

Idea of Proof

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Can upgrade for block convergence (eigenvalues not of distinct magnitude), SOT convergence etc.

Questions

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2. When do we gain convergence to a diagonal operator and in what sense? ✓
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Non Normal Operators

Set Up

Assume the following (M now finite):

(A1) $T \in \mathcal{B}(\mathcal{H})$ is an invertible operator and there is an orthogonal projection P of finite rank M with image invariant under T.

(A2) There exist $\alpha > \beta > 0$ such that

$$\|Tx\| \geq \alpha\|x\| \quad \forall x \in \mathrm{ran}(P),$$
$$\|(I-P)T(I-P)\| \leq \beta.$$

(A3) $\{\tilde{P}e_j\}_{j=1}^{M}$ are linearly independent ($\tilde{P}$ canoncal defined later).

Define for orthogonal projections E, F onto $S_1, S_2 \subset \mathcal{H}$ the distance between subspaces

$$\hat{\delta}(S_1, S_2) = \|E - F\| \in [0, 1]$$

and the subspace angle

$$\phi(S_1, S_2) = \sin^{-1}\left(\hat{\delta}(S_1, S_2)\right).$$

Result

Theorem

There exists a canonical M dimensional T^*-invariant subspace S with orthogonal projection $\tilde{P}$ with

(i) The subspace angle $\phi(\text{span}\{e_j\}_{j=1}^M, S) < \pi/2$ and we have

$$\hat{\delta}(\text{span}\{Q_n e_j\}_{j=1}^M, \text{ran}(P)) \leq \frac{\sin\left(\phi(\text{span}\{e_j\}_{j=1}^M, \text{ran}(P))\right)}{\cos\left(\phi(\text{span}\{e_j\}_{j=1}^M, S)\right)} \left(1 + \frac{\|PT(I-P)\|}{\alpha - \beta}\right) \frac{\beta^n}{\alpha^n},$$

(ii) Every subsequence of $\{Q_n^* T Q_n\}_{n \in \mathbb{N}}$ has a convergent subsequence $\{Q_{n_k}^* T Q_{n_k}\}_{k \in \mathbb{N}}$ such that

$$Q_{n_k}^* T Q_{n_k} \xrightarrow{\text{WOT}} \sum_{j=1}^{M} \xi_j \otimes e_j \bigoplus \sum_{i=M+1}^{\infty} \zeta_i \otimes e_i,$$

$$\xi_j \in \overline{\text{span}\{e_j\}_{j=1}^M}, \quad \zeta_i \in \mathcal{H}.$$

Questions

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How To Compute

Some Definition

Definition

Let T be an infinite matrix acting as a bounded operator on $l^2(\mathbb{N})$ with basis $\{e_j\}_{j\in\mathbb{N}}$. For $f:\mathbb{N}\to\mathbb{N}$ non-decreasing with $f(n)\geq n$ we say that T has quasi-banded subdiagonals with respect to f if $\langle Te_j, e_i\rangle = 0$ when $i > f(j)$.

A Theorem

Theorem

Let $T \in \mathcal{B}(l^2(\mathbb{N}))$ have quasi-banded subdiagonals with respect to f and let T_n be the n-th element in the QR iteration, i.e. $T_n = Q_n^* \cdots Q_1^* T Q_1 \cdots Q_n$, where

$$Q_j = \operatorname*{SOT-lim}_{l \to \infty} \; U_1^j \cdots U_l^j$$

and U_l^j is a Householder transformation. Let P_m be the usual projection onto $\mathrm{span}\{e_j\}_{j=1}^m$ and denote the a-fold iteration of f by $\underbrace{f \circ f \circ \ldots \circ f}_{a \text{ times}} = f_a$. Then

$$\begin{aligned} P_m T_n P_m = {} & P_m U_m^n \cdots U_1^n U_{f_1(m)}^{n-1} \cdots U_1^{n-1} \cdots U_{f_{(n-2)}(m)}^2 \cdots U_1^2 U_{f_{(n-1)}(m)}^1 \cdots U_1^1 \\ & \cdot P_{f_n(m)} T P_{f_n(m)} \\ & \cdot U_1^1 \cdots U_{f_{(n-1)}(m)}^1 U_1^2 \cdots U_{f_{(n-2)}(m)}^2 \cdots U_1^{n-1} \cdots U_{f_1(m)}^{n-1} U_1^n \cdots U_m^n P_m. \end{aligned}$$

Why?

In the subcase of invertibility, a consequence of the fact that if T has quasi-banded subdiagonals with respect to f then

$$P_m T^n P_m = P_m (P_{f_n(m)} T P_{f_n(m)})^n P_m.$$

Why?

In the subcase of invertibility, a consequence of the fact that if T has quasi-banded subdiagonals with respect to f then

$$P_m T^n P_m = P_m (P_{f_n(m)} T P_{f_n(m)})^n P_m.$$

We can apply Gram-Schmidt (or a more stable modified version) to the columns of $P_{f_n(m)} T P_{f_n(m)}$ and truncate the resulting matrix!

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Can also extend to compute the IQR iterates with error control if we can evaluate an increasing family of increasing functions $g^j : \mathbb{N} \to \mathbb{N}$ such that defining the matrix $T_{(j)}$ with columns $\{P_{g^j(n)} T e_n\}$ we have that $T_{(j)}$ is invertible and

$$\left\| (P_{g^j(n)} - I) T e_n \right\| \leq \frac{1}{j}.$$

Questions

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Numerical Examples

Example 1

Take unilateral shift $U : e_n \to e_{n+1}$ acting on $l^2(\mathbb{Z})$ (with the natural choice of indexing $\mathbb{Z}$) and perturb by the compact diagonal operator

$$D(e_n) = \frac{5\sin(n)^2}{\sqrt{|n|+1}} e_n.$$

Hence the spectrum of the full operator $T = U + D$ consists of the unit circle and a collection of eigenvalues in the discrete spectrum.

Example 1

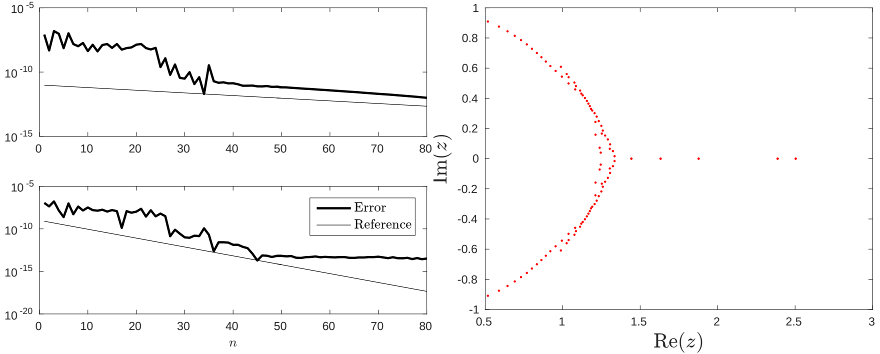

Figure: Left: Error in approximating λ_1 (top) and λ_2 through taking finite sections $P_{100}Q_n^*TQ_n|_{P_{100}\mathcal{H}}$. We have shown the expected rates of convergence as references. Right: The spectrum of $P_{100}Q_{500}^*TQ_{500}|_{P_{100}\mathcal{H}}$ demonstrating convergence to the extremal parts.

Example 2

Almost Mathieu related to a wealth of mathematical/physical problems:

$$(H_1 x)_n = x_{n-1} + x_{n+1} + 2\cos(2\pi n\alpha + \nu)x_n,$$

on $l^2(\mathbb{Z})$. Hamiltonian represents crystal electron in a uniform magnetic field and the spectrum the allowed energies of the system. No discrete spectrum!

Example 2

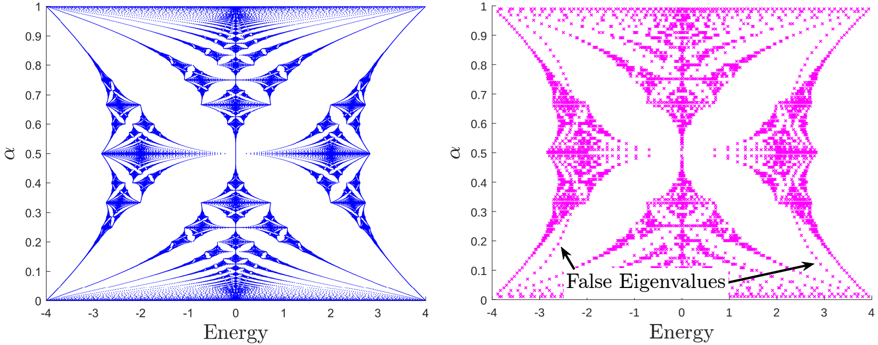

Figure: The spectrum of H_1 calculated analytically for rational α and the output of finite section for $m = 100$. Note that the finite section method causes strong spectral pollution.

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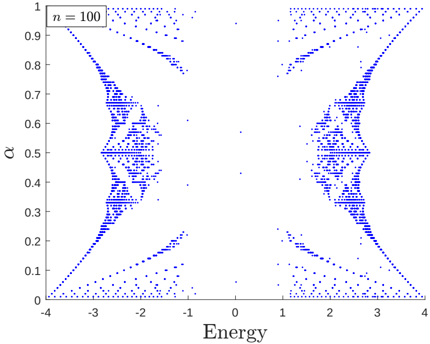


Figure: IQR for $m = 100, n = 100$ and the same for $m = 100, n = 5000$. IQR algorithm is more robust, preserving the structure of the spectrum whilst converging to the boundary of the essential spectrum.

Example 3

Toeplitz operator

$$N = \frac{1}{2}(U_3 + U_{-1})$$

where U_m acts on $l^2(\mathbb{Z})$ by the shift $e_j \to e_{j+m}$ on the standard basis. Not invertible and has no eigenvalues. With no shift, $Q_n^* N Q_n$ appeared

to converge strongly to the operator

$$\tilde{N} = \begin{pmatrix} A & & \\ & A & \\ & & \ddots \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Spectrum equal to $\{\pm 1, \pm 1i\}$ which are the extremal points of $\sigma(N)$. Shift to $Q_n^*(N + I)Q_n$, then we appeared to converge to the diagonal

operator $D = 2I$. BUT curious case of reduced rate of convergence...

Example 3

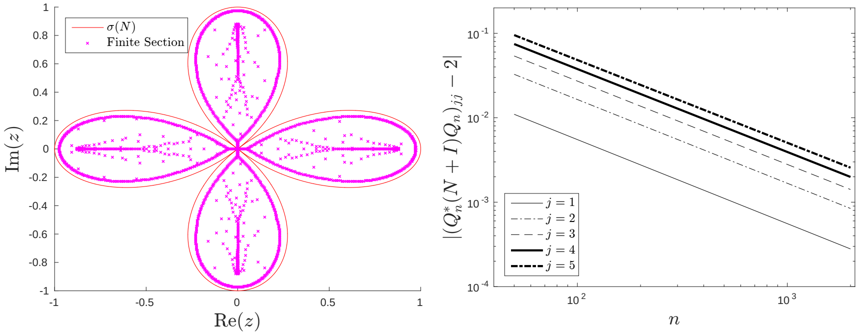


Figure: Left: Spectrum of the normal operator N and finite section approximates. Right: Convergence of first five diagonal entries of $Q_n^*(N+I)Q_n$ to 2. Convergence of the rate $\mathcal{O}(1/n)$ for this part of the essential spectrum as opposed to the linear convergence rate $\mathcal{O}(r^n)$ seen in the first example.

Example 4

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ 1 & 0 & a_{23} & a_{24} & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & a_{45} & a_{46} & \dots \\ 0 & 0 & 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & 1 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

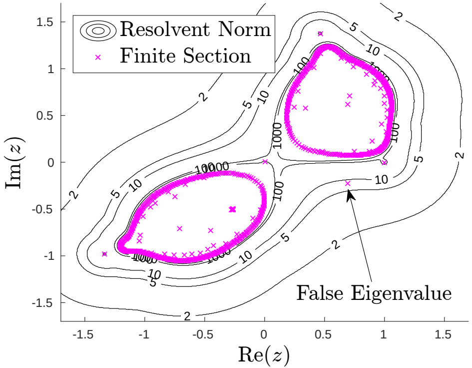
where $a_{2j,2j+1} = i$, and $a_{2j,2j+2} = -i$ if j is prime and $a_{2j,2j+2} = 0$ otherwise.

Example 4

$$T = \begin{pmatrix} 2.5+0.5i & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ 1 & 3-0.5i & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 1.7 & 0.05 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0.05 & t_4 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & t_5 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & 1 & t_6 & 0 & \dots \\ 0 & 0 & 0 & 0 & 0 & 1 & t_7 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

where $t_j = 1 + 0.5(\sin(j) + i\cos(j))$ for $j \geq 4$.

Example 4



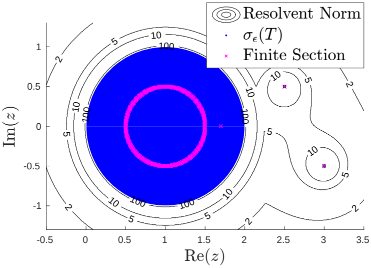


Figure: Left: $\sigma(P_n A|_{P_n\mathcal{H}})$ for $n = 1000$ with the false eigenvalue (recall that $\sigma(A) \subseteq \sigma_\epsilon(A)$). Right: $\sigma(P_n T|_{P_n\mathcal{H}})$ for $n = 500$ along with contours of the resolvent norm and $\sigma_\epsilon(T)$ for $\epsilon = 2\sqrt{\epsilon_{\mathrm{mach}}}$.

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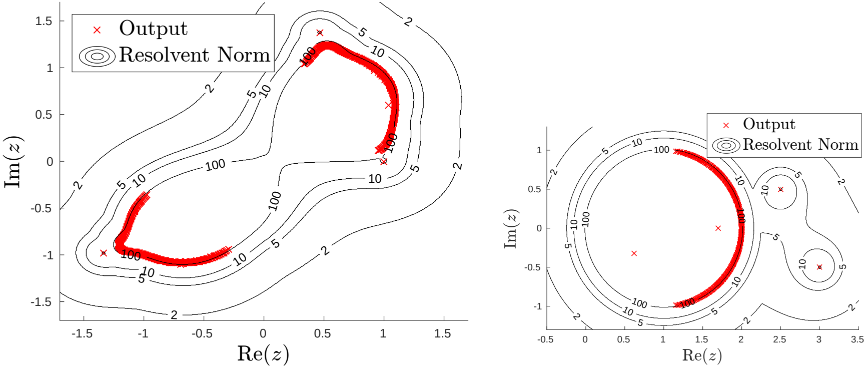

Figure: The figures show $\sigma(P_m Q_n^* A Q_n|_{P_m \mathcal{H}})$ (left), $\sigma(P_m Q_n^* T Q_n|_{P_m \mathcal{H}})$ (right) for $n = 1000, m = 1000$ and $n = 1500, m = 500$ respectively.

Example 4

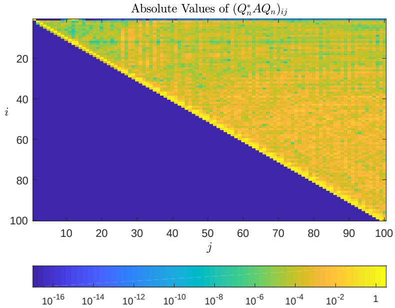

Figure: Left: Absolute values of entries of $Q_{1000}^* A Q_{1000}$. Right: Absolute values of entries of $Q_{1500}^* T Q_{1500}$. We appear to gain convergence to a diagonally dominated upper triangular matrix.

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7. Paper available soon!

Future Work

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3. Many more open computational spectral problems - spectral measures, IQR for unbounded operators etc.

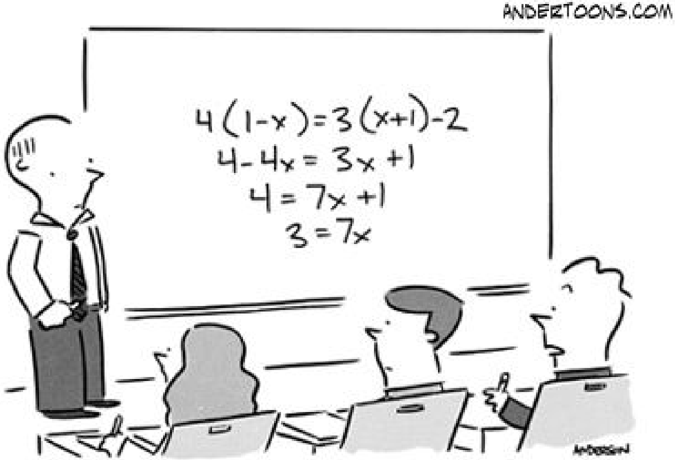
References

Only two main references:

1. First appearance of the algorithm for real symmetric infinite matrices: P Deift, LC Li, and C Tomei. Toda flows with infinitely many variables. Journal of functional analysis, 64(3):358402, 1985.
2. Existence of QR decomposition for non invertible operators and eigenvector convergence theorem for normal operators: AC Hansen. On the approximation of spectra of linear operators on Hilbert spaces. J. Funct. Anal., 254(8):20922126, 2008.

Other SCI results: In progress!

Thanks for listening!
Any questions?



"Wouldn't it be more efficient to just find who's complicating equations and ask them to stop?"