Filter analysis for the stochastic estimation of eigenvalue counts

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Abstract

To estimate the number of eigenvalues of a Hermitian matrix that are located in a given interval, existing methods include polynomial filtering and rational filtering. Both filtering approaches are based on stochastic approximations for matrix trace. In this paper, we analyze a rational filtering method that is based on polynomial filtering in which the solutions to the linear systems are approximated by a Krylov subspace method. Our analysis and numerical experiments indicate that the rational filtering method is effective when the eigenvalues of a given matrix are sparsely distributed in the target interval.

Keywords eigenvalue counts, stochastic estimation, Krylov subspace methods

Research Activity Group Algorithms for Matrix / Eigenvalue Problems and their Applications

1. Introduction

We consider estimating the number of eigenvalues of a Hermitian matrix that are located in a given interval. Estimations of eigenvalue counts are useful for several applications. For example, the band gap of energy state in materials science can be obtained by estimating the eigenvalue counts in an interval where eigenvalues are sparsely distributed (e.g. see [1]). Estimations of eigenvalue counts are also useful for finding parameters in some kinds of eigensolvers to achieve high efficiency. For these purposes, exact eigenvalue counts are not always necessary.

For estimating the number of eigenvalues, the polynomial filtering method[2] and the rational filtering method[3] are reasonable choices. Both filtering approaches are based on stochastic approximations of a band-pass filter function for the target interval. The polynomial filtering method utilizes filtering techniques based on the Chebyshev polynomials, and the rational filtering method uses a contour integration.

The rational filtering method requires solving linear systems. For a rough estimation of the eigenvalue counts, highly accurate solutions of the linear systems are not required [2]. By applying a Krylov subspace method to the linear systems, we can get an approximation of the eigenvalue counts at each iteration.

In this paper, we analyze the filter function and the error of the estimated eigenvalue counts of the rational filtering method when applying the Krylov subspace method to the linear systems. It is shown that the rational filtering method estimates eigenvalue counts effectively when the target interval lies in a sparse region of

the eigenvalue distribution.

The remainder of this paper is organized as follows. In Section 2, we review the polynomial and rational filtering methods for the eigenvalue counts. In Section 3, we present how to approximate the band-pass filter function and the error of the estimated eigenvalue counts in the rational filtering method when using a Krylov subspace method applied to the linear systems with a fixed number of iterations. In Section 4, we confirm our results by some numerical experiments. Finally, our conclusions are presented in Section 5.

2. Polynomial and rational filtering methods

In this section, we introduce the polynomial filtering method[2] and the rational filtering method[3] for eigenvalue counts. Let $A \in \mathbb{C}^{n \times n}$ be a Hermitian matrix, and let λ_i , $i = 1, 2, \dots, n$ be the eigenvalues. The number of eigenvalues m in an interval $[a, b]$ is given by $m = \sum_{i=1}^n h(\lambda_i)$, where $h(\lambda_i)$ is the band-pass filter function for the interval $[a, b]$ and is defined by

$$h(\lambda_i) = \begin{cases} 1 & (a \leq \lambda_i \leq b), \\ 0 & (\text{otherwise}). \end{cases}$$

The polynomial filtering method uses the Chebyshev polynomials to approximate the band-pass filter $h(\lambda_i)$:

$$h(\lambda_i) \approx P_p(\lambda_i) := \sum_{j=0}^p \gamma_j T_j(\lambda_i),$$

where $T_j(\cdot)$ is the Chebyshev polynomial of the first kind of degree j , and γ_j is the expansion coefficient of the

band-pass filter function[2]. Without loss of generality, it is assumed in the polynomial filtering method that all of the eigenvalues lie in the interval $[-1, 1]$. The number of eigenvalues m can be estimated by

$$m \approx m_P^{(p)} = \sum_{i=1}^n P_p(\lambda_i) = \text{tr}(P_p(A)), \quad (1)$$

where $\text{tr}(\cdot)$ is the matrix trace. The polynomial filtering method produces Gibbs oscillations. To reduce this behavior, the Jackson coefficients[4] can be used.

Next, we introduce the rational filtering method for the eigenvalue counts[3]. Let Γ be a positively oriented closed Jordan curve which intersects the real axis at a and b . The number of eigenvalues m in $[a, b]$ can be computed by

$$m = \frac{1}{2\pi i} \oint_{\Gamma} \text{tr}((zI - A)^{-1}) dz,$$

where $i = \sqrt{-1}$. This is approximated by the N -point quadrature rule

$$m \approx \hat{m}_R = \sum_{k=1}^N w_k \text{tr}((z_k I - A)^{-1}), \quad (2)$$

where w_k is a quadrature weight and z_k is an integration node on Γ [3].

The matrix trace can be approximated by using the stochastic estimation described in [5, 6]:

$$\text{tr}(A) \approx \frac{n}{L} \sum_{\ell=1}^L v_{\ell}^T A v_{\ell}, \quad (3)$$

where v_{ℓ} , $\ell = 1, 2, \dots, L$ are real random vectors such that the mean of their entries is zero and $\|v_{\ell}\|_2 = 1$. The polynomial filtering method[2] applies (3) to (1):

$$m_P^{(p)} \approx \tilde{m}_P^{(p)} = \frac{n}{L} \sum_{\ell=1}^L v_{\ell}^T P_p(A) v_{\ell}. \quad (4)$$

The rational filtering method[3] applies (3) to (2):

$$\hat{m}_R \approx \tilde{m}_R = \frac{n}{L} \sum_{\ell=1}^L \sum_{k=1}^N w_k v_{\ell}^T (z_k I - A)^{-1} v_{\ell}. \quad (5)$$

3. Filter analysis for the rational filtering method

The most time-consuming step in evaluating (5) is solving the $L \times N$ independent linear systems $(z_k I - A)x_{k,\ell} = v_{\ell}$. However, we do not always require the exact value of the eigenvalue counts, and in this case $\tilde{m}_R$ can be approximated by using the approximate solutions $\tilde{x}_{k,\ell}$ of the linear systems:

$$\tilde{m}_R \approx \frac{n}{L} \sum_{\ell=1}^L \sum_{k=1}^N w_k v_{\ell}^T \tilde{x}_{k,\ell}.$$

When applying a Krylov subspace method to these linear systems, we obtain estimated eigenvalue counts at each iteration, and the filter function for the rational filtering method varies according to the iteration. In this section we analyze the filter function and the error of the estimated eigenvalue counts in the rational filtering

method at each iteration. We use the polynomial expression of the Krylov subspace method.

3.1 Filter function for the rational filtering method

Let $x_{k,\ell}^{(p+1)}$ be the $(p+1)$ -st approximate solution obtained by a Krylov subspace method for a linear system $(z_k I - A)x_{k,\ell}$ with a zero initial guess. Then we have $x_{k,\ell}^{(p+1)} = S_p^{(k,\ell)}(z_k I - A)v_{\ell}$, where $S_p^{(k,\ell)}(z_k I - A)$ is the polynomial of degree p . Using $S_p^{(k,\ell)}(z_k I - A)$, $\tilde{m}_R$ in (5) is approximated as

$$\begin{aligned} \tilde{m}_R &\approx \tilde{m}_R^{(p)} = \frac{n}{L} \sum_{k=1}^N \sum_{\ell=1}^L w_k v_{\ell}^T S_p^{(k,\ell)}(z_k I - A) v_{\ell} \\ &= \frac{n}{L} \sum_{\ell=1}^L v_{\ell}^T Q_p^{(N,\ell)}(A) v_{\ell}. \end{aligned} \quad (6)$$

The linear combination of $S_p^{(k,\ell)}(z_k I - A)$ can be represented as $Q_p^{(N,\ell)}(A)$ because of the shift invariance of the Krylov subspace[7]:

$$Q_p^{(N,\ell)}(A) = \sum_{k=1}^N w_k S_p^{(k,\ell)}(z_k I - A).$$

As shown in Section 2, the polynomial filtering method approximates the band-pass filter $h(\lambda_i)$ by $P_p(\lambda_i)$. The rational filtering method uses the Krylov subspace method to approximate $h(\lambda_i)$. Let Λ be a diagonal matrix whose diagonal elements are eigenvalues of A , and let U be a unitary matrix whose i -th column is the eigenvector u_i of A , that is, $A = U\Lambda U^H$. The estimated eigenvalue counts in (6) can be written as

$$\begin{aligned} \tilde{m}_R^{(p)} &= \frac{n}{L} \sum_{\ell=1}^L v_{\ell}^T U Q_p^{(N,\ell)}(\Lambda) U^H v_{\ell} \\ &= \sum_{i=1}^n \frac{n}{L} \sum_{\ell=1}^L Q_p^{(N,\ell)}(\lambda_i) |v_{\ell}^T u_i|^2. \end{aligned}$$

Therefore, the rational filtering method approximates the band-pass filter $h(\lambda_i)$ by

$$R_p^{(N,L)}(\lambda_i) := \frac{n}{L} \sum_{\ell=1}^L Q_p^{(N,\ell)}(\lambda_i).$$

In practice, the value of p is decided when the $(p+1)$ -st residual norm of the linear systems or $|\tilde{m}_R^{(p)} - \tilde{m}_R^{(p-1)}|$ is smaller than a tolerance. The number of iterations of the Krylov subspace method is same as the degree p of $R_p^{(N,L)}(\lambda_i)$. The coefficients of the filter function $P_p(\lambda_i)$ do not depend on the eigenvalue distribution. Therefore, $P_p(\lambda_i)$ has a fixed form that depends on p and $[a, b]$. On the other hand, the coefficients of the filter function $R_p^{(N,L)}(\lambda_i)$ depend on the eigenvalue distribution. Therefore, $R_p^{(N,L)}(\lambda_i)$ has a transmuted form that depends on p , $[a, b]$, v_i , w_k , z_k and $\lambda_1, \lambda_2, \dots, \lambda_n$.

3.2 Error of the estimated eigenvalue counts

Let $e_R = \tilde{m}_R^{(p)} - \tilde{m}_R$ be the error of the estimated eigenvalue counts. Using (5) and (6), e_R can be written

as

$$e_R = \frac{n}{L} \sum_{\ell=1}^L \sum_{k=1}^N w_k v_\ell^T (z_k I - A)^{-1} r_{k,\ell}^{(p+1)},$$

where $r_{k,\ell}^{(p+1)} = v_\ell - (z_k I - A)x_{k,\ell}^{(p+1)}$ is the $(p+1)$ -st residual. The $(p+1)$ -st residual $r_\sigma^{(p+1)}$ of the COCG method applied to $(\sigma I - A)x = v_\ell$ with a zero initial guess satisfies $r_{k,\ell}^{(p+1)} = \xi_{k,\ell}^{(p+1)} r_\sigma^{(p+1)} = \xi_{k,\ell}^{(p+1)} C_{p+1}^{(\ell)}(\sigma I - A)v_\ell$, where $C_{p+1}^{(\ell)}(\sigma I - A)$ is the residual polynomial, and $\xi_{k,\ell}^{(p+1)}, \sigma \in \mathbb{C}$. Then, the error e_R can be written as

$$\begin{aligned} e_R &= \frac{n}{L} \sum_{\ell=1}^L \sum_{k=1}^N w_k v_\ell^T (z_k I - A)^{-1} \xi_{k,\ell}^{(p+1)} C_{p+1}^{(\ell)}(\sigma I - A)v_\ell \\ &= \frac{n}{L} \sum_{\ell=1}^L \sum_{i=1}^n g_{p+1}^{(\ell)}(\lambda_i) \|r_\sigma^{(p+1)}\|_2^{-1} C_{p+1}^{(\ell)}(\sigma - \lambda_i) |v_\ell^T u_i|^2, \end{aligned}$$

where $g_{p+1}^{(\ell)}(\lambda_i) = \|r_\sigma^{(p+1)}\|_2 \sum_{k=1}^N w_k \xi_{k,\ell}^{(p+1)} / (z_k - \lambda_i)$. Here, if $\sigma I - A$ is Hermitian positive definite, then the polynomial $C_{p+1}^{(\ell)}(\lambda_i)$ is constructed so that it minimizes $\sum_{i=1}^n (\sigma - \lambda_i)^{-1} |C_{p+1}^{(\ell)}(\sigma - \lambda_i) v_\ell^T u_i|^2$. It is expected that $g_{p+1}^{(\ell)}(\lambda_i)$ is a function which decays outside the given interval, i.e. $g_{p+1}^{(\ell)}(\lambda_i) \approx 0$ for $\lambda_i \notin [a, b]$. Therefore, we expect e_R is small when eigenvalues sparsely distribute in the target interval.

4. Numerical experiments

Two numerical examples are presented in this section. The first example depicts how polynomials work as filter functions in the stochastic estimation methods. The second example depicts how the degrees of the polynomials in (4) and (6) affects the estimation of the eigenvalue counts. All the computations were performed using MATLAB 8.3. The elements of the sample vectors were constructed by the MATLAB function `randn` of ‘twister’ type with seed 0.

4.1 Example 1

In this example, we explore the behavior of the filter functions in the polynomial and rational filtering methods by changing the distribution of the eigenvalues. The test matrices are diagonal. The diagonal elements of $A = \{a_{ii}\}_{i=1,2,\dots,1000}$ were set for the two cases: case 1: $a_{ii} = c_i$; and case 2: $a_{ii} = \text{sign}(c_i) * \sqrt{|c_i|}$, where the values of c_i are linearly spaced in the interval $[-1, 1]$, that is, $c_i = -1 + 2*(i-1)/999$, and $\text{sign}(\cdot)$ is the signum function. The target interval $[a, b]$ was set to $[-0.035, 0.035]$. The exact eigenvalue counts for the matrices of cases 1 and 2 are 34 and 2, respectively. The parameters were set to $p = 200$, $L = 30$, and $N = 16$, and the integral path Γ was taken to be a circle centered at $(b+a)/2$ with radius $(b-a)/2$. The linear systems were dealt with the shifted COCG method (s-COCG) [8], and $\sigma = 2 > \max(\lambda_i)$.

The filter functions and $g_{p+1}^{(\ell)}(\lambda)$ for the cases 1 and 2 are shown in Figs. 1 and 2, respectively. The horizontal axes indicate the eigenvalues. Markers indicate the approximated filter function for each eigenvalue, as obtained by the polynomial filtering method $P_p(\lambda)$,

Fig. 1. Approximated filter functions for the case 1.

Fig. 2. Approximated filter functions for the case 2.

the polynomial filtering method with the Jackson coefficient $P_p^J(\lambda)$, and the rational filtering method $R_p^{(N,L)}(\lambda)$. Here, $h(\lambda)$ is the exact band-pass filter. We can see that $P_p(\lambda)$ and $P_p^J(\lambda)$ have the same form for each case, whereas $R_p^{(N,L)}(\lambda)$ has a different form for each case, and $g_{p+1}^{(\ell)}(\lambda)$ decays outside the target interval. In Fig. 2, we can see that $R_p^{(N,L)}(\lambda)$ and $g_{p+1}^{(\ell)}(\lambda)$ decay more rapidly outside the given interval than the case 1. These results indicate that the rational filtering method is more effective when the distribution of the eigenvalues in a given interval is sparse.

4.2 Example 2

In this example, we investigated how the estimated eigenvalue counts varied as the degree p of the polynomial increased. The test matrix was taken from the ELSEs matrix library[9], and its physical origin was a thermally vibrating carbon nanotube. This matrix is a real symmetric matrix of dimension $n = 4000$. The target intervals $[a, b]$ were set to $[0.1, 0.15]$, $[-0.125, -0.075]$, and $[0.33, 0.38]$; note that these all have the same width. The exact eigenvalue counts in these intervals are 32, 4, and 0. Here, p was set to 10, 20, 50, 100, 150, and 200, and $\sigma = 2 > \max(\lambda_i)$, and $\lambda_1, \lambda_2, \dots, \lambda_n$ were computed by the MATLAB function `eig`. The other parameter values were the same as in Example 1.

The estimated eigenvalue counts for these intervals are given in Tables 1, 2, and 3, and the approximated filter functions and $g_{p+1}^{(\ell)}(\lambda)$ are shown in Figs. 3, 4, and 5. The value $\tilde{m}_p^{(p)}(\text{Jackson})$ indicates the estimated eigenvalue counts of the polynomial filtering method using the Jackson coefficients. In Table 3, we can see that

Fig. 3. Approximated filter functions for the case of $[0.1, 0.15]$. Fig. 4. Approximated filter functions for the case of $[-0.125, -0.075]$. Fig. 5. Approximated filter functions for the case of $[0.33, 0.38]$.

$\tilde{m}_R^{(p)}$ estimates eigenvalue counts with a smaller degree p of the polynomial than that estimated by $\tilde{m}_P^{(p)}$ and $\tilde{m}_P^{(p)}$ (Jackson) for the interval $[0.33, 0.38]$. Fig. 5 shows that $R_p^{(N,L)}(\lambda)$ and $g_{p+1}^{(\ell)}(\lambda)$ decay more rapidly outside the given interval than other cases. These results indicate that the rational filtering method estimates eigenvalue counts effectively when the target interval lies in a sparse region of the eigenvalue distribution.

5. Conclusion

In this paper, we analyzed the filter function in the rational filtering method in which the solutions of the linear systems are approximated by a fixed iteration of a Krylov subspace method. We showed that the rational filtering method is effective in an interval where the eigenvalues are sparsely distributed, and it was confirmed by some numerical experiments. As an area of future work, we intend to analyze the filter function of the stochastic estimation method for generalized non-

Table 1. Estimated eigenvalue counts for the case of $[0.1, 0.15]$.

p	$\tilde{m}_P^{(p)}$	$\tilde{m}_P^{(p)}$ (Jackson)	$\tilde{m}_R^{(p)}$
10	134.83	110.55	279.15
20	72.75	118.51	159.12
50	24.30	88.22	33.80
100	34.18	52.55	36.75
150	32.45	42.54	31.13
200	31.52	38.62	31.19
m	32	32	32

Table 2. Estimated eigenvalue counts for the case of $[-0.125, -0.075]$.

p	$\tilde{m}_P^{(p)}$	$\tilde{m}_P^{(p)}$ (Jackson)	$\tilde{m}_R^{(p)}$
10	86.22	115.63	223.48
20	22.80	101.49	89.00
50	2.52	49.83	7.07
100	1.39	18.71	4.24
150	3.22	9.57	3.98
200	4.49	6.38	3.96
m	4	4	4

Table 3. Estimated eigenvalue counts for the case of $[0.33, 0.38]$.

p	$\tilde{m}_P^{(p)}$	$\tilde{m}_P^{(p)}$ (Jackson)	$\tilde{m}_R^{(p)}$
10	96.86	154.60	0.00
20	8.50	122.17	0.00
50	6.01	41.10	0.01
100	3.93	11.05	0.02
150	0.86	3.86	0.02
200	0.33	1.43	0.02
m	0	0	0

symmetric eigenvalue problems.

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References

- [1] R. L. Chern, C. C. Chang, C. C. Chang and R. R. Hwang, Numerical study of three-dimensional photonic crystals with large band gaps, *J. Phys. Soc. Jpn.*, **73** (2004), 727–737.
- [2] E. D. Napoli, E. Polizzi and Y. Saad, Efficient estimation of eigenvalue counts in an interval, *arXiv:cs/1308.4275v2*, 2014.
- [3] Y. Futamura, H. Tadano and T. Sakurai, Parallel stochastic estimation method for eigenvalue distribution, *JSIAM Letters*, **2** (2010), 127–130.
- [4] L. O. Jay, H. Kim, Y. Saad and J. R. Chelikowsky, Electronic structure calculations using plane wave codes without diagonalization, *J. Comput. Appl. Math.*, **118** (1999), 21–30.
- [5] Z. Bai, M. Fahey and G. Golub, Some large scale matrix computation problems, *J. Comput. Appl. Math.*, **74** (1996), 71–89.
- [6] M. F. Hutchinson, A stochastic estimator of the trace of the influence matrix for laplacian smoothing splines, *Commun. Stat.-Simul. Comput.*, **19** (1990), 433–450.
- [7] B. Jegerlehner, Krylov space solvers for shifted linear systems, *arXiv:hep-lat/9612014v1*, 1996.
- [8] R. Takayama, T. Hoshi, T. Sogabe, S.-L. Zhang and T. Fujiwara, Linear algebraic calculation of Green's function for large-scale electronic structure theory, *Phys. Rev. B*, **73** (2006), 165108.
- [9] ELSIES matrix library, <http://www.elses.jp/matrix/>.