An Algorithm for Dense Nonlinear Eigenvalue Problems

Gian Maria Negri Porzio
gianmaria.negriporzio@manchester.ac.uk

Françoise Tisseur
francoise.tisseur@manchester.ac.uk

The University of Manchester

Manchester Numerical Analysis

Definition

Given a nonempty, open, bounded set $\Omega \subset \mathbb{C}$, and a meromorphic function $F\colon \Omega \to \mathbb{C}^{n\times n}$, derive and implement a reliable eigensolver to compute all the *eigenpairs* $(\lambda, v) \in \Omega \times \mathbb{C}^n \setminus \{0\}$ such that

$$F(\lambda)v = 0$$

for n not too large.

Idea

Use a contour integral approach. Replace $F(\lambda)v = 0$ with $(M - \lambda I)u = 0$, where $M = V_0^* B_1 W_0 \Sigma_0^{-1}$ has the same e'vals of F inside Ω, with $B_0 = V_0 \Sigma_0 W_0^*$ (economy-size SVD), and

$$B_0 = \begin{bmatrix} A_0 & \dots & A_{m-1} \\ \vdots & & \vdots \\ A_{m-1} & \dots & A_{2m-2} \end{bmatrix}, \qquad B_1 = \begin{bmatrix} A_1 & \dots & A_m \\ \vdots & & \vdots \\ A_m & \dots & A_{2m-1} \end{bmatrix},$$

with $B_i \in \mathbb{C}^{mn\times mp}$, and A_k being the kth moment

$$A_k = \int_{\partial\Omega} z^k F(z)^{-1} P \, dz \in \mathbb{C}^{n\times p},$$

where $P \in \mathbb{C}^{n\times p}$ is a random probing matrix.

Difficulties

Main focus is on the choice of the parameters:

- Optimal values of the size of the probing matrix $P \in \mathbb{C}^{n\times p}$? Optimal number of moments m?
- Which quadrature rule to approximate A_k? How many quadrature points N? How much does this approximation influence the backward error of the computed eigenvalues?

Computational cost

Assume N_e eigenvalues in Ω. Then the asymptotical computational cost is

$$\frac{2}{3}n^3 Np + \frac{14n}{p}N_e^3 + \text{cost of } \texttt{eig}$$

$\implies$ Computational cost heavily influenced by number of eigenvalues N_e inside Ω. A small problem can be very expensive to solve if $N_e \gg n$.

Advantages

- Find all the eigenvalues in Ω at the same time.
- Easily parallelizable. Each linear system in $A_k \approx \frac{1}{N}\sum_{j=1}^{N} z_j^{k+1} F(z_j)^{-1} P$ can be solved by different processors.
- Weak hypotheses on $F(z)$: can cope with singularities inside Ω and only need to compute $F(z)$ or $F(z)^{-1}P$ at specific points z.

Contour integral methods to reliably solve dense **nonlinear eigenvalue problems.**

Quadrature approximation and eigenvalues

$A_k^{(N)} \approx A_k$ with N trapezoidal points. Influence on eigenvalues computation? In Fig. 1(a) and Fig. 2(a) error $\|A_k^{(N)} - A_k^{(2N)}\|_\infty / (1 + \|A_k^{(N)}\|_\infty)$ for each moment A_k using N trapezoidal points for two NEPs, `butterfly` and `sleeper`. In Fig. 1(b) and Fig. 2(b) bound for the backward error for each eigenpair (λ_i, v_i):

$$\varepsilon_i = \frac{\|F(\lambda_i)v_i\|_2}{\|F(\lambda_i)\|_F \|v_i\|_2}.$$

- In `sleeper`, increasing N improves final approximation of eigenvalues.
- In `butterfly`, bad approximation of A_k still returns "good eigenvalues".

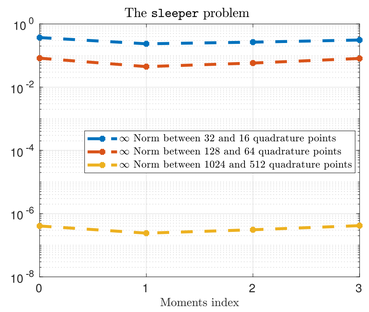

Figure 1(a).

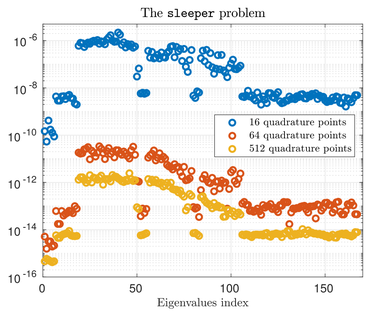

Figure 1(b).

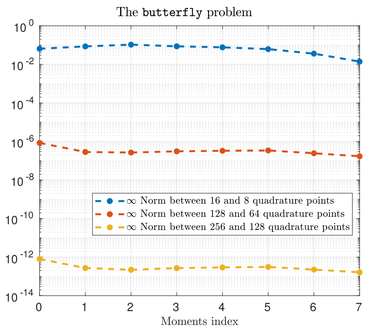

Figure 2(a).

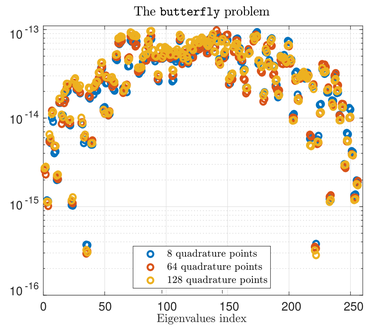

Figure 2(b).

Possible refinements

Backward error for $\overline{N_e}$ eigepairs may be too large. Three different refinements:

- Global: If $\overline{N_e} \gg 1$ and $p < n$, increase the size of probing matrix P.
- Local: If $\overline{N_e}$ quite small, use Newton-Raphson method to refine each of them. One or two steps are enough.
- Clusters: If $\overline{N_e} \gg 1$ and those eigenvalues can be divided in clusters, apply again the algorithm on smaller contours.

Further comments

- Approximate the moments with Gauss–Kronrod quadrature rule (exponential convergence). No need to choose the number of quadrature points N.
- Necessary that $mp > N_e$. We can compute N_e using the Residues Theorem. Numerical experiments show that, keeping mp constant, a larger probing matrix P produces better numerical results.

Numerical examples

Table 1 considers 3 NEPs from the NLEVP 4.0 collection. Keeping mp (almost) constant, we have smaller backward errors

$$\varepsilon = \max_{\lambda_i \in \Lambda(F)} \frac{\|F(\lambda_i)v_i\|_2}{\|F(\lambda_i)\|_F \|v_i\|_2}$$

with a larger probing matrix P.

Table 1.

Problem	$p\ell$	p	ℓ	ε
`butterfly` $n = 64$, $N_e = 256$	260	4	65	3.19e−13
	264	8	33	2.06e−11
	266	14	19	1.07e−8
`hadeler` $n = 30$, $N_e = 117$	120	4	30	2.45e−11
	126	7	18	1.06e−8
	126	9	14	5.01e−5
`sleeper` $n = 120$, $N_e = 167$	180	2	90	3.46e−12
	180	4	45	1.08e−10
	180	9	20	4.63e−2

References

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- N. J. Higham, G. M. Negri Porzio, and F. Tisseur. *"An Updated Set of Nonlinear Eigenvalue Problems"*. In: *MIMS EPrint* 2019.5, 12pp, 2019.