ICMS 2010, Sep. 13-17, 2010 at Kobe University.

Filter Diagonalization Method by Resolvents for Symmetric Eigenproblems

Hiroshi MURAKAMI

Department of Mathematics and Information Sciences,
Tokyo Metropolitan University
1-1, Minami-Osawa, Hachi-oji,
Tokyo, 192-0397, Japan.
⟨mrkmhrsh@tmu.ac.jp⟩

Filter Diagonalization Method

- **We solve symmetric definite generalized matrix eigenproblem:**
$$A\,\mathbf{v} = \lambda\,B\,\mathbf{v}.$$
- **Only those eigenpairs are required whose eigenvalues are in $\mathcal{I} = [\alpha, \beta]$.**
- **Let $\mathcal{S}_{\mathcal{I}}$ be an invariant subspace spanned by eigenvectors whose eigenvalues are in $\mathcal{I}$.**
- **Filter $\mathcal{F}$ is a well designed linear operator which maps any input vector to an output vector relatively very close to $\mathcal{S}_{\mathcal{I}}$.**

- **When sufficiently many B-orthonormal vectors are filtered, output vectors will span $\mathcal{S}_{\mathcal{I}}$ approximately.**
- **SVD analysis with B-metric is applied to the output vectors, and those singular vectors are rejected whose singular values are relatively smaller than a certain tiny threshold.**
- **The subspace method is applied to the set of remained B-orthonormal singular vectors, and approximated eigenpairs are obtained whose eigenvalues are in the neighbor of $\mathcal{I}$.**
- **The approximations of eigenpairs are quickly improved by a few cycles of Rayleigh inverse-iteration or Ritz simultaneous inverse-iteration.**

Filter Operator by a Combination of Resolvents

- **Let** $R(\tau) \equiv (A - \tau B)^{-1}B$ **be the** ***generalized*** **resolvent.**
- **Filter operator is a linear combination of** $2n$ **resolvents** $R(\tau_p)$ **and an identity operator:**

$$\mathcal{F} \equiv c_\infty I + \sum_{p=1}^{2n} \gamma_p \, R(\tau_p).$$

The tuning parameters are the integer n **and the complex numbers** γ_p**,** τ_p**,** $p{=}1, 2, \ldots, 2n$**, and** c_∞**.**

- **For an eigenpair** $(\lambda^{(\nu)}, \mathbf{v}^{(\nu)})$**, since** $R(\tau)\mathbf{v}^{(\nu)} = \mathbf{v}^{(\nu)} \cdot \frac{1}{\lambda^{(\nu)} - \tau}$**, we have** $\mathcal{F}\,\mathbf{v}^{(\nu)} = \mathbf{v}^{(\nu)} \cdot f(\lambda^{(\nu)})$**, where** $f(\lambda) \equiv c_\infty + \sum_{p=1}^{2n} \dfrac{\gamma_p}{\lambda - \tau_p}$**.**

For any eigenvector whose eigenvalue is λ**, the rational function** $f(\lambda)$ **gives the output/input ratio of the filter.**

Use of Complex Conjugate Symmetry

For the typical filters, the poles of $f(\lambda)$ are imaginary n complex conjugate pairs. For the pair of complex conjugate poles, their coefficients are also complex conjugates.

Therefore, a real vector v can be filtered using only n resolvents whose shifts have positive imaginary parts:

$$\sum_{p=1}^{2n} \gamma_p \, R(\tau_p) \, \mathbf{v} = \sum_{\mathrm{Im}\tau_q > 0} \mathrm{Re}\{2\gamma_q \, R(\tau_q) \, \mathbf{v}\} \; .$$

By this approach, even the complex arithmetics are included, the result is clearly a real vector.

Requirements for the Filter

- **The transfer function of the ideal bandpass filter with passband interval $\mathcal{I} = [\alpha, \beta]$ is the characteristic function of the interval, which is not a rational function.**
- **Therefore, a rational function approximation of the characteristic function is used as the transfer function.**
- **This is similar to the approach for the bandpass filters of analog electronic circuits[1][3].**
- **The magnitude of the transfer function $|f(\lambda)|$ will be:**
  - **near unity, when λ is in the passband.**
  - **quite small (near zero), when λ is separated from the passband.**

Typical Filters

- **Typical filter designs for the analog circuits are:**
  1. ***Butterworth*** **,**
  2. ***Chebyshev*** **,**
  3. ***inverse-Chebyshev*** **,**
  4. ***elliptic*** **.**
- **By the analogy, the above filter designs are available for the diagonalization method also.**

Recipe for Filter Design

- **We define $g(t) = f(\lambda)$ by the linear map between the intervals $\lambda \in [\alpha, \beta]$ and $t \in [-1, 1]$ as:**

$$\lambda = \mathcal{L}(t) = \mathcal{L}' \cdot t + \mathcal{L}(0) \equiv \frac{\beta - \alpha}{2} t + \frac{\beta + \alpha}{2}.$$

- **When the fractional expansion of the transfer function $g(t)$ in the normalized coordinate t is:**

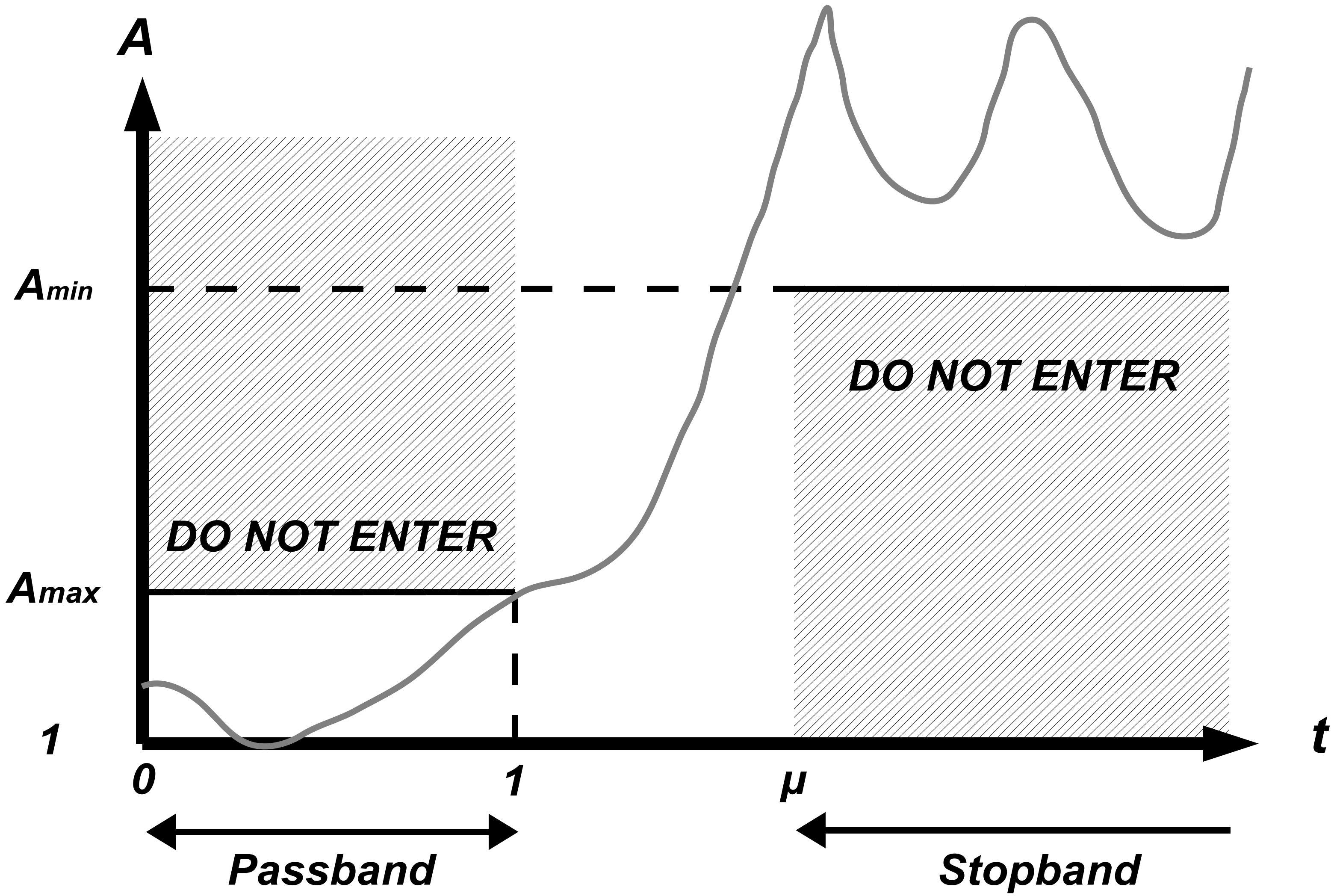
$$g(t) = c_\infty + \sum_{p=1}^{2n} \frac{c_p}{t - t_p},$$

then the corresponding filter operator is:

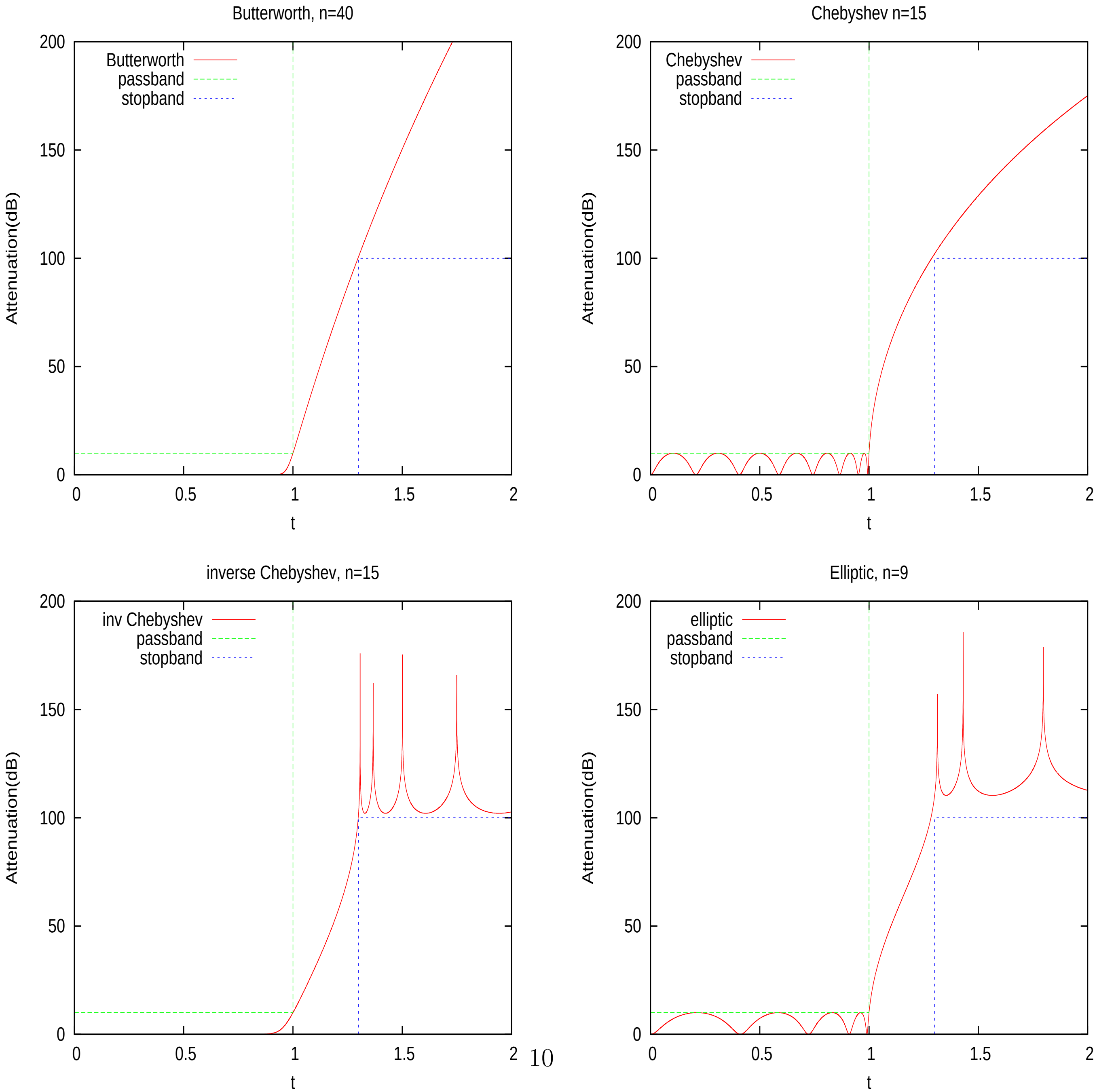
$$\mathcal{F} = c_\infty I + \sum_{p=1}^{2n} \gamma_p R(\tau_p), \text{ where } \tau_p = \mathcal{L}(t_p) \text{ and } \gamma_p = \mathcal{L}' \cdot c_p.$$

- **The attenuation function is defined as the reciprocal of the transfer function: $\mathcal{A}(t) \equiv 1/g(t)$.**

Three Shape Parameters of the Attenuation Function.



Sample Graphs of Attenuation Functions.
μ=1.3, $\mathcal{A}_{\max}$=10[dB], $\mathcal{A}_{\min}$=100[dB].



Selection of Filter Shape Parameters and the degree n

- **Select the type of the filter from:**
  ***Butterworth*, *Chebyshev*, *inverse-Chebyshev*, *elliptic*.**
- **Give the three shape parameters for the attenuation function:** $\mu(>1)$, $\mathcal{A}_{\max}$, $\mathcal{A}_{\min}$.

  The passband is $|t| \le 1$**, and the stopbands are** $\mu \le |t|$**, where** t **is the normalized coordinate by the linear map** $\lambda = \mathcal{L}(t)$**.**

  $\mathcal{A}_{\max}$ **: the upper bound of** $\mathcal{A}$ **in the passband.**
  $\mathcal{A}_{\min}$ **: the lower bound of** $\mathcal{A}$ **in the stopbands.**
  (Hereafter we define $L_{\min} \equiv \sqrt{(\mathcal{A}_{\min}-1)/(\mathcal{A}_{\max}-1)}$**.)**

- **From requirements for the shape of attenuation function, the minimal degree $n_{\min}$ of the filter is calculated. The degree n of the filter must be set $n_{\min}$ or more.**

Case 1. Butterworth Filter

The attenuation function is a degree $2n$ polynomial of t :

$$\mathcal{A}(t) \equiv 1 + \epsilon^2 t^{2n} .$$

1.1 Determination of degree for Butterworth filter

Since $\mathcal{A}_{\max} = 1 + \epsilon^2$, $\mathcal{A}_{\min} \le 1 + \epsilon^2 \mu^{2n}$.

Then we have $\epsilon^2 = \mathcal{A}_{\max} - 1$ **and** $\mu^n \ge L_{\min}$

Therefore, $n_{\min} = \text{ceil}\left(\ln(L_{\min}) / \ln(\mu)\right)$.

The degree n **must be no less than** $n_{\min}$.

1.2 Poles and their coefficients of Butterworth filter

The poles of $g(t)$ **are:**

$$t_p = \frac{1}{\epsilon^{1/n}} \left(\cos\theta_p + \sqrt{-1}\,\sin\theta_p \right),$$

where

$$\theta_p \equiv \frac{(2p-1)\pi}{2n},\ \ p=1,2,\ldots,2n.$$

The poles are on the circle in the complex plane. Their imaginary parts are positives for $p=1,2,\ldots,n$**.**

The coefficient of pole c_p **and the value** c_∞ **are:**

$$c_p = \frac{-t_p}{2n},\ \text{and}\ c_\infty = 0.$$

Case 2. Chebyshev Filter

The attenuation function is a degree $2n$ polynomial of t :

$$\mathcal{A}(t) \equiv 1 + \epsilon^2 T_n^2(t)$$

By allowing ripples in the passband, the *Chebyshev* filter attains the required bandpass property with lower degree than the *Butterworth*.

2.1 Determination of degree for Chebyshev filter

Since $\mathcal{A}_{\max} = 1 + \epsilon^2$, $\mathcal{A}_{\min} \leq 1 + \epsilon^2 {T_n}^2(\mu)$.

Then we have $\epsilon^2 = \mathcal{A}_{\max} - 1$ **and** $T_n(\mu) \geq L_{\min}$.

Therefore, $n_{\min} = \mathrm{ceil}\left(\cosh^{-1}(L_{\min}) / \cosh^{-1}(\mu)\right)$.

The degree n **must be no less than** $n_{\min}$.

2.2 Poles and their coefficients of Chebyshev filter

The poles of $g(t)$ are:

$$t_p = \cosh\tau \cdot \cos\theta_p + \sqrt{-1}\,\sinh\tau \cdot \sin\theta_p\,,$$

where

$$\tau = \frac{1}{n}\sinh^{-1}(\frac{1}{\epsilon}),\ \ \theta_p = \frac{(2p{-}1)\pi}{2n},\ \ p{=}1,2,\ldots,2n.$$

In the complex plane, the poles are located on the ellipse whose foci are -1 and 1. Their imaginary parts are positives for $p{=}1,2,\ldots,n$.

The residues c_p and c_∞ are:

$$c_p = \frac{-T_n(t_p)}{2T'_n(t_p)} = \frac{-T_n(t_p)}{2nU_{n-1}(t_p)},\ \ \text{and } c_\infty{=}0.$$

Here, $U_k(x)$ denotes the degree k polynomial of Chebyshev of the 2nd kind.

Case 3. Inverse-Chebyshev Filter

The attenuation is a degree $2n$ rational function of t :

$$\mathcal{A}(t) \equiv 1 + \epsilon^2 \left[\frac{T_n(\mu)}{T_n(\mu/t)} \right]^2 .$$

<u>3.1 Determination of degree for inverse-Chebyshev filter</u>

Since $\mathcal{A}_{\max} = 1 + \epsilon^2$, $\mathcal{A}_{\min} \leq 1 + \epsilon^2 {T_n}^2(\mu)$.

Then we have $\epsilon^2 = \mathcal{A}_{\max} - 1$ and $T_n(\mu) \geq L_{\min}$.

Therefore, $n_{\min} = \operatorname{ceil}\left(\cosh^{-1}(L_{\min}) / \cosh^{-1}(\mu)\right)$.

The degree n has to be set no less than $n_{\min}$.

The formula of $n_{\min}$ for the inverse-Chebyshev filter is <u>identical</u> to that of the Chebyshev filter.

By allowing ripples in the stopband, the *inverse-Chebyshev* filter attains the required bandpass property with lower degree than the *Butterworth*.

3.2 Poles and their coefficients of inverse-Chebyshev filter

We define $\frac{1}{c} = \epsilon\, T_n(\mu)$**,** $\tau{=}\frac{1}{n}\sinh^{-1}(\frac{1}{c})$ **and** $\theta_p{=}\frac{2(p-1)\pi}{2n}$**,** $p{=}1, 2, \ldots, 2n$**.**

The poles of $g(t) = 1/\mathcal{A}(t)$ **are** $t_p = \mu/x_p$ **,**
where $x_p = \cosh\tau \cdot \cos\theta_p - \sqrt{-1}\,\sinh\tau \cdot \sin\theta_p$**.**

(The zeros of $g(t)$ **are** $z_j = \mu/\cos\theta_j$**,** $j{=}1, 2, \ldots, 2n$**.)**

The residues c_p **are:**

$$c_p = \frac{-\mu}{2{x_p}^2}\frac{T_n(x_p)}{T_n'(x_p)} = \frac{-\mu}{n{x_p}^2}\frac{T_n(x_p)}{nU_{n-1}(x_p)}.$$

The value of c_∞ **is** 0 **for odd** n**,** $\frac{1}{1+(1/c)^2}$ **for even** n**.**

Case 4. Elliptic Filter

The attenuation is a degree $2n$ rational function of t :

$$\mathcal{A}(t) \equiv 1 + \epsilon^2 {R_n}^2(t).$$

The rational function R_n of degree n has a parametric representation by Jacobi's elliptic functions as:

$$R_n(t) = \mathrm{sn}\left[K(L^{-1})(nu + \delta_n), L^{-1}\right], \; t = \mathrm{sn}[K(\mu^{-1})u, \mu^{-1}],$$

where $K(k)$ is the 1st kind complete elliptic integral, the symbol δ_n is 0 for odd n, $(-1)^{n/2}$ for even n.

4.1 Determination of degree for elliptic filter

Since $\mathcal{A}_{\max} = 1 + \epsilon^2$, $\mathcal{A}_{\min} \leq 1 + \epsilon^2 {R_n}^2(\mu)$.

Then we have $\epsilon^2 = \mathcal{A}_{\max} - 1$ and $R_n(\mu) \geq L_{\min}$.

Therefore, $n_{\min} = \text{ceil}\left(\frac{K'(L_{\min}^{-1})}{K(L_{\min}^{-1})}\frac{K(\mu^{-1})}{K'(\mu^{-1})}\right)$**,** **where** $K(k)$ **denotes the elliptic complete integral of the 1st kind, and** $K'(k) \equiv K(\sqrt{1-k^2})$**.**

The degree n **is set no less than** $n_{\min}$**.**

By allowing the ripples in both the passband and the stopband, the *elliptic* filter attains the required bandpass property with lower degree than the *Chebyshev* or the *inverse-Chebyshev*.

The value of L **is calculated from the value of** μ **and** n **as:**

$$L^{-1} = \mu^{-n} \prod_{j=1}^{\text{floor}(n/2)} \text{sn}^4 \left[\frac{(2j-1)K(\mu^{-1})}{n}, \mu^{-1}\right].$$

4.2 Poles and their coefficients of elliptic filter

The poles t_p of $g(t) = 1/\mathcal{A}(t)$ are calculated by

$b \equiv F(\tan^{-1}(\epsilon^{-1}), \sqrt{1-L^{-2}})$,

$F(\phi, k) \equiv \int_0^\phi (1-k^2 \sin^2 x)^{-\frac{1}{2}} dx$ **is 1st kind elliptic integral.**

$\tau \equiv \frac{K(\mu^{-1})b}{K(L^{-1})n}$, $\theta_p = (2p+1-\mathrm{mod}(n,2))\frac{K(\mu^{-1})}{n}$,

then $t_p = \mathrm{sn}(\theta_p + \sqrt{-1}\,\tau, \mu^{-1})$, $p = 1, 2, \ldots, 2n$.

The coefficients of poles are also given by:

$c_p = \zeta \cdot \sqrt{-1}\,\mathrm{cn}(\theta_p + \sqrt{-1}\,\tau, \mu^{-1})\,\mathrm{dn}(\theta_p + \sqrt{-1}\,\tau, \mu^{-1})$,

where $\zeta = \frac{-1}{2n}\frac{K(\mu^{-1})}{K(L^{-1})}\sqrt{\frac{\epsilon^2}{(1+\epsilon^2)(\epsilon^2+L^{-2})}}$.

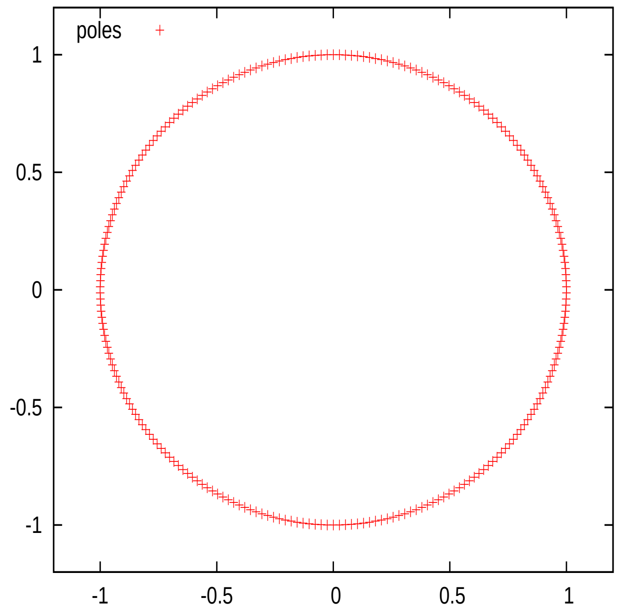
The value of c_∞ is 0 for odd n, $\frac{1}{1+\epsilon^2 L^2}$ for even n.

Note: c_∞ may be Neglected

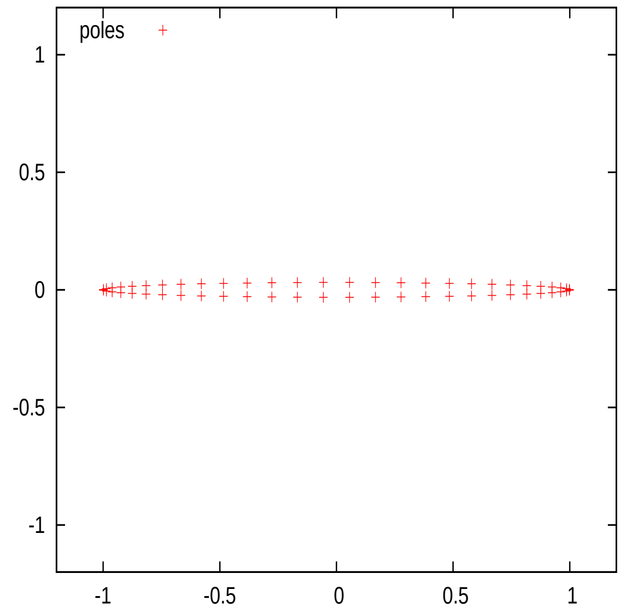
- **For the cases of Butterworth and Chebyshev, c_∞ is always zero.**
  For the inverse-Chebyshev and the elliptic cases, c_∞ is zero for odd n and non-zero for even n.
- **However, even in the case c_∞ is non-zero, the term with coefficient c_∞ may be dropped off from the filter's fractional expansion.**
  Because, $\mathcal{A}_{\min}$ is usually taken to a very large value therefore $c_\infty = g(\infty) \leq 1/\mathcal{A}_{\min}$ is a very small value and negligible.

Sample Plots of the Complex Poles of Filters.
μ=1.1, $\mathcal{A}_{\max}$=3[dB], $\mathcal{A}_{\min}$=100[dB].

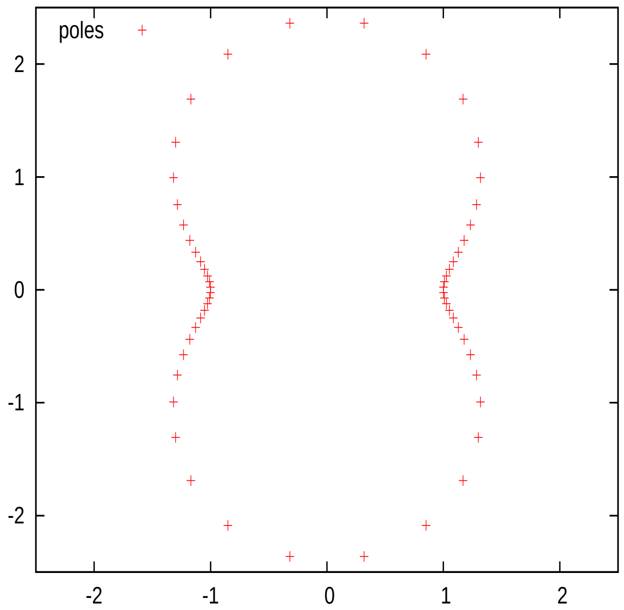
Butterworth filter, degree n=121



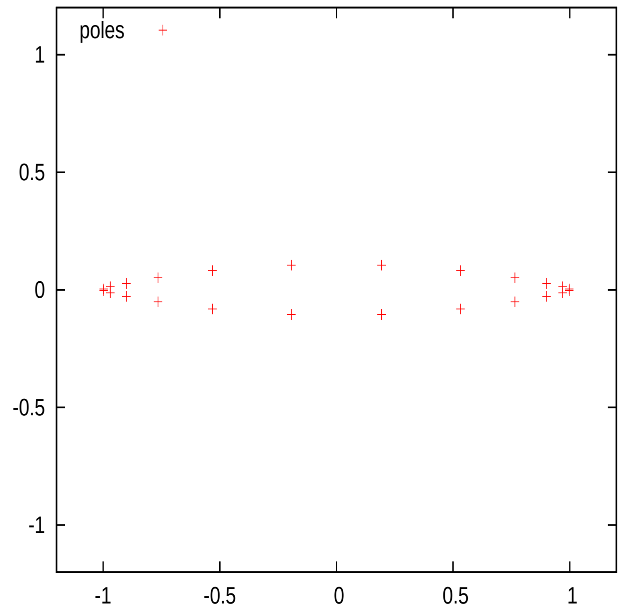
Chebyshev filter, degree n=28



inverse Chebyshev filter, degree n=28



elliptic filter, degree n=12



Tables of Values of $n_{\min}$.

$\mathcal{A}_{\max}$=3[dB], $\mathcal{A}_{\min}$=150[dB]

μ	$n_{\min}$		
	Butter	Cheb	elliptic
1.001	17281	402	35
1.003	5766	232	30
1.005	3463	180	28
1.01	1736	128	26
1.03	585	74	22
1.05	355	58	20
1.1	182	41	17
1.2	95	29	15
1.3	66	24	13
1.5	43	19	12

$\mathcal{A}_{\max}$=3[dB], $\mathcal{A}_{\min}$=100[dB]

μ	$n_{\min}$		
	Butter	Cheb	elliptic
1.001	11522	274	24
1.003	3845	158	21
1.005	2309	123	20
1.01	1158	87	18
1.03	390	50	15
1.05	237	39	14
1.1	121	28	12
1.2	64	20	10
1.3	44	17	9
1.5	29	13	8

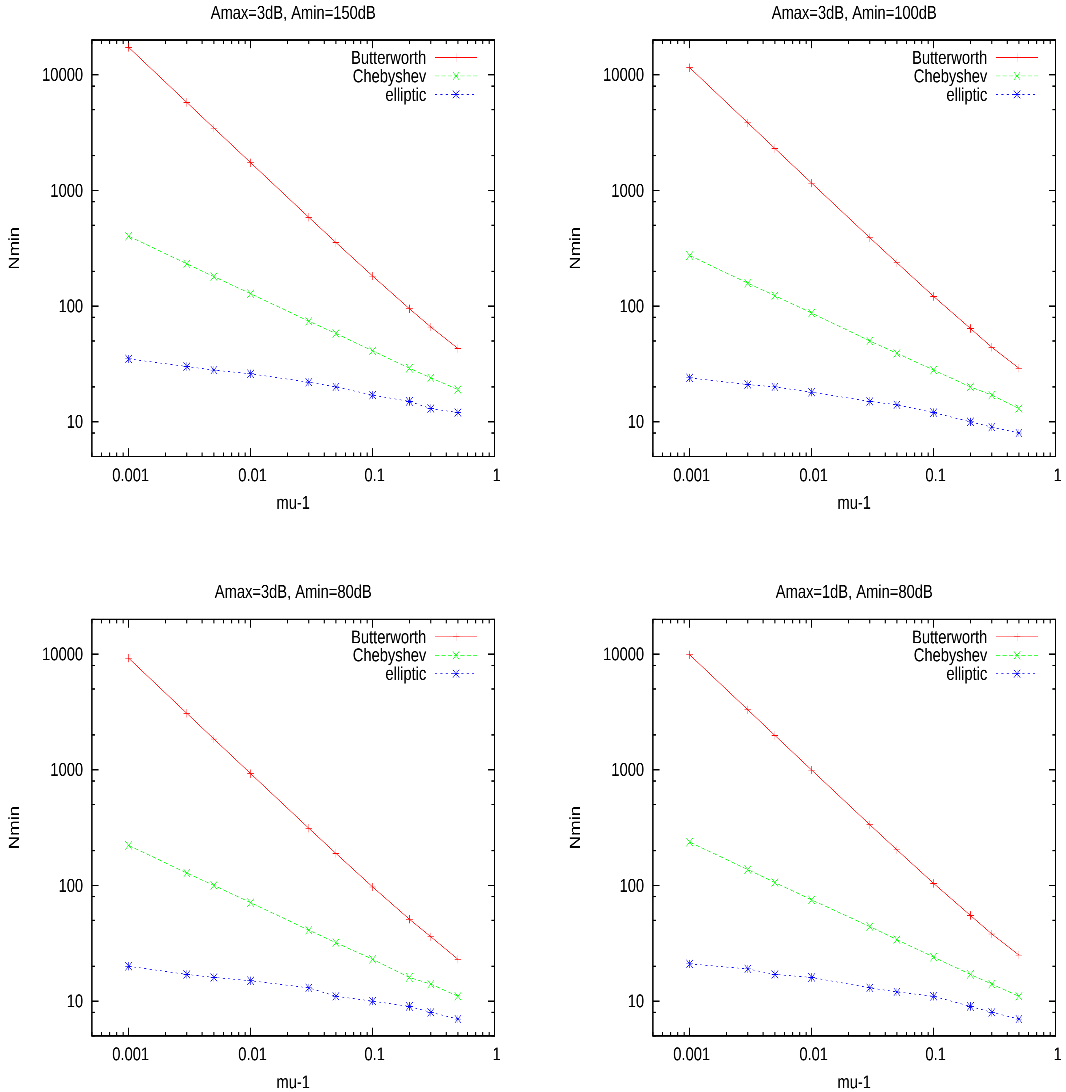
$\mathcal{A}_{\max}$=3[dB], $\mathcal{A}_{\min}$=80[dB]

μ	$n_{\min}$		
	Butter	Cheb	elliptic
1.001	9218	222	20
1.003	3076	128	17
1.005	1848	100	16
1.01	926	71	15
1.03	312	41	13
1.05	189	32	11
1.1	97	23	10
1.2	51	16	9
1.3	36	14	8
1.5	23	11	7

$\mathcal{A}_{\max}$=1[dB], $\mathcal{A}_{\min}$=80[dB]

μ	$n_{\min}$		
	Butter	Cheb	elliptic
1.001	9891	237	21
1.003	3301	137	19
1.005	1983	106	17
1.01	994	75	16
1.03	335	44	13
1.05	203	34	12
1.1	104	24	11
1.2	55	17	9
1.3	38	14	8
1.5	25	11	7

Graphs of Values of $n_{\min}$.



Behaviors of the Degree of Filters when $\mu \to 1$.

The asymptotic behaviors for $\mu \to 1$ or $\ln \mu \to 0$ for the cases of the filters are derived below. The superiority of the elliptic filter should be stressed.

Case of Butterworth

For $\mu \to 1$ then we have $\ln \mu \approx \mu - 1$. Therefore, $n_{\min} = \frac{\ln L_{\min}}{\ln(\mu)} \approx \frac{\ln L_{\min}}{\mu - 1}$ or in logarithm: $\log n_{\min} \approx \log(\ln L_{\min}) - \log(\mu - 1)$.

Cases of Chebyshev and inverse-Chebyshev

For $\mu \to 1$ then we have $\cosh^{-1} \mu \approx \sqrt{2(\mu - 1)}$. Because $L_{\min}$ is a very large number, we also have $\cosh^{-1} L_{\min} \approx \ln\{2L_{\min}\}$. Therefore we have $n_{\min} = \frac{\cosh^{-1} L_{\min}}{\cosh^{-1} \mu} \approx \frac{\ln(2L_{\min})}{\sqrt{2(\mu - 1)}}$ or in logarithm:

$\log n_{\min} \approx \log(\frac{1}{\sqrt{2}} \ln(2L_{\min})) - \frac{1}{2} \log(\mu - 1)$.

Cases of elliptic

We have defined $K(k) \equiv \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}}$**.**

For $k \ll 1$**, from well known formulae [Abramowitz and Stegan,Chap.17]:**

$$K(k) \approx \frac{\pi}{2} + O(k^2).$$

$$q(k) \equiv \exp\left(-\pi \frac{K'(k)}{K(k)}\right) = \frac{k^2}{16} + O(k^4).$$

And $k \to 1$**,**

$$\lim_{k \to 1} \left\{ K(k) - \frac{1}{2}\ln\left(\frac{16}{1-k^2}\right) \right\} = 0.$$

Therefore, for the case of $\mu \to 1$**,**

$$K'(\mu^{-1}) = K(\sqrt{1-\mu^{-2}}) \approx \frac{\pi}{2}\left(1 + O(1-\mu^{-2})\right).$$

And, $K(\mu^{-1}) \approx \frac{1}{2}\ln(\frac{16}{1-\mu^{-2}})$**.**

Since $1-\mu^{-2} = \frac{\mu+1}{\mu^2}(\mu-1) \approx 2(\mu-1)+O\left((\mu-1)^2\right)$**, and** $K'(\mu^{-1}) \approx \frac{\pi}{2}\left(1 + O(\mu-1)\right)$**. So,**

$$\{K'(\mu^{-1})/K(\mu^{-1})\}^{-1} \approx \frac{1}{\pi}\ln(\frac{8}{\mu-1})\{1 + O(\mu-1)\}.$$

Eventually, we have obtained a good asymptotic approximation of $n_{\min}$ **for** $\mu \ll 1$**:**

$$n_{\min} = \left\{\frac{K'(L_{\min}^{-1})}{K(L_{\min}^{-1})}\right\} / \left\{\frac{K'(\mu^{-1})}{K(\mu^{-1})}\right\} \approx \frac{2}{\pi^2}\ln\left(4L_{\min}\right)\ln(\frac{8}{\ln\mu})$$

or in logarithm:

$$\log n_{\min} \approx \log\left\{\frac{2}{\pi^2}\ln(4L_{\min})\right\} + \log\left\{\ln\left(\frac{8}{\ln\mu}\right)\right\}.$$

Summary of the Asymptotic Behavior of $n_{\min}$.

If we let $x \equiv 1/(\mu - 1)$ **then** $\mu \to 1$ **means** $x \to \infty$.

The asymptotic behaviors of $n_{\min}$ **can be rewritten:**

Butterworth	$\approx \ln(L_{\min})\, x$,
Chebyshev	$\approx \ln(2L_{\min})\, \sqrt{x/2}$,
inverse-Chebyshev	$\approx \ln(2L_{\min})\, \sqrt{x/2}$,
elliptic	$\approx (2/\pi^2)\ln(4L_{\min})\ \ln(8x)$.

Here, $L_{\min} \equiv \sqrt{(\mathcal{A}_{\min} - 1)/(\mathcal{A}_{\max} - 1)}$.

Value of Relative Threshold for SVD Analysis

After the filter is applied, the SVD analysis with B-metric is made.
The regularization is added to reduce the effects of round-off errors.
(Those singular vectors are removed whose singular values are relatively very small.)

When the relative threshold is set to $\varepsilon_{\mathrm{SVD}}$, the round-off errors in the remained vectors could be magnified relatively $\varepsilon_{\mathrm{SVD}}^{-1}$ times.

- **Since random vectors are filtered, the magnitudes of eigenvectors in the output vectors are distributed as the statistical variables.**

- **The value of relative threshold cannot be set less than $r \equiv \mathcal{A}_{\mathrm{max}}/\mathcal{A}_{\mathrm{min}}$.**
- **A suitable value of the threshold would be some tiny value such as between $r^{2/3}$ and $r^{1/3}$.**
- **By the numerical calculation, the precision of the computation limits the attainable value of $\mathcal{A}_{\mathrm{min}}$. Therefore, the suitable value of the threshold depends also on the precision.**

  For the higher precision computations, the risk to miss some eigenpairs will be reduced if the threshold is reduced.
- **Theoretical considerations on the statistics would be necessary.**

Some Examples by Experiments

System: CPU: intel Core i7 920(only single core is used); Memory:12Gbytes DDR3-1333; Compiler:intel Fortran v11 for intel64 with option -fast; FP numbers: IEEE 64-bit float; OS: Fedora10 for intel64.

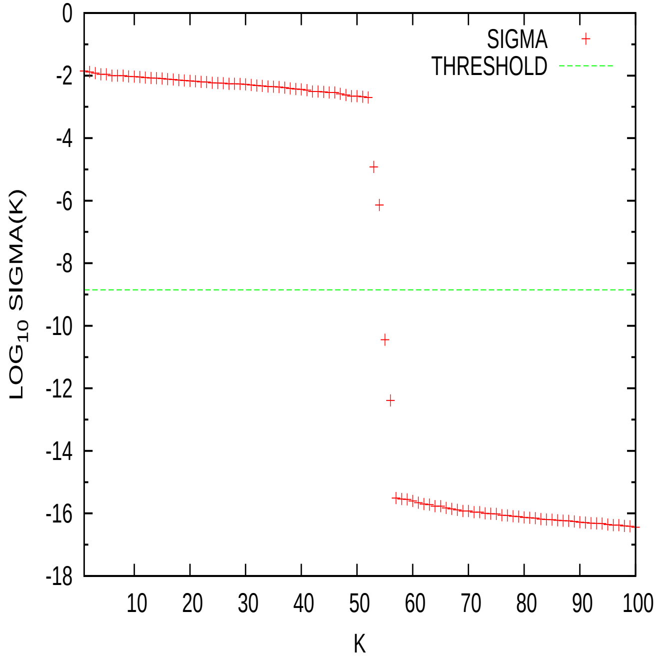
A, B **are size** N **real symmetric banded matrices with lower bandwidth** h **(matrix elements** $a_{i,j}, b_{i,j}$ **have values only when** $|i-j| \leq h$**). The matrix elements inside the bandwidth are** $a_{i,j} \equiv \max(i,j) - 1$, $b_{i,j} \equiv 1/(i+j-1) + \delta_{i,j}$**. Where,** $\delta_{i,j}$ **denotes the Kronecker's symbol. And** $N = 10^6$, $h = 10$**, the interval is** $[-10, 10]$**. There are 52 eigenpairs whose eigenvalues are in this interval.**

For an approximated eigenpair $(\lambda, \mathbf{v})$**, the norm of the residual vector** $\mathbf{r} \equiv (A - \lambda B)\mathbf{v}$ **is defined by** $\Delta \equiv \sqrt{\mathbf{r}^T B^{-1} \mathbf{r}}$ **which gives an upper-bound of the distance of the calculated eigenvalue from some true eigenvalue. This norm can be used to estimate the qualities of approximated pairs.**

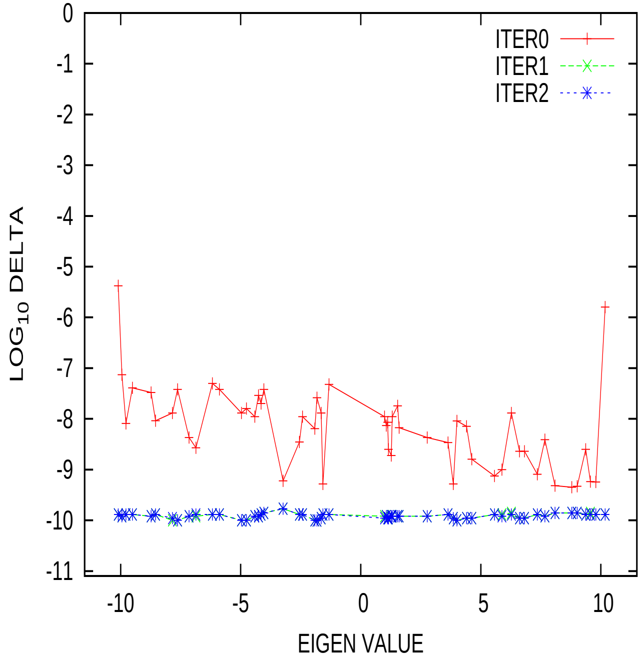
In graphs, `ITER0` **plots eigenpairs by the filter diagonalization method.** `ITER1` **plots eigenpairs corrected once by the Rayleigh quotient inverse iteration.** `ITER2` **plots eigenpairs corrected twice.**

TEST1: With the triplet conditions (μ=1.1, $\mathcal{A}_{\max}$=3[dB], $\mathcal{A}_{\min}$=150[dB]), the elliptic filter is selected. The degree n is set to the minimal value 17.

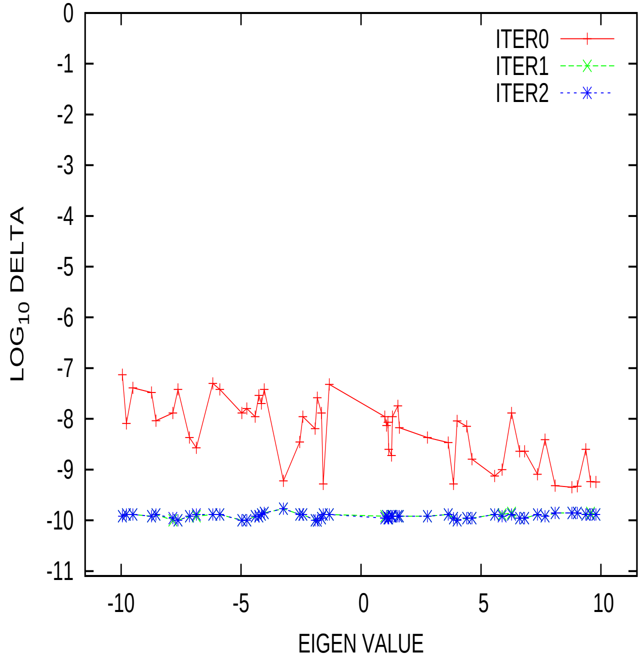
The input vectors are 100 random vectors orthonormalized in B-metric. The relative threshold 10^{-7} is used to cut the singular values. After the cut-off, the rank of the singular vectors is 54. There are 52 approximated pairs whose eigenvalues are in the interval. The elapsed times are 456 seconds for the filter diagonalization method, and 85 seconds for the two cycles of the inverse iterations.



Distribution of Singular Values



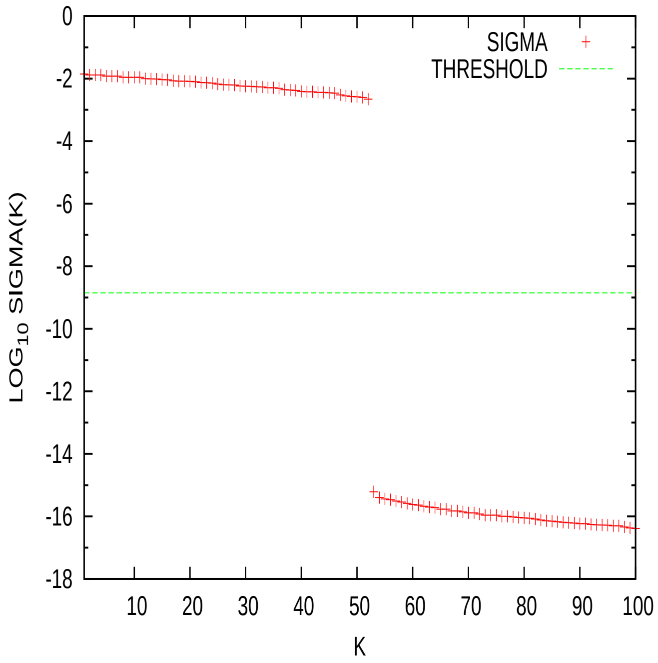
Qualities of all pairs in the subspace



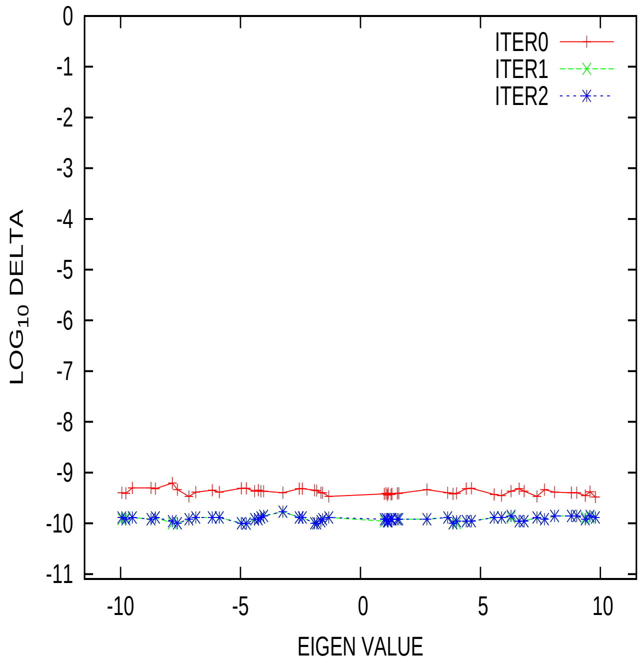
Qualities of pairs in the interval

TEST2: With the triplet conditions (μ=1.01, $\mathcal{A}_{\max}$=3[dB], $\mathcal{A}_{\min}$=150[dB]), the elliptic filter is selected. The degree n is set to the minimal value 26.

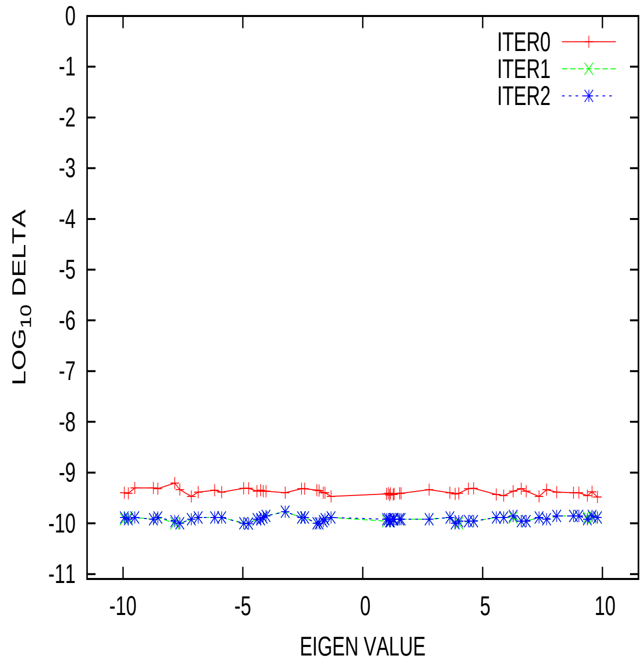
The input vectors are 100 random vectors orthonormalized in B-metric. The relative threshold 10^{-7} is used to cut the singular values. After the cut-off, the rank of the singular vectors is 52. There are 52 approximated pairs whose eigenvalues are in the interval. The elapsed times are 644 seconds for the filter diagonalization method, and 82 seconds for the two cycles of inverse iterations.



Distribution of Singular Values



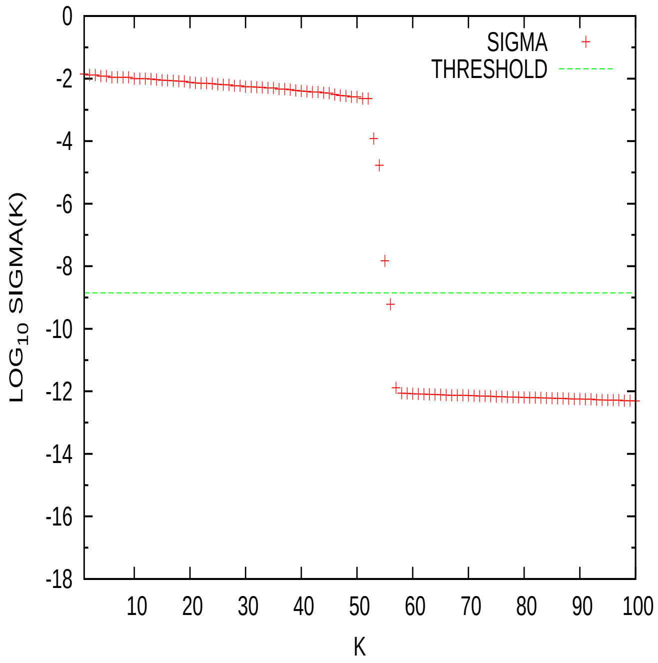
Qualities of all pairs in the subspace



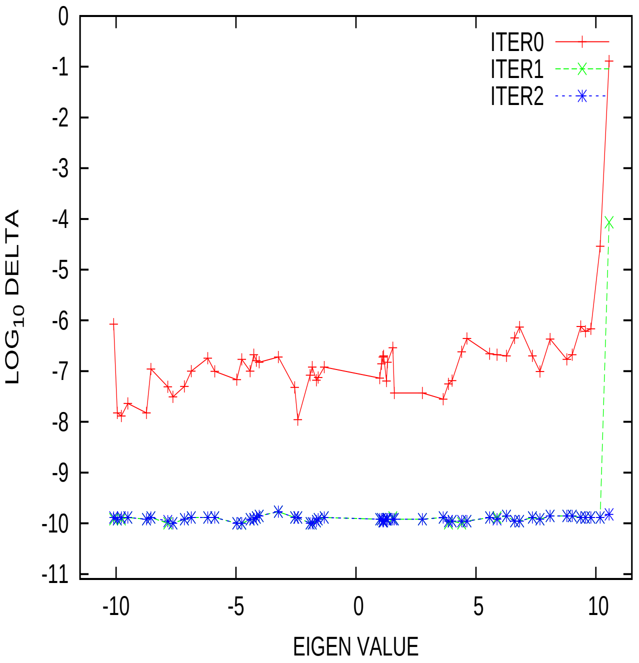
Qualities of pairs in the interval

TEST3: With the triplet conditions (μ=1.1, $\mathcal{A}_{\max}$=3[dB], $\mathcal{A}_{\min}$=100[dB]), the elliptic filter is selected. The degree n is set to the minimal value 12.

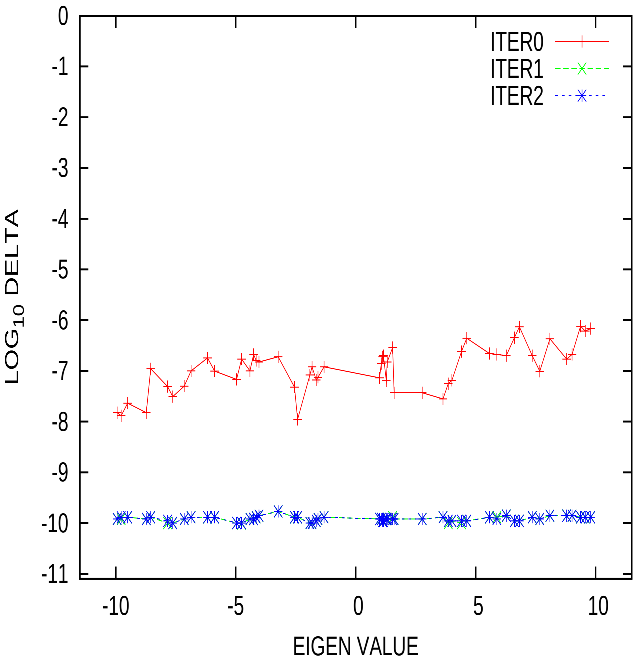
The input vectors are 100 random vectors orthonormalized in B-metric. The relative threshold 10^{-7} is used to cut the singular values. After the cut-off, the rank of the singular vectors is 55. There are 52 approximated pairs whose eigenvalues are in the interval. The elapsed times are 352 seconds for the filter diagonalization method, and 87 seconds for the two cycles of inverse iterations.



Distribution of Singular Values



Qualities of all pairs in the subspace



Qualities of pairs in the interval

References

[1] R.W. Daniels: ***Approximation Methods for Electronic Filter Design***, McGraw-Hill, 1974.

[2] W.J. Thompson: ***Atlas for Computing Mathematical Functions***, Chap.17:"Elliptic Integrals and Elliptic functions", Wiley-Interscience, 1997.

[3] M.D. Lutovac, D.Y. Tošić and B.L. Evans: ***Filter Design for Signal Processing***, Prentice Hall, 2001.

[4] Toledo, S. and Rabani, E.: Very Large Electronic Structure Calculations Using an Out-of-Core Filter-Diagonalization Method, *J. Comput. Phys.*, Vol.180, No.1, pp.256–269 (2002).

[5] Sakurai, T. and Sugiura, H: A projection method for generalized eigenvalue problems using numerical integration, *J. Comp. Appl. Math.*, Vol.159, pp.119–128 (2003).

[6] Saad, Y.: Diagonalization algorithms in real space methods for electronic structure calculations, *PMAA-06, IRISA, Rennes, Sep. 8th (2006), Dept. Comput. Sci. and Eng., Univ. of Minnesota* (2006).

[7] H. Murakami: The Filter Diagonalization Method by the Shifted Inverses, Conference Abstracts of ICCM2007, p.126 (2007); CD-ROM Proceeding paper(p126_G7-8_proc.pdf).

[8] H. Murakami: "Application of Filter Diagonalization Method to Numerical Solution of Algebraic Equations", Proceedings of SNC2009, pp.95–104 (2009).

[9] **Polizzi, E.: Density-matrix-based algorithm for solving eigenvalue problems,** *Phys. Rev. B*, **Vol.79, No.11, p.115112(6pages), (2009).**