Numerical methods for the banded quadratic eigenvalue problem

Bor Plestenjak
Department of Mathematics
University of Ljubljana
Slovenia

Quadratic eigenvalue problem (QEP)

$Q(\lambda) = \lambda^2 M + \lambda C + K$, where M, C, K are $n \times n$ matrices. If a scalar λ and a nonzero vector x satisfy $Q(\lambda)x = 0$ then λ is an eigenvalue and x is the (right) eigenvector.

If M is nonsingular then there are $2n$ finite eigenvalues. They are usually computed by a linearization, e.q., from the $2n \times 2n$ generalized eigenvalue problem

$$\begin{bmatrix} 0 & I \\ -K & -C \end{bmatrix} \begin{bmatrix} x \\ u \end{bmatrix} = \lambda \begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} x \\ u \end{bmatrix}.$$

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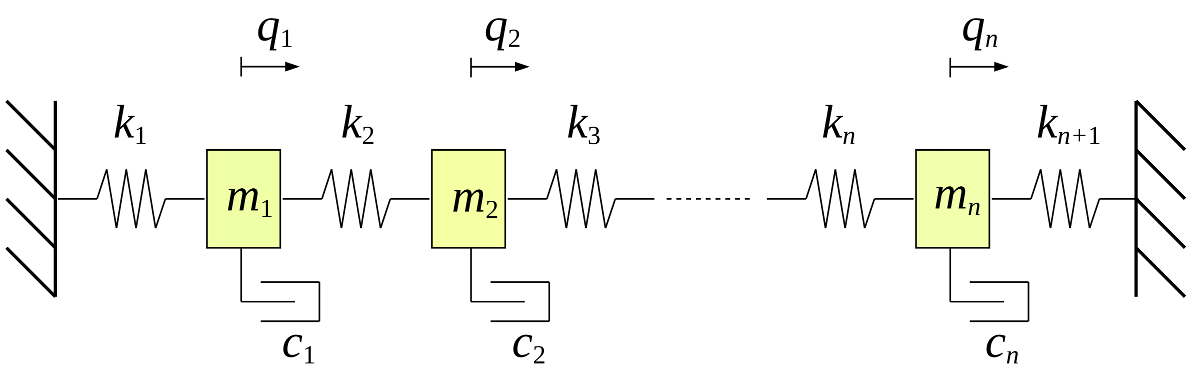
We will show that the eigenvalues of banded QEP can be efficiently computed as the zeros of the characteristic polynomial $f(\lambda) = \det(Q(\lambda))$.

We first consider a special case where

- M, C, K are real symmetric tridiagonal matrices and
- QEP is hyperbolic.

The eigenvectors can be obtained later by inverse iteration (e.g., Dhillon (1990)).

Example: a damped mass-spring system



A damped system of n masses and $n+1$ springs leads to the QEP

$$\lambda^2 M + \lambda C + K,$$

where $M = \mathrm{diag}(m_1, \dots, m_n)$, $C = \mathrm{diag}(c_1, \dots, c_n)$, and

$$K = \begin{bmatrix} k_1 + k_2 & -k_2 & & \\ -k_2 & \ddots & \ddots & \\ & \ddots & \ddots & -k_n \\ & & -k_n & k_n + k_{n+1} \end{bmatrix}.$$

M is the mass matrix, C is the damping matrix, and K is the stiffness matrix. The eigenvalues are the squares of the natural frequencies of the modes of vibration.

Overview

- Hyperbolic QEP
- Divide-and-conquer approach
- Laguerre's and Ehrlich–Aberth's method
- Efficient computation of $\det(Q(\lambda))$ and its derivatives
- Numerical experiments

Hyperbolic QEP

Symmetric $Q(\lambda) = \lambda^2 M + \lambda C + K$ is hyperbolic if $M > 0$ and

$$(x^T C x)^2 - 4(x^T M x)(x^T K x) > 0$$

for all $x \neq 0$. Properties:

- all eigenvalues and eigenvectors are real,
- a gap between n largest (primary) and n smallest (secondary) eigenvalues,
- n linearly independent eigenvectors associated with the primary (secondary) eigenvalues.
- Markus (1988): Symmetric Q with $M > 0$ is hyperbolic iff exists γ such that $Q(\gamma) < 0$.
- Let $\nu(\mu)$ be the number of negative eigenvalues of $Q(\mu)$. Can show:
  a) if $\gamma \leq \mu$ then $\nu(\mu)$ equals the number of eigenvalues of Q that are greater than μ,
  b) if $\mu \leq \gamma$ then $\nu(\mu)$ equals the number of eigenvalues of Q that are smaller than μ.

We can compute the k-th eigenvalue by bisection.

Faster methods

We can compute all eigenvalues by bisection, but the convergence is slow.

We apply other numerical methods for the roots of the characteristic polynomial:

- Laguerre's method
  - Li, Li (1993): symmetric tridiagonal eigenproblem
  - Li, Li, Zeng (1994): generalized symmetric tridiagonal eigenproblem
  - suitable for the hyperbolic QEP
- Ehrlich–Abert's method
  - Bini, Gemignani, Tisseur (2003): nonsymmetric tridiagonal eigenproblem
  - suitable also for a general QEP

The above methods require good initial approximations and stable and efficient computation of

$$f(\lambda) = \det(Q(\lambda)), \quad f'(\lambda)/f(\lambda), \text{ and } \quad f''(\lambda)/f(\lambda).$$

Divide-and-conquer (D&C)

$$Q(\lambda) = \begin{bmatrix} a_1 & b_1 & & & 0 \\ b_1 & a_2 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{n-2} & a_{n-1} & b_{n-1} \\ 0 & & & b_{n-1} & a_n \end{bmatrix},$$

where $a_i = a_i(\lambda)$ and $b_i = b_i(\lambda)$. We choose $m \approx n/2$ and set $b_m = 0$. We obtain

$$Q_0(\lambda) = \begin{bmatrix} Q_1(\lambda) & 0 \\ 0 & Q_2(\lambda) \end{bmatrix}.$$

We take the eigenvalues $\widetilde{\lambda}_{2n} \leq \cdots \leq \widetilde{\lambda}_1$ of Q_0 as approximations to the eigenvalues $\lambda_{2n} \leq \cdots \leq \lambda_1$ of Q (and repeat this recursively for Q_1 and Q_2).

Theorem: If Q is hyperbolic, so is Q_0 and the eigenvalues of Q_0 and Q interlace:

a) $\lambda_{2n} \leq \widetilde{\lambda}_{2n}$ and $\widetilde{\lambda}_1 \leq \lambda_1$,

b) $\widetilde{\lambda}_{i+1} \leq \lambda_i \leq \widetilde{\lambda}_{i-1}$ for $i = 2, \ldots, n-1$ and $i = n+2, \ldots, 2n-1$,

c) $\widetilde{\lambda}_{n+1} \leq \lambda_{n+1} < \lambda_n \leq \widetilde{\lambda}_n$.

Laguerre's method

Laguerre's iteration for $f(\lambda) = \det(Q(\lambda))$ is

$$L_\pm(x) = x + \frac{2n}{\left(\frac{-f'(x)}{f(x)} \pm \sqrt{(2n-1)\left((2n-1)\left(\frac{-f'(x)}{f(x)}\right)^2 - 2n\frac{f''(x)}{f(x)}\right)}\right)}.$$

Has cubic convergence close to a simple eigenvalue.

Global convergence: if we add $\lambda_{2n+1} = -\infty$ and $\lambda_0 = \infty$ then for $x \in (\lambda_{i+1}, \lambda_i)$ we have

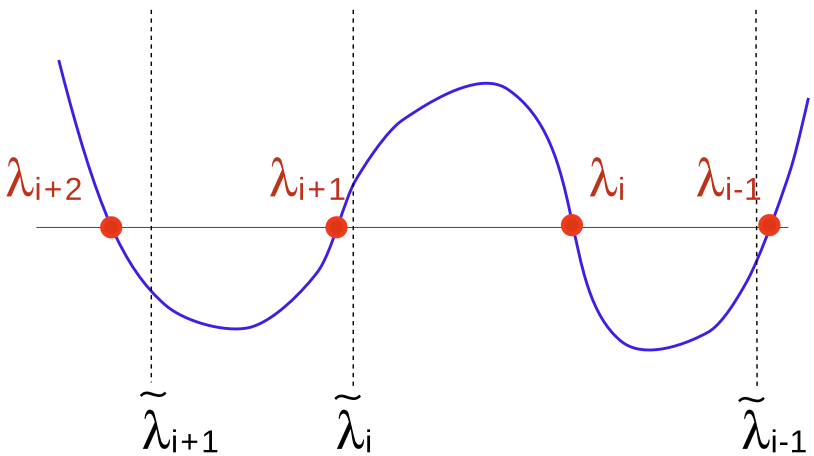
$$\lambda_{i+1} < L_-(x) < x < L_+(x) < \lambda_i.$$

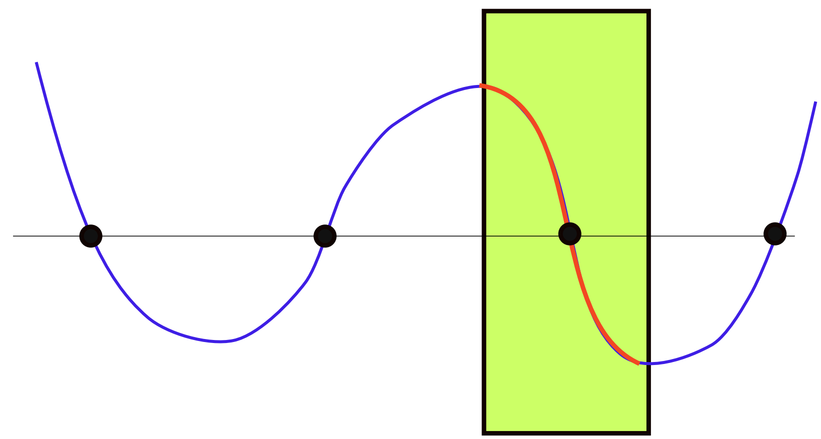
Divide-and-conquer:

- interlation shows that $\widetilde{\lambda}_i$ is good initial approximation for λ_i,
- from $\nu(Q(\widetilde{\lambda}_i))$ we see if $\lambda_i < \widetilde{\lambda}_i$ or $\widetilde{\lambda}_i < \lambda_i$ and then use L_- or L_+ sequence.

Bisection and Laguerre's method

If $\widetilde{\lambda}_i$ is close to λ_{i-1} or λ_{i+1}, then the convergence can be very slow.





The necessary condition for the cubic convergence near a single eigenvalue λ is

$$\frac{f'(x)}{f(x)}(x-\lambda) > 0.$$

We first use bisection on $[\widetilde{\lambda}_i, \widetilde{\lambda}_{i+1}]$ (or $[\widetilde{\lambda}_i, \widetilde{\lambda}_{i-1}]$) until the condition is achieved.

Ehrlich–Aberth's method

The method simultaneously approximates all the zeros of a polynomial $f(\lambda) = \det(Q(\lambda))$. From an initial approximation $x^{(0)} \in \mathbb{C}^{2n}$ the method generates a sequence $x^{(j)} \in \mathbb{C}^{2n}$ which locally converges to the eigenvalues of Q. The equation is

$$x_j^{(k+1)} = x_j^{(k)} - \frac{\frac{f\left(x_j^{(k)}\right)}{f'\left(x_j^{(k)}\right)}}{1 - \frac{f\left(x_j^{(k)}\right)}{f'\left(x_j^{(k)}\right)} \sum_{\substack{l=1 \\ l \neq j}}^{2n} \frac{1}{x_j^{(k)} - x_l^{(k)}}}$$

for $j = 1, \ldots, 2n$.

If implemented in the Gauss–Seidel style then the convergence for simple roots is cubical.

To eliminate multiple values in the initial approximation obtained by the D&C we slightly perturb the eigenvalues of Q_0.

Computation of $\det(Q(\lambda))$ from the three term recurrences

Let

$$Q(\lambda) = \begin{bmatrix} a_1 & b_1 & & & 0 \\ b_1 & a_2 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{n-2} & a_{n-1} & b_{n-1} \\ 0 & & & b_{n-1} & a_n \end{bmatrix},$$

where $a_i = a_i(\lambda)$ and $b_i = b_i(\lambda)$. Then

$f_0 = 1,\ f_1 = a_1, \quad f_{r+1} = a_{r+1} f_r - b_r^2 f_{r-1}.$

$f_0' = 0,\ f_1' = a_1', \quad f_{r+1}' = a_{r+1}' f_r + a_{r+1} f_r' - 2 b_r b_r' f_{r-1} - b_r^2 f_{r-1}'.$

$f_0'' = 0,\ f_1'' = a_1'', \quad f_{r+1}'' = a_{r+1}'' f_r + 2 a_{r+1}' f_r' + a_{r+1} f_r'' - 2 b_r'^2 f_{r-1} - 2 b_r b_r'' f_{r-1} - 4 b_r b_r' f_{r-1}' - b_r^2 f_{r-1}''.$

Because of possible overflow–underflow problems, we rather use simillar recurrences for

$$d_i = \frac{f_i}{f_{i-1}}, \quad g_i = \frac{f_i'}{f_i}, \quad h_i = \frac{f_i''}{f_i}.$$

Computation of $\det(Q(\lambda))$ from the LU decomposition

Bohte (1979): If $\det(Q(\lambda)) \neq 0$ and $PQ(\lambda) = LU$ is a LU decomposition of $Q(\lambda)$, then

$$f(\lambda) = \det(Q(\lambda)) = \det(P) \cdot u_{11} u_{22} \cdots u_{nn}.$$

It follows $PQ'(\lambda) = L'U + LU' = MU + LV$, where $M = L'$ is lower triangular with zero diagonal and $V = U'$ is upper triangular.

M and V can be computed from $Q'(\lambda)$, P, L, and U. Then

$$\frac{f'(\lambda)}{f(\lambda)} = \sum_{i=1}^{n} \frac{v_{ii}}{u_{ii}}.$$

Remarks:

- generalization for f'' is straightforward,
- implementation for banded matrices computes f'/f and f''/f in $\mathcal{O}(n)$.

Numerical example 1: hyperbolic tridiagonal QEP

- M and K: diagonals and codiagonals are random from $[0.5, 1]$ and $[0, 0.1]$, respectively,
- C: diagonals and codiagonals are random from $[4, 5]$ and $[0, 0.5]$, respectively.
- ZGGEV: linearization + Lapack routine for the generalized eigenvalue problem

n	Ehrlich-Aberth $\mathbb{R}$	Laguerre-bisection	ZGGEV
average number of iterations in the last D&C			
100	1.88	1.86	
200	1.76	2.09	
400	1.57	1.20	
800	1.55	1.26	
time in seconds			
100	0.02	0.02	0.60
200	0.05	0.06	5.02
400	0.13	0.23	52.95
800	0.48	0.83	684.63
maximum relative error			
100	5e-15	5e-15	5e-14
200	5e-15	5e-15	9e-14
400	5e-15	5e-15	1e-13
800	5e-15	5e-15	1e-13

Numerical example 2: general tridiagonal QEP

QEP 1:

- M: diagonals and codiagonals are random from $[0,1]$ and $[0,0.1]$, respectively,
- C: diagonals and codiagonals are random from $[0,1]$ and $[0,0.5]$, respectively,
- K: diagonals and codiagonals are random from $[0,1]$ and $[0,0.2]$, respectively.

QEP 2: Example from Tisseur and Meerbergen (2000)

- $M = \text{tridiag}(0.1, 1, 0.1)$, $C = \text{tridiag}(-3, 9, -3)$, $K = \text{tridiag}(-5, 15, -5)$
- all eigenvalues are simple, D&C approximations are double.

	QEP 1					QEP 2				
	ZGGEV		Ehrlich–Aberth $\mathbb{C}$			ZGGEV		Ehrlich–Aberth $\mathbb{C}$		
n	time	error	time	avg. iter	error	time	error	time	avg. iter	error
100	0.75	4e-13	0.03	1.94	1e-13	0.59	7e-15	0.23	20.10	2e-15
200	6.16	3e-12	0.11	1.72	9e-15	5.23	4e-14	1.02	19.52	2e-15
400	67.09	4e-12	0.39	1.56	4e-14	46.64	6e-14	4.09	18.88	4e-15

Numerical example 3: banded QEP

We can apply the Ehrlich-Aberth method if an efficient method for the computation of the characteristic polynomial and its derivative is available. For banded matrices we can use the method based on the LU factorization.

The initial approximations are obtained by the D&C scheme from the eigenvalues of

$$Q_0(\lambda) = \begin{bmatrix} Q_1(\lambda) & 0 \\ 0 & Q_2(\lambda) \end{bmatrix}.$$

We take `M=randn(n)`, `C=randn(n)`, and `K=randn(n)`, set $m_{ij} = c_{ij} = k_{ij} = 0$ for $|i-j| > p$, where p is the bandwidth, and apply the Ehrlich-Aberth method. Table shows the average number of iterations in the last D&C step.

p	$n = 50$	$n = 100$	$n = 200$
1	3.91	2.85	2.32
2	5.78	4.18	3.31
3	6.23	5.31	4.44
4	6.42	5.91	5.33
5	9.27	6.44	6.37

Conclusions

- Two methods for the tridiagonal hyperbolic QEP.
- All methods can be easily parallelized.
- This approach might be applied to:
  - nonsymmetric and non hyperbolic tridiagonal quadratic eigenvalue problems,
  - tridiagonal polynomial problems,
  - banded polynomial eigenvalue problems.
- Algorithm based on LU decomposition might be used for an efficient computation of the derivative of the determinant.