Numerical methods for tridiagonal quadratic eigenvalue problems

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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 that are the zeros of the characteristic polynomial $f(\lambda) = \det(Q(\lambda))$ and the eigenvalues of the $2n \times 2n$ matrix

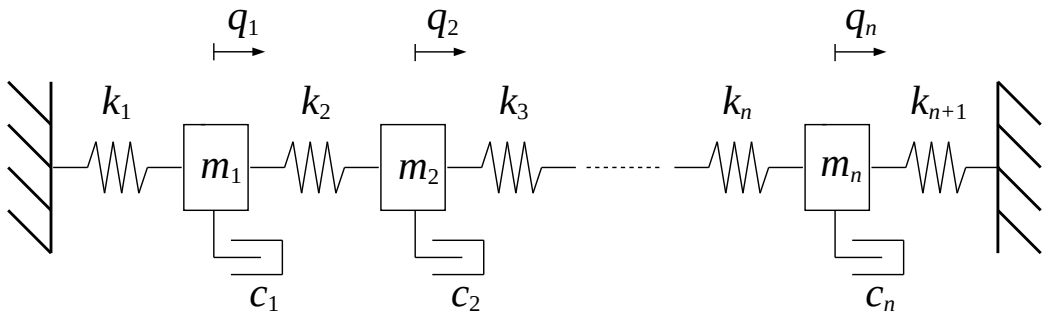
$$\begin{bmatrix} 0 & I \\ -M^{-1}K & -M^{-1}C \end{bmatrix}.$$

We consider a special case where

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

Our goal is to compute all the eigenvalues. 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

$$M = \begin{bmatrix} m_1 & & \\ & \ddots & \\ & & m_n \end{bmatrix}, \; C = \begin{bmatrix} c_1 & & \\ & \ddots & \\ & & c_n \end{bmatrix}, \; K = \begin{bmatrix} k_1 + k_2 & -k_2 & & \\ -k_2 & \ddots & \ddots & \\ & \ddots & \ddots & -k_n \\ & & -k_n & k_n + k_{n+1} \end{bmatrix}.$$

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
- Inertia of a hyperbolic QEP
- $\det(Q(\lambda))$ and its derivatives
- Rank two divide and conquer approach
- Laguerre's method and bisection
- Ehrlich–Aberth's method
- Durand–Kerner's method
- Numerical experiments
- Conclusion

Hyperbolic QEP

$Q(\lambda) = \lambda^2 M + \lambda C + K$ 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
- eigenvalues are semisimple
- a gap between n largest (primary) and n smallest (secondary) eigenvalues
- n linearly independent eigenvectors associated with the primary and the secondary eigenvalues, respectively
- (Markus 1988)
  Selfadjoint Q with $M > 0$ is hyperbolic iff there exists λ_0 such that $Q(\lambda_0) < 0$.

Minimax principle

For each $x \neq 0$, the equation $x^T Q(\mu) x = 0$

$$\mu^2 x^T M x + \mu x^T C x + x^T K x = 0$$

has two real solutions $\mu_1(x) < \mu_2(x)$.

Minimax principle (Duffin 1955): If $\lambda_{2n} \leq \cdots \leq \lambda_1$ are eigenvalues of a hyperbolic QEP Q then

$$\lambda_i = \max_{\substack{S \subset \mathbb{R}^n \\ \dim(S) = i}} \min_{0 \neq x \in S} \mu_2(x)$$

and

$$\lambda_{n+i} = \max_{\substack{S \subset \mathbb{R}^n \\ \dim(S) = i}} \min_{0 \neq x \in S} \mu_1(x)$$

for $i = 1, \ldots, n$.

Inertia of a hyperbolic QEP

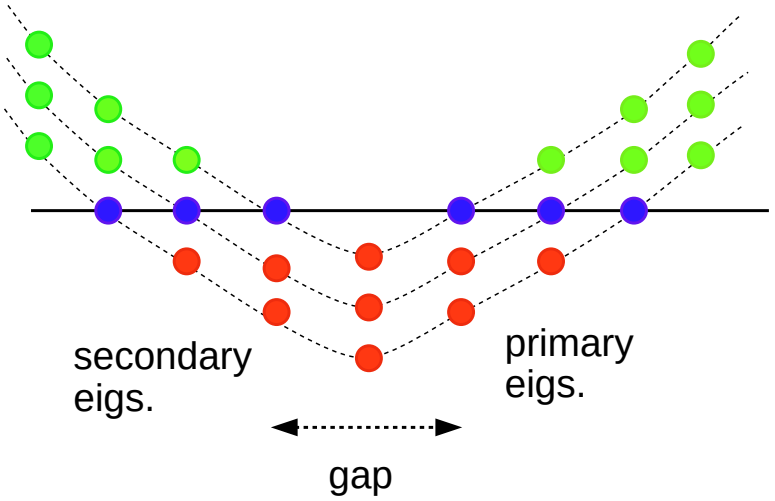
$$Q(\lambda) = \lambda^2 M + \lambda C + K$$

Inertia of a symmetric matrix A is a triple $(\nu(A), \zeta(A), \pi(A))$, where ν, ζ and π are the numbers of negative, zero and positive eigenvalues of A, respectively.

Theorem: Let γ be such that $Q(\gamma) < 0$.

a) If $\gamma \leq \mu$ then $\nu(Q(\mu))$ equals the number of eigenvalues of Q that are greater than μ.

b) If $\mu \leq \gamma$ then $\nu(Q(\mu))$ equals the number of eigenvalues of Q that are smaller than μ.



Bisection and other methods

Based on the inertia we can use bisection to obtain the k-th eigenvalue, but the convergence is slow. Therefore we apply methods that were successfully applied to tridiagonal generalized eigenproblems.

- Laguerre's method
  - K. Li, T.Y. Li (1993) - symmetric tridiagonal eigenproblem
  - K. Li, T.Y. Li, Z. Zeng (1994) - generalized symmetric tridiagonal eigenproblem
- Ehrlich–Abert's method
  - D.A. Bini, L. Gemignani, F. Tisseur (2003) - nonsymmetric tridiagonal eigenproblem
- Durand–Kerner's method
  - K. Li (1999) - generalized symmetric tridiagonal eigenproblem

The above methods require stable and efficient computation of $\nu(Q(\lambda))$, $f(\lambda)$, $f'(\lambda)/f(\lambda)$ and $f''(\lambda)/f(\lambda)$, where $f(\lambda) = \det(Q(\lambda))$.

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

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

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

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

As the above recurrences may suffer from overflow–underflow problems, we define $d_i = \frac{f_i}{f_{i-1}}$, $g_i = \frac{f_i'}{f_i}$, $h_i = \frac{f_i''}{f_i}$:

$$d_1 = a_1, \qquad d_{r+1} = a_{r+1} - \frac{b_r^2}{d_r}.$$

$$g_0 = 0,\ g_1 = \frac{a_1'}{a_1}, \quad g_{r+1} = \frac{1}{d_{r+1}}\left(a_{r+1}' + a_{r+1} g_r - \frac{1}{d_r}(2 b_r b_r' + b_r^2 g_{r-1})\right).$$

$$h_0 = 0, h_1 = \frac{a_1''}{a_1}, \quad h_{r+1} = \frac{1}{d_{r+1}}\left(a_{r+1}'' + 2 a_{r+1}' g_r + a_{r+1} h_r - \frac{1}{d_r}(2 b_r'^2 + 2 b_r b_r'' + 4 b_r b_r' g_{r-1} + b_r^2 h_{r-1})\right).$$

Using QR decomposition

It is known that

$$f'(\lambda)/f(\lambda) = \mathrm{Tr}(Q(\lambda)^{-1}Q'(\lambda)).$$

Bini, Gemignani, Tisseur (2003): A stable $\mathcal{O}(n)$ computation for $\mathrm{Tr}(A^{-1})$, where A is unreduced nonsymmetric tridiagonal matrix.

Kressner (2004): Generalization to $\mathcal{O}(n)$ algorithm for the computation of $\mathrm{Tr}(A^{-1}B)$ where A and B are tridiagonal.

Using LU decomposition

Bohte (1979): Suppose that $\det(Q(\lambda)) \neq 0$ and that $PQ(\lambda) = LU$ is LU decomposition for $Q(\lambda)$. Then

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

By differentiation we have $PQ'(\lambda) = L'U + LU' = MU + LV$, where $M = L'$ is lower triangular with zero diagonal and $V = U'$ is upper triangular. M and V of the proper form and such that $PQ'(\lambda) = MU + LV$ can be computed from $Q'(\lambda)$, P, L, and U. It follows that

$$f'(\lambda) = \det(P) \sum_{i=1}^{n} v_{ii} \prod_{\substack{j=1 \\ j \neq i}}^{n} u_{jj}$$

and

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

For the second derivative we have $PQ''(\lambda) = L''U + 2L'U' + LU'' = NU + 2MV + LW$, where $N = L''$ is lower triangular with zero diagonal and $V = U''$ is upper triangular. It follows that

$$f''(\lambda)/f(\lambda) = \sum_{i=1}^{n} \frac{w_{ii}}{u_{ii}} + \left(\sum_{i=1}^{n} \frac{v_{ii}}{u_{ii}} \right)^2 - \sum_{i=1}^{n} \frac{v_{ii}^2}{u_{ii}^2}.$$

Divide and conquer

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

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

Q_0 is hyperbolic. 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.

We repeat the procedure recursively for the eigenvalues of Q_1 and Q_2.

Interlacing property

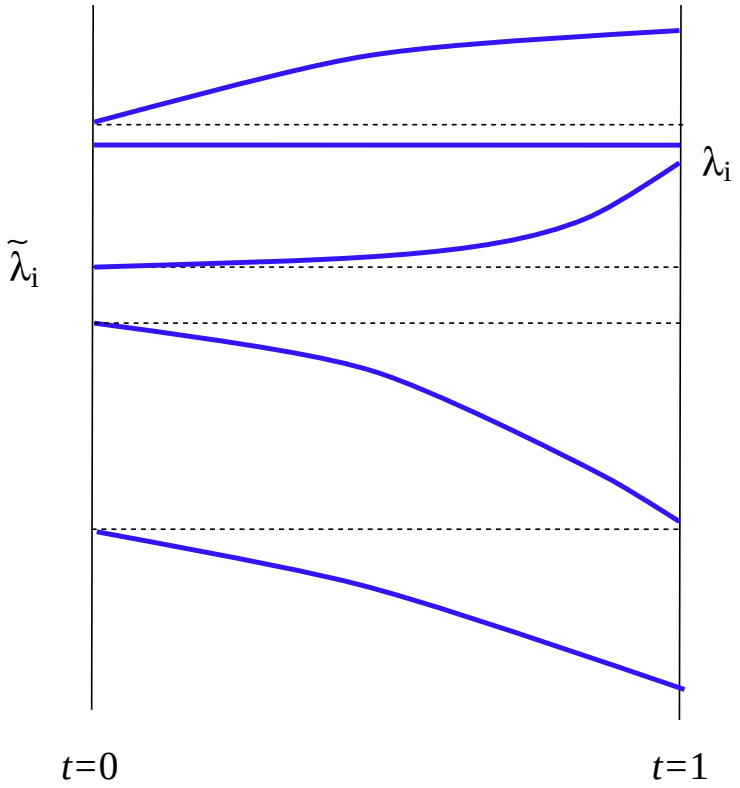
$$Q_0(\lambda) = \begin{bmatrix} Q_1(\lambda) & 0 \\ 0 & Q_2(\lambda) \end{bmatrix}$$

Theorem: Let $\widetilde{\lambda}_{2n} \leq \cdots \leq \widetilde{\lambda}_1$ be the eigenvalues of Q_0 and $\lambda_{2n} \leq \cdots \leq \lambda_1$ the eigenvalues of Q. Then

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

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

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

The method has cubic convergence in a neighbourhood of 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

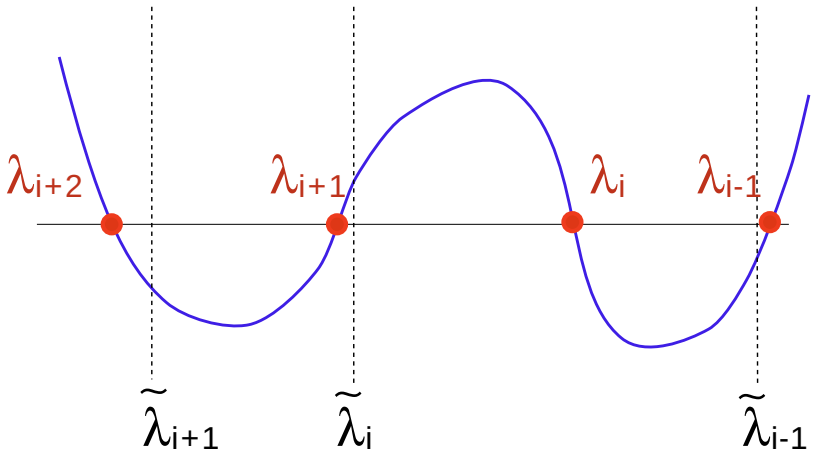
$$\lambda_{i+1} < L_-(x) < x < L_+(x) < \lambda_i.$$

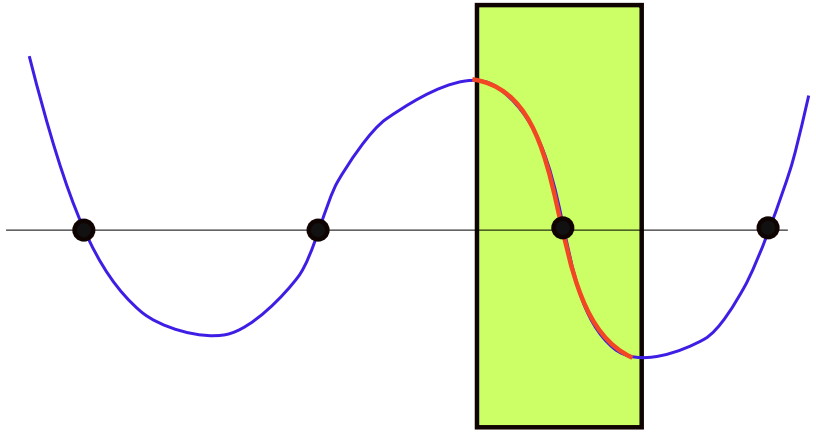
Divide and conquer: eigenvalues $\widetilde{\lambda}_{2n} \leq \cdots \leq \widetilde{\lambda}_1$ of $Q_0(\lambda)$ are initial approximations for $\lambda_{2n} \leq \cdots \leq \lambda_1$.

As $\widetilde{\lambda}_{i+1} \leq \lambda_i \leq \widetilde{\lambda}_{i-1}$ we can always use $\widetilde{\lambda}_i$ as an 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 that the sign of $f'(x)/f(x)$ agrees with the sign of $x - \lambda$. To improve the convergence we first use bisection on interval $[\widetilde{\lambda}_i, \widetilde{\lambda}_{i+1}]$ (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

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

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

If we implement the method in the Gauss–Seidel style then the convergence for simple roots is cubical and linear for multiple roots. We iterate only those eigenvalues that have not converged yet.

For initial approximations we again use divide and conquer with rank two modifications. To eliminate multiple values in the initial approximation we slightly perturb the eigenvalues of Q_0.

Durand–Kerner's method

Another method that simultaneously approximates all the zeros of a polynomial. As the method requires that the leading coefficient of the polynomial is one we apply it on

$$p(\lambda) = \frac{1}{\det(M)} \det(Q(\lambda)).$$

Similar to Ehrlich–Aberth the method generates a sequence $x^{(j)} \in \mathbb{C}^{2n}$ which locally converges to the eigenvalues of Q. The equation for $j = 1, \ldots, 2n$ is

$$x_j^{(k+1)} = x_j^{(k)} - \frac{p(x_j^{(k)})}{\prod_{\substack{l=1 \\ l \neq j}}^{2n} (x_j^{(k)} - x_l^{(k)})}.$$

If we implement the method in the Gauss–Seidel style then the convergence for simple roots is superquadratical and linear for multiple roots. As before, we iterate only the eigenvalues that have not converged yet.

Comparison and numerical results

In Matlab 7.0 we tested all three methods on a limited set of tridiagonal QEPs. We compared the average number of iterations. In all three methods one step (for one eigenvalue approximation) has linear time complexity. Three term recurrences were used for the computation of $\det(Q(\lambda))$ and its derivatives.

- One step of Durand–Kerner's method is the cheapest as it requires only values of f.
- One step of Ehrlich–Aberth's method requires f and f' and is roughly equivalent to 1.6 Durand–Kerner steps.
- One step of Laguerre's method is the most expensive. It requires f, f' and f'', and is roughly equivalent to 2.4 Durand–Kerner steps.

Numerical example 1

- M and K: diagonals are random values from $[0.5, 1]$, codiagonals are random values from $[0, 0.1]$,
- C: diagonals are random values from $[4, 5]$, codiagonals are random values from $[0, 0.5]$,

n	Ehrlich-Aberth $\mathbb{R}$	Durand-Kerner $\mathbb{R}$	Ehrlich-Aberth $\mathbb{C}$	Durand-Kerner $\mathbb{C}$	Laguerre-bisection	polyeig
avg. iteration in last D&C						
50	2.46	5.25	2.52	5.29	2.19	
100	2.15	6.47	2.26	6.61	1.71	
200	1.99	9.85	2.17	9.84	1.91	
400	1.86	4.48	2.04	4.59	1.16	
800	1.85	4.51	2.03	4.60	1.22	
time						
50	0.34	0.64	0.52	1.05	0.45	0.09
100	0.72	1.69	1.22	3.27	1.03	0.53
200	1.55	4.88	3.31	11.84	2.53	4.75
400	3.59	11.28	9.28	30.41	5.98	53.25
800	9.25	32.00	29.19	89.67	15.38	924.53
error						
50	2e-16	2e-16	2e-16	2e-16	7e-15	5e-15
100	2e-16	2e-16	4e-16	2e-16	6e-15	1e-14
200	2e-16	2e-16	2e-16	3e-16	4e-15	1e-14
400	3e-16	2e-16	2e-16	3e-16	2e-15	2e-14
800	2e-16	3e-16	2e-16	3e-16	5e-15	2e-14

- all eigenvalues are simple,
- as the dimension of the matrices increases, better the eigenvalues of $Q_0(\lambda)$ approximate eigenvalues of $Q(\lambda)$ and fewer steps are required in the final divide and conquer phase.

Numerical example 2

- $M = \mathrm{tridiag}(0.1, 1, 0.1)$, $C = \mathrm{tridiag}(0.5, 5, 0.5)$, $K = \mathrm{tridiag}(0.2, 1, 0.2)$
- all eigenvalues are simple, divide and conquer approximations are double

n	Ehrlich-Aberth $\mathbb{R}$	Durand-Kerner $\mathbb{R}$	Ehrlich-Aberth $\mathbb{C}$	Durand-Kerner $\mathbb{C}$	Laguerre-bisection	polyeig
avg. iterations in last D&C						
50	13.55	47.23	10.66	18.39	4.32	
100	12.91	115.65	10.17	23.76	4.34	
200	12.38	> 500	9.51	19.32	4.32	
400	11.87	> 500	9.05	21.82	4.30	
800	11.25	> 500	8.53	23.86	4.29	
time						
50	0.77	1.86	1.13	2.00	0.53	0.19
100	1.94	10.08	3.38	7.61	1.34	0.52
200	5.09	> 93	10.39	24.50	3.42	5.00
400	13.78	> 354	33.09	94.59	9.14	57.83
800	39.72	> 1495	111.63	372.38	26.20	1126.36
error						
50	4e-16	4e-16	4e-16	4e-16	3e-15	5e-15
100	5e-16	2e-11	5e-16	5e-16	3e-15	4e-15
200	6e-16	3e-02	5e-16	4e-16	5e-15	5e-15
400	5e-16	2e+00	5e-16	6e-16	5e-15	5e-15
800	5e-16	2e-02	5e-16	3e-06	6e-15	7e-15

Numerical example 3

- $Q(\lambda) = \begin{bmatrix} Q_1(\lambda) & A(\lambda) & \\ A(\lambda)^T & Q_1(\lambda) & A(\lambda) \\ & A(\lambda)^T & Q_1(\lambda) \end{bmatrix}$, where $A(\lambda) = \begin{bmatrix} 0 & 0 \\ 10^{-4}\lambda & 0 \end{bmatrix}$ and Q_1 is from the first numerical example.
- eigenvalues appear in clusters of size three

n	Ehrlich-Aberth $\mathbb{R}$	Durand-Kerner $\mathbb{R}$	Ehrlich-Aberth $\mathbb{C}$	Durand-Kerner $\mathbb{C}$	Laguerre-bisection	polyeig
avg. iteration in last D&C						
51	6.00	96.01	10.13	29.77	12.76	
102	7.64	52.92	16.10	37.67	9.60	
201	8.72	52.20	17.53	39.29	6.71	
402	8.42	> 500	17.85	57.18	4.04	
time						
51	0.39	4.63	0.80	2.39	0.69	0.08
102	0.92	6.80	2.94	8.80	1.44	0.48
201	2.36	18.34	9.67	30.17	3.28	4.61
402	5.70	> 239	34.11	152.53	7.55	50.41
error						
51	1e-14	1e-07	7e-16	1e-15	1e-13	5e-15
102	2e-14	6e-08	8e-16	2e-15	2e-13	9e-15
201	2e-14	1e-08	9e-16	2e-15	9e-14	2e-14
402	2e-14	1e-05	1e-15	3e-08	7e-10	2e-14

Ehrlich-Aberth and general tridiagonal QEP

- M: diagonals are random values from $[0, 1]$, codiagonals are random values from $[0, 0.1]$,
- C: diagonals are random values from $[0, 1]$, codiagonals are random values from $[0, 0.5]$,
- K: diagonals are random values from $[0, 1]$, codiagonals are random values from $[0, 0.2]$,
- all eigenvalues are simple.

	`polyeig`		Ehrlich-Aberth $\mathbb{C}$			Durand-Kerner $\mathbb{C}$		
n	time	error	time	avg. iter	error	time	avg. iter	error
50	0.11	1e-14	0.72	2.29	9e-16	1.27	4.72	9e-16
100	0.86	5e-14	2.03	2.34	8e-15	4.64	5.88	6e-15
200	6.38	9e-14	4.05	2.14	7e-15	10.45	6.21	1e-14
400	68.11	2e-13	11.30	2.09	3e-15	33.06	3.98	1e-14

Example from Tisseur and Meerbergen (2000)

- $M = \mathrm{tridiag}(0.1, 1, 0.1)$, $C = \mathrm{tridiag}(-3, 9, -3)$, $K = \mathrm{tridiag}(-5, 15, -5)$
- all eigenvalues are simple, $\mathrm{Re}(\lambda) < 0$, divide and conquer approximations are double.

	`polyeig`		Ehrlich-Aberth $\mathbb{C}$			Durand-Kerner $\mathbb{C}$		
n	time	error	time	avg. iter	error	time	avg. iter	error
50	0.11	8e-15	1.42	13.59	2e-15	2.94	30.09	4e-15
100	0.63	1e-14	4.28	13.10	1e-15	9.25	24.59	1e-15
200	5.13	1e-14	13.30	12.73	3e-15	32.47	22.60	3e-15
400	50.05	3e-14	43.06	12.06	4e-15	137.05	28.93	2e-15

Conclusions

Three eigensolvers for tridiagonal hyperbolic QEPs.

Generalizations:

- All methods can be easily parallelized.
- Similar approach (EA and DK) 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 computing of the derivative of the determinant.

Future work:

- handling of multiple eigenvalues
- more numerical tests
- stable computation of f, f' and f''.
- could continuation and path following be competitive to the presented three methods