FIRST AND SECOND ORDER SPECTRAL SHIFT FUNCTIONS FOR PAIRS OF SELF-ADJOINT MATRICES

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Abstract. We explore properties and representations of first and second order spectral shift functions evaluated for pairs of self-adjoint matrices guided by examples. We examine the conditions sufficient for the first and second order spectral shift functions to be identically 0 in 3.11, 4.10, and 4.13.

1. Introduction

Spectral shift functions of the first order emerged from I.M. Lifshits's work on theoretical physics during 1947–1952 wherein he was looking for efficient formulas to calculate how the free energy of a pure crystal changes when small impurities are added to the crystal [1]. Spectral shift functions have now become fundamental objects in perturbation theory.

Spectral shift functions contain information about the change of the spectrum of a matrix, or more generally, a bounded linear operator, under the influence of a perturbation. Operators that are functions of other operators can be encountered in quantum mechanics, and perturbation theory can help in examining systems obtained by perturbations of simpler systems.

The first order spectral shift function $\xi(x)$, given in (14), can be thought of as a measure of how many eigenvalues of a matrix passed the real parameter x in the positive direction as the matrix was perturbed. The first order spectral shift function also appears in a version of the fundamental theorem of calculus for functions of bounded linear operators in (13). The second order spectral shift function $\eta(x)$, given in (20), can be thought of as a measure of how much the eigenvalues shift when the matrix is perturbed.

2. Linear Algebra Preliminaries

In this section, we gather facts from standard linear algebra that will be applied in our study of spectral shift functions. Most of these facts can be found in textbooks on linear algebra. The facts that we need are collected in [2] and [3].

Definition 2.1. ([2, Definition 3.4]) *A square matrix A is called diagonalizable if there is a diagonal matrix D and an invertible matrix S such that*

$$A = SDS^{-1}. \tag{1}$$

Theorem 2.2. ([2, Theorem 3.5]) *An $n \times n$ matrix A is diagonalizable if and only if A has n linearly independent eigenvectors. The elements on the diagonal of the matrix D in the decomposition* (1) *are the eigenvalues of A and the columns of S are the respective eigenvectors of A.*

Definition 2.3. ([2, Definition 3.9]) *The adjoint of a matrix, A^*, is the transpose of the matrix A with every element replaced with its complex conjugate.*

Definition 2.4. ([2, Definition 3.10]) *A matrix is unitary if and only if its adjoint equals its inverse, $U^* = U^{-1}$.*

Definition 2.5. ([2, Definition 3.10]) *A matrix is self-adjoint if and only if it equals its adjoint, $A = A^*$.*

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Proposition 2.6. ([2, Exercise 3.11]) *A matrix U in $\mathbb{C}^{n\times n}$ is unitary if and only if its column vectors form an orthonormal basis in $\mathbb{C}^n$.*

Proposition 2.7. ([2, Exercise 3.13]) *The spectrum, the set of eigenvalues, of a self-adjoint matrix is a subset of $\mathbb{R}$.*

Theorem 2.8 (The Spectral Theorem)**.** ([2, Theorem 3.12]) *An $n \times n$ matrix A is self-adjoint if and only if it is diagonalizable with a unitary matrix S.*

Let us collect and connect what we know so far. The eigenvalues of a self-adjoint matrix are real numbers, even if the matrix itself has complex entries. Self-adjoint matrices are diagonalizable with unitary matrices. Unitary matrices have orthonormal columns, which will be important later for the second order spectral shift function. The columns of the diagonalizing matrix are also the eigenvectors of the self-adjoint matrix.

Proposition 2.9. ([2, Proposition 4.9]) *If A is a self-adjoint matrix with eigenvalues $\lambda_1, ..., \lambda_n$, then the decomposition of A into SDS^{-1} can be represented as the linear combination*

$$A = \sum_{i=1}^{n} \lambda_i S E_{ii} S^{-1}. \tag{2}$$

where the matrix E_{ij}, called an elementary matrix, has one nonzero entry, the $i, j-th$ entry, and this entry is always 1.

Definition 2.10. ([3, Theorem 5.13.9]) *A matrix P is an orthogonal projection if and only if $P = P^2$ and $P = P^*$.*

Definition 2.11. ([3, Definition of Orthogonal Complement]) *For a subset M of an inner-product space V, the orthogonal complement, denoted $M^\perp$, is defined to be the set of all vectors in V that are orthogonal to every vector in M.*

Definition 2.12. ([3, Theorem 5.11.1]) *If M is a subspace of a finite-dimensional inner-product space V, then $V = M \oplus M^\perp$, the direct sum of the orthocomplementary subspaces. This means that for every $v \in V$, $v = x + y$ for a unique x and y, where $x \in M, y \in M^\perp$.*

Lemma 2.13. ([4, Lemma 2.6]) *For P and Q orthogonal projections,*

$$Q - P = QP^\perp - Q^\perp P. \tag{3}$$

Proof. Let P be defined on V and let X be the image space of the projection P. To prove this lemma, we need to establish that $P + P^\perp = I$ for an orthogonal projection P onto a subspace X of a finite-dimensional inner-product space V. We know $V = X + X^\perp$ and $X \cap X^\perp = 0$ by the properties of orthocomplementary subspaces. For every $v \in V$, there are unique vectors $x \in X$ and $y \in X^\perp$ such that $v = x + y$. Additionally, a pair of orthocomplementary subspaces X and $X^\perp$ in V defines an orthogonal projection P onto X and an orthogonal projection $P^\perp$ onto $X^\perp$ such that $Pv = x$ and $P^\perp v = y$. Thus for every $v \in V$, $v = x + y = Pv + P^\perp v = (P + P^\perp)v$, and since $v = (P + P^\perp)v$, it must be that $(P + P^\perp) = I$.

Now we can rewrite the equation (3) in the following way:

$$Q - P = Q(P + P^\perp) - (Q + Q^\perp)P = QP + QP^\perp - QP - Q^\perp P = QP^\perp - Q^\perp P.$$

□

Proposition 2.14. *Let S be the diagonalizing unitary matrix of a self-adjoint matrix A, then $SE_{ii}S^{-1}$ is an orthogonal projection.*

Proof. To show that $SE_{ii}S^{-1}$ is an orthogonal projection, we need to demonstrate that it satisfies the two properties from 2.10. First recall from 2.4 that since S is unitary we can rewrite $SE_{ii}S^{-1}$ as $SE_{ii}S^*$. This gives us $SE_{ii}S^{-1} = (SE_{ii}S^{-1})^*$ because

$$(SE_{ii}S^*)^* = (S^*)^* E_{ii}^* S^* = SE_{ii}S^*.$$

For the second property, observe that an elementary matrix is a projection, so $E_{ii}^2 = E_{ii}$. This gives us $SE_{ii}S^{-1} = (SE_{ii}S^{-1})^2$ because

$$(SE_{ii}S^{-1})^2 = (SE_{ii}S^{-1})(SE_{ii}S^{-1}) = SE_{ii}(S^{-1}S)E_{ii}S^{-1} = S(E_{ii}E_{ii})S^{-1} = SE_{ii}S^{-1}.$$

□

Definition 2.15. ([2, Definition 4.11]) *Let A be a self-adjoint matrix and let f be a bounded, scalar-valued function defined on the real numbers. We define the function f of the matrix A to be*

$$f(A) = Sf(D)S^{-1} = \sum_{i=1}^{n} f(\lambda_i)SE_{ii}S^{-1}. \tag{4}$$

There are two functions that are used to define the first and second order spectral shift function. The first function is the characteristic, or indicator, function of a set.

Definition 2.16. *The characteristic function $\chi_{(a,b)}(x)$ is defined on $\mathbb{R}$. It maps a scalar to 1 if the scalar is in the specified interval, and maps the scalar to 0 otherwise, that is,*

$$\chi_{(a,b)}(x) = \begin{cases} 1, & \text{if } x \in (a,b) \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

The matrix valued characteristic function of a self-adjoint matrix can be viewed as a linear sum of matrices as in (4) which uses the scalar valued characteristic function $\chi_{(a,b)}(\lambda_i)$ as $f(\lambda_i)$.

$$\chi_{(a,b)}(A) = S\chi_{(a,b)}(D)S^{-1} = \sum_{i=1}^{n} \chi_{(a,b)}(\lambda_i)SE_{ii}S^{-1}. \tag{6}$$

We can also represent $\chi_{(a,b)}(A)$ applied to a vector x using the dot product with the set of eigenvectors of A, $\{f_j\}_{j=1}^n$.

$$\chi_{(a,b)}(A)x = \sum_{\lambda \in (a,b)} \langle x, f_j \rangle f_j. \tag{7}$$

Example 2.17. We will now inspect a simple example of the matrix valued characteristic function.

$$\chi_{(0,1.5)}(A) = \chi(\begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix})$$

Since A is a triangular matrix, the eigenvalues are the numbers on the diagonal; $\lambda_1 = 1$, and $\lambda_2 = 2$. We can see that $\chi_{(0,1.5)}(1) = 1$ and $\chi_{(0,1.5)}(2) = 0$. Since A is a diagonal matrix with real entries, it is self-adjoint. The diagonalizing matrix for a diagonal matrix is the identity matrix, which is its own inverse.

$$S = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = S^{-1}$$

The SDS^{-1} decomposition of A is

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Putting it all into equation (6) gives us

$$\chi_{(0,1.5)}(A) = (1)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + (0)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

The second function we need to define the first and second order spectral shift functions is the trace of matrix.

Definition 2.18. *The trace of a matrix is defined to be the sum of the diagonal entries,*

$$tr(A) = \sum_{i=1}^{n} a_{ii}. \tag{8}$$

The trace can also be defined using the dot product,

$$tr(A) = \sum_{j=1}^{n} \langle Af_j, f_j \rangle \tag{9}$$

where the vectors $\{f_j\}_{j=1}^{n}$ *are the eigenvectors of* A.

The trace function maps a matrix to a scalar, and in our work this scalar is a real number. The trace function has the properties that it is linear and cyclic. Given three matrices A, B and C and two scalars c and d, we have

$$tr(cA + dB) = c(tr(A)) + d(tr(B)), \tag{10}$$

$$tr(ABC) = tr(CAB) = tr(BCA). \tag{11}$$

3. The First Order Spectral Shift Function

When examining matrix valued functions it is often useful to ask how $f(A)$ changes if we perturb A to $A+V$ where both matrices are self-adjoint. The scalar version of the Fundamental Theorem of Calculus allows us to see how a scalar valued function $f(a)$ changes when $a \in \mathbb{R}$ is perturbed to $a + v \in \mathbb{R}$. One can think of the scalars a and $a + v$ as 1×1 matrices which are trivially self-adjoint.

$$f(a + v) - f(a) = \int_{a}^{a+v} f'(x)dx \tag{12}$$

It is reasonable to expect that integration will be involved in the case of matrix valued functions as well, and that there is an analog of the fundamental theorem of calculus for matrix valued functions. We can begin to gain some insight by using the scalar valued characteristic function to rewrite the integrand and the bounds of the integral in the fundamental theorem of calculus for scalars.

$$\int_{a}^{a+v} f'(x)dx = \int_{-\infty}^{\infty} f'(x)\chi_{(a,a+v]}(x)dx$$

$$\int_{-\infty}^{\infty} f'(x)\chi_{(a,a+v]}(x)dx = \int_{-\infty}^{\infty} f'(x)(\chi_{(a,\infty)}(x) - \chi_{(a+v,\infty)}(x))dx$$

$$\int_{-\infty}^{\infty} f'(x)(\chi_{(a,\infty)}(x) - \chi_{(a+v,\infty)}(x))dx = \int_{-\infty}^{\infty} f'(x)(\chi_{(-\infty,x)}(a) - \chi_{(-\infty,x)}(a + v))dx.$$

Now we have a different form for the right hand side of (12).

$$f(a + v) - f(a) = \int_{-\infty}^{\infty} f'(x)(\chi_{(-\infty,x)}(a) - \chi_{(-\infty,x)}(a + v))dx.$$

It is known that for matrices

$$tr(f(A + V) - f(A)) = \int_{-\infty}^{\infty} f'(x)\, tr(\chi_{(-\infty,x)}(A) - \chi_{(-\infty,x)}(A + V))\, dx. \tag{13}$$

This equation looks very similar to (5) except the scalars a and $a + v$ have been replaced by the matrices A and $A + V$ and the trace function appears on each side of the equation. The equation (13) is named *Krein's Trace Formula* and references to it can be found in [4]. This equation is in fact the analog to the Fundamental Theorem of Calculus we were looking for.

Definition 3.1. *Let A and V be two self-adjoint matrices of the same dimension. Then, the first order spectral shift function for the pair A and $A+V$ is defined by*

$$\xi(x) := tr(\chi_{(-\infty,x)}(A) - \chi_{(-\infty,x)}(A+V)). \tag{14}$$

It can be interpreted as the net number of the eigenvalues of a matrix that crossed x in the positive direction as A is perturbed to $A+V$.

This first order spectral shift function can also be expressed in an equivalent and much easier to use form.

Definition 3.2. *The first order spectral shift function for the pair A and $A+V$ can be defined by*

$$\xi(x) = Card\{i : \lambda_i < x\} - Card\{j : \mu_j < x\}, \tag{15}$$

where Card stands for the cardinality of the set, $\{i : \lambda_i < x\}$ is the set of eigenvalues of A that are less than x, and $\{j : \mu_j < x\}$ is the set of eigenvalues of $A+V$ that are less than x. We prove this in the proposition below.

Proposition 3.3. *For two $n \times n$ self-adjoint matrices, A and $A+V$, with eigenvalues $\{\lambda_i\}_{i=1}^n$ and $\{\mu_i\}_{i=1}^n$, respectively,*

$$tr(\chi_{(-\infty,t)}(A) - \chi_{(-\infty,t)}(A+V)) = L - M,$$

where $L = \mathrm{Card}\{i : \lambda_i < t\}$ and $M = \mathrm{Card}\{j : \mu_j < t\}$.

Proof. Let S denote the diagonalizing matrix of A and T denote the diagonalizing matrix of $A+V$. Let D_A denote the diagonal matrix of the eigenvalues of A and D_{A+V} denote the diagonal matrix of the eigenvalues of $A+V$. Finally, let $\{\lambda_i\}_{i=1}^n$ be the eigenvalues of A and $\{\mu_j\}_{j=1}^n$ be the eigenvalues of $A+V$.

Given equation (6), we know

$$\chi_{(-\infty,x)}(A) = \sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) S^{-1} E_{ii} S,$$

from which we get

$$tr\left(\chi_{(-\infty,x)}(A) - \chi_{(-\infty,x)}(A+V)\right) = tr\left(\sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) S^{-1} E_{ii} S - \sum_{j=1}^{n} \chi_{(-\infty,x)}(\mu_j) T^{-1} E_{jj} T\right).$$

By linearity and cyclicity of the trace given in (10) and (11) respectively,

$tr(\sum_{i=1}^n \chi_{(-\infty,x)}(\lambda_i) S^{-1} E_{ii} S - \sum_{j=1}^n \chi_{(-\infty,x)}(\mu_j) T^{-1} E_{jj} T)$

$$
\begin{aligned}
&= tr(\sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) S^{-1} E_{ii} S) - tr(\sum_{j=1}^{n} \chi_{(-\infty,x)}(\mu_j) T^{-1} E_{jj} T) \\
&= \sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) tr(S^{-1} E_{ii} S) - \sum_{j=1}^{n} \chi_{(-\infty,x)}(\mu_j) tr(T^{-1} E_{jj} T) \\
&= \sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) tr(S S^{-1} E_{ii}) - \sum_{j=1}^{n} \chi_{(-\infty,x)}(\mu_j) tr(T T^{-1} E_{jj}) \\
&= \sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) tr(I E_{ii}) - \sum_{j=1}^{n} \chi_{(-\infty,x)}(\mu_j) tr(I E_{jj}) \\
&= \sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) tr(E_{ii}) - \sum_{j=1}^{n} \chi_{(-\infty,x)}(\mu_j) tr(E_{jj}).
\end{aligned}
$$

Since the trace of E_{ii} is always equal to 1,

$$
\sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) tr(E_{ii}) - \sum_{j=1}^{n} \chi_{(-\infty,x)}(\mu_j) tr(E_{jj}) = \sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) - \sum_{j=1}^{n} \chi_{(-\infty,x)}(\mu_j).
$$

Furthermore,

$$
\sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) - \sum_{j=1}^{n} \chi_{(-\infty,x)}(\mu_j) = \sum_{\{i:\lambda_i<x\}} 1 - \sum_{\{j:\mu_j<x\}} 1
$$

because $\chi_{(-\infty,x)}(\lambda_i)$ is equal to 1 if $\lambda_i < x$ and 0 otherwise, i.e. 1 is added to the sum for each eigenvalue less than x. Finally,

$$
\sum_{\{i:\lambda_i<x\}} 1 - \sum_{\{j:\mu_j<x\}} 1 = \text{Card}\{i : \lambda_i < x\} - \text{Card}\{j : \mu_j < x\}.
$$

□

There is yet another way to view $\xi(x)$ that involves viewing the matrix product $SE_{ii}S^{-1}$ as an orthogonal projection, named the spectral projection, onto the span of the eigenvector associated with λ_i.

Proposition 3.4. *The first order spectral shift function can be defined as*

$$
\xi(x) = tr(\chi_{(-\infty,x)}(A+V)\chi_{[x,\infty)}(A) - \chi_{[x,\infty)}(A+V)\chi_{(-\infty,x)}(A)). \tag{16}
$$

Proof. We can view $\chi_{(-\infty,x)}(A)$ as

$$
\chi_{(-\infty,x)}(A) = \sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) S E_{ii} S^{-1} = \sum_{i=1}^{n} \chi_{(-\infty,x)}(\lambda_i) P_i. \tag{17}
$$

From this representation we see that $\chi_{(-\infty,x)}(A)$ is an orthogonal projection itself. The orthogonal complement of $\chi_{(-\infty,x)}(A)$ is $\chi_{[x,\infty)}(A)$.

Now we write the first order spectral shift function in the form given by (14). We can then apply (3) with $Q = \chi_{(-\infty,x)}(A)$ and $P = \chi_{(-\infty,x)}(A+V)$. Thus we simply have

$$
tr(\chi_{(-\infty,x)}(A) - \chi_{(-\infty,x)}(A+V)) = tr(\chi_{(-\infty,x)}(A+V)\chi_{[x,\infty)}(A) - \chi_{[x,\infty)}(A+V)\chi_{(-\infty,x)}(A)).
$$

□

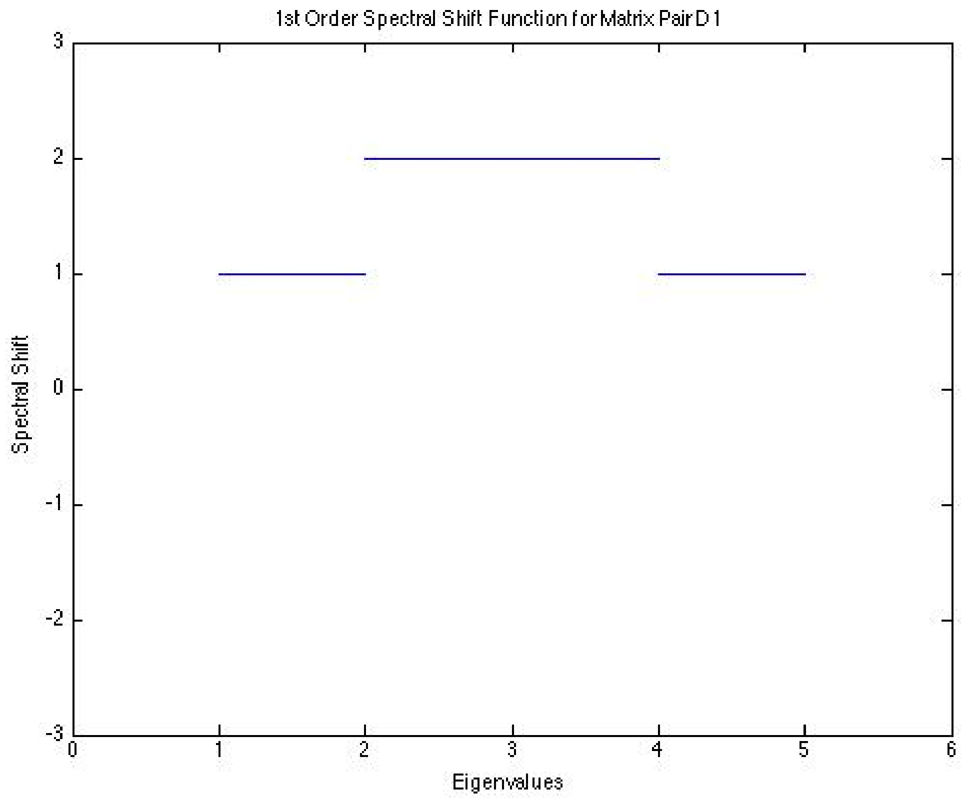
What follows are several examples of $\xi(x)$ with graphs to accompany them. Notice from the graphs that $\xi(x)$ can only be nonzero on the interval $[a, b]$, where $a = min\{\lambda_i, \mu_j\}_{i,j=1}^n$ and $b = max\{\lambda_i, \mu_j\}_{i,j=1}^n$. This follows when one considers $\xi(x)$ as in equation (14). When $x < a$ none of the eigenvalues in $\{\lambda_i, \mu_j\}_{i,j=1}^n$ are less than x, so the difference in equation (14) is 0, and when $x > b$ all of the eigenvalues are less than x, so the difference in equation (14) is again 0. Notice that ξ is a piece-wise constant function.

Example 3.5. **Diagonal Pair D1**

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \quad A + V = \begin{bmatrix} 4 & 0 \\ 0 & 5 \end{bmatrix}$$

$$\sigma(A) = \{1, 2\} \quad \sigma(A + V) = \{4, 5\}$$

$$\xi(t) = \begin{cases} 2, & \text{if } t \in (2, 4] \\ 1, & \text{if } t \in (1, 2] \; or \; (4, 5] \\ 0, & \text{otherwise} \end{cases}$$

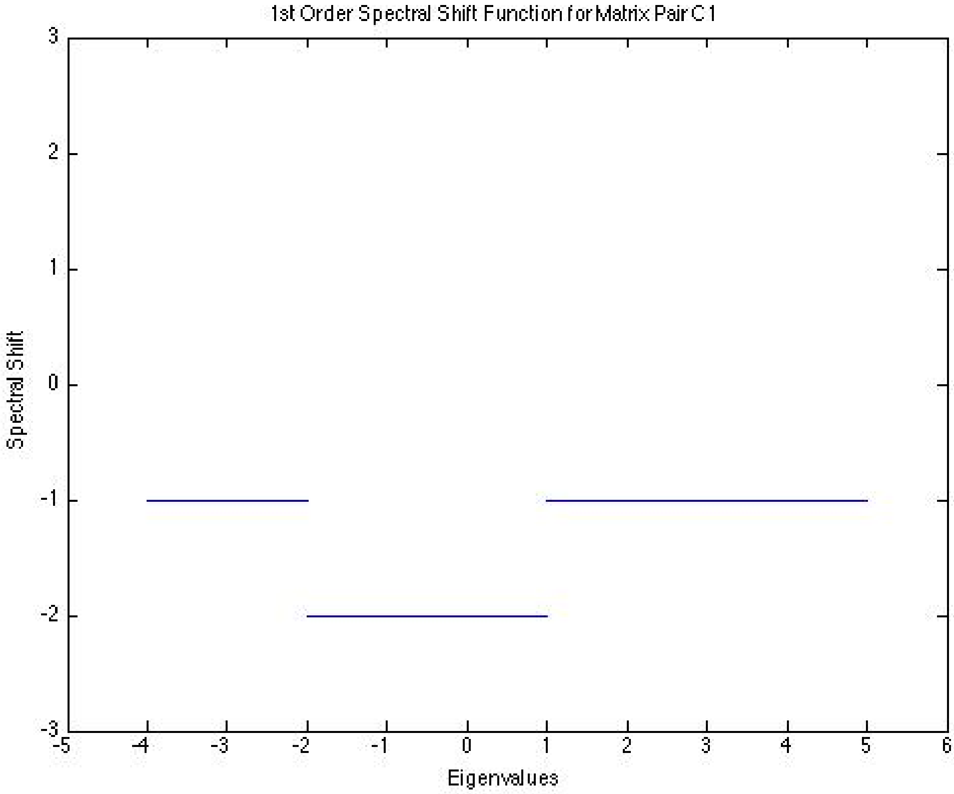


Example 3.6. **Commuting Pair C1**

$$A = \begin{bmatrix} 3 & 2i \\ -2i & 3 \end{bmatrix} \quad A + V = \begin{bmatrix} -3 & i \\ -i & -3 \end{bmatrix}$$

$$\sigma(A) = \{1, 5\} \quad \sigma(A + V) = \{-4, -2\}$$

$$\xi(t) = \begin{cases} -2, & \text{if } t \in (-2, 1] \\ -1, & \text{if } t \in (-4, -2] \; or \; (1, 5] \\ 0, & \text{otherwise} \end{cases}$$

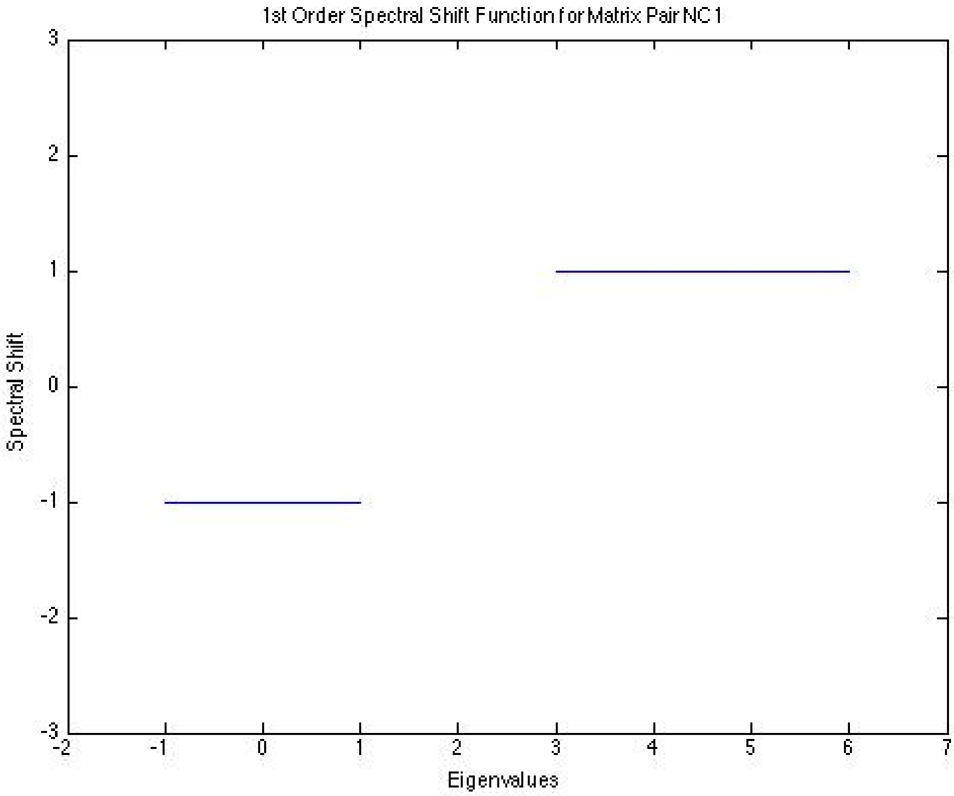


Example 3.7. **Noncommuting Pair NC1**

$$A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \quad A + V = \begin{bmatrix} 1 & 3+i \\ 3-i & 4 \end{bmatrix}$$

$$\sigma(A) = \{1, 3\} \quad \sigma(A+V) = \{-1, 6\}$$

$$\xi(t) = \begin{cases} -1, & \text{if } t \in (-1, 1] \\ 1, & \text{if } t \in (3, 6] \\ 0, & \text{otherwise} \end{cases}$$

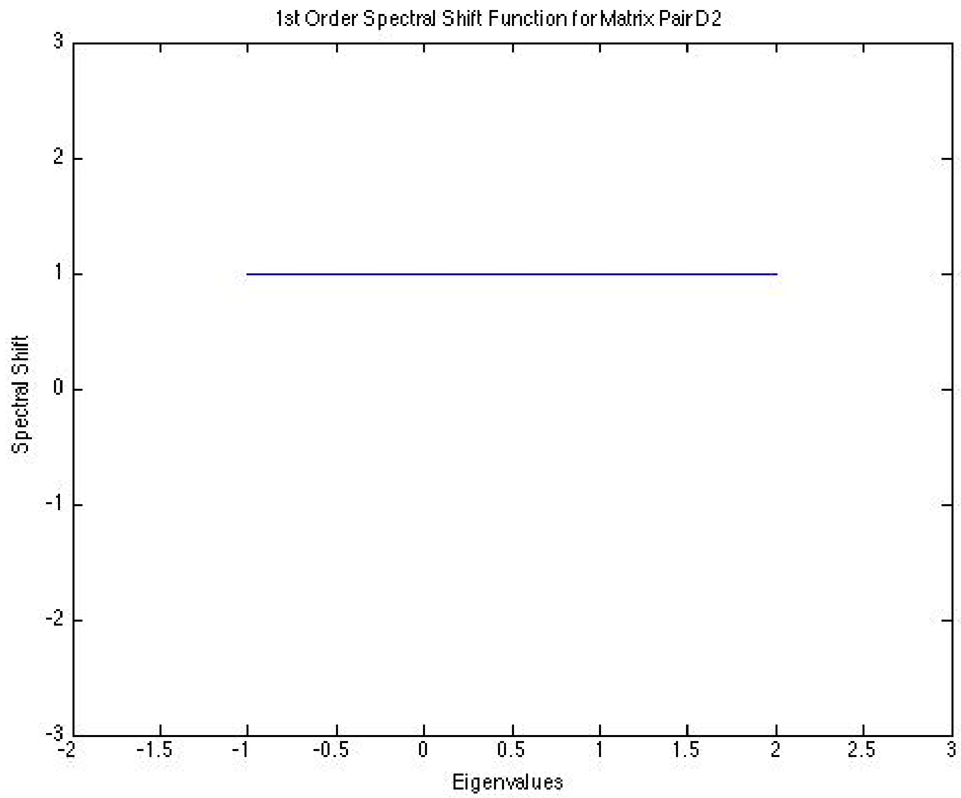


Example 3.8. **Diagonal Pair D2**

$$A = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad A + V = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

$$\sigma(A) = \{-1, 0, 1\} \quad \sigma(A+V) = \{0, 1, 2\}$$

$$\xi(t) = \begin{cases} 1, & \text{if } t \in (-1, 2] \\ 0, & \text{otherwise} \end{cases}$$

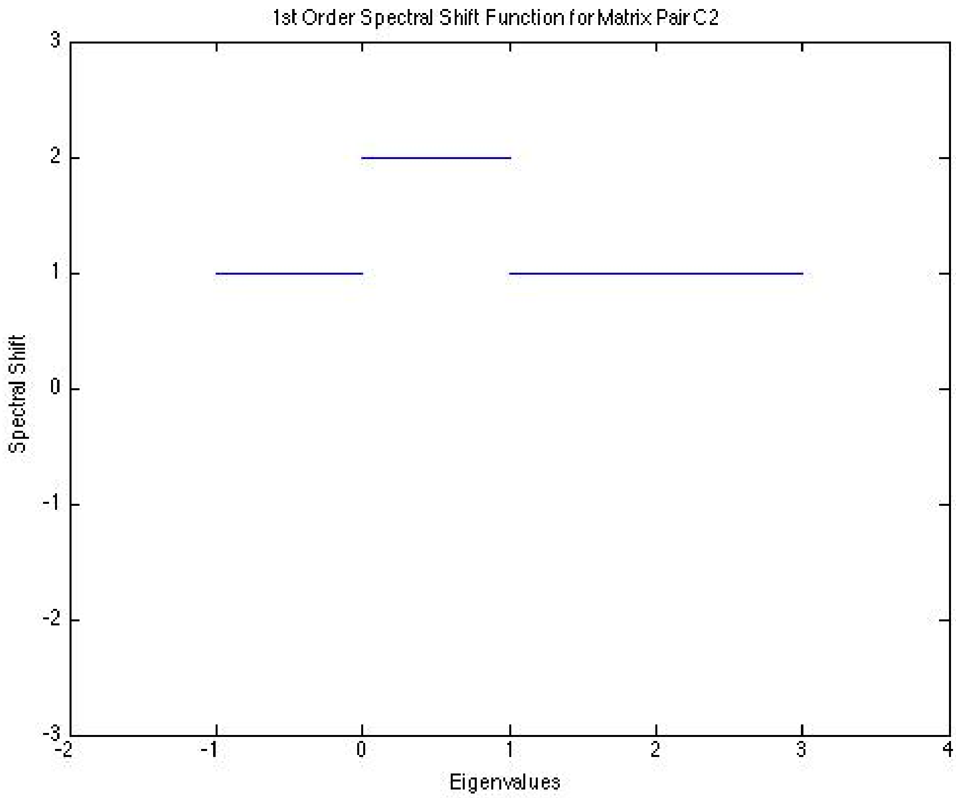


Example 3.9. **Commuting Pair C2**

$$A = \begin{bmatrix} 1 & i & 0 \\ -i & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix} \quad A + V = \begin{bmatrix} 2 & i & 0 \\ -i & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

$$\sigma(A) = \{-1, 0, 2\} \quad \sigma(A + V) = \{1, 2, 3\}$$

$$\xi(t) = \begin{cases} 1, & \text{if } t \in (-1, 0] \ or \ (1, 3] \\ 2, & \text{if } t \in (0, 1] \\ 0, & \text{otherwise} \end{cases}$$

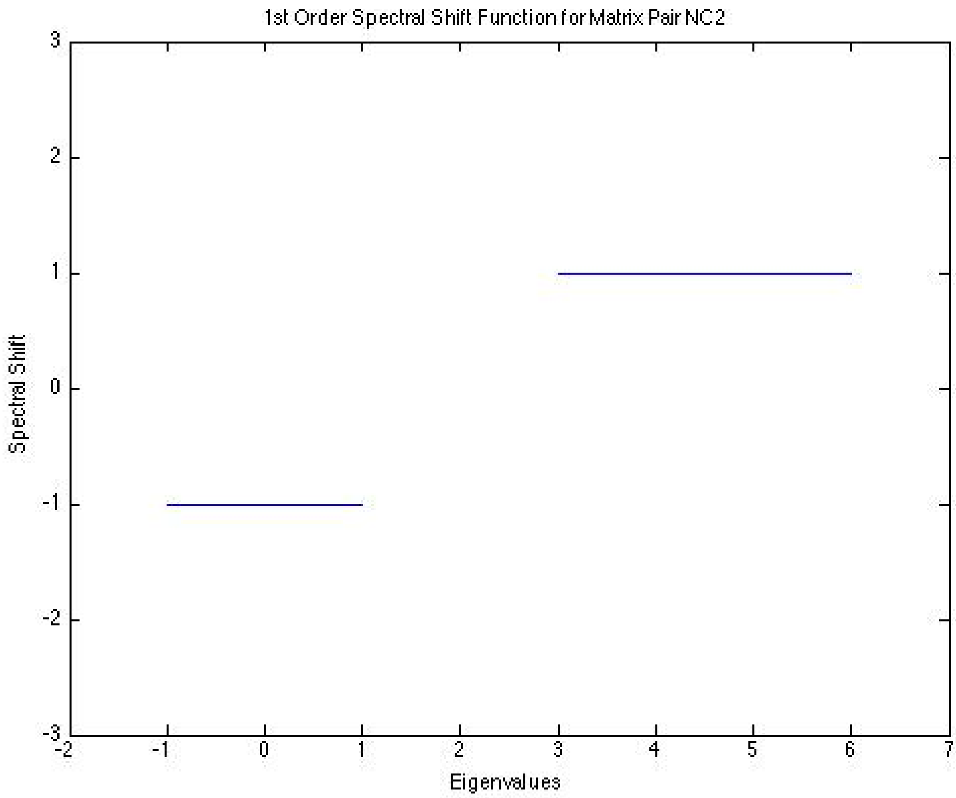


Example 3.10. **Noncommuting Pair NC2**

$$A = \begin{bmatrix} 2 & 0 & -i \\ 0 & 3 & 0 \\ i & 0 & 2 \end{bmatrix} \quad A + V = \begin{bmatrix} 3 & 2-i & -3i \\ 2+i & 0 & 1-i \\ 3i & 1+i & 0 \end{bmatrix}$$

$\sigma(A) = \{1, 3\} \quad \sigma(A+V) = \{-2, -1, 6\}$

$$\xi(t) = \begin{cases} -1, & \text{if } t \in (-1, 1] \\ 1, & \text{if } t \in (3, 6] \\ 0, & \text{otherwise} \end{cases}$$



It can be insightful to ask when $\xi(x)$ is zero everywhere. This occurs when the spectra are equal and multiplicities of the respective eigenvalues are equal.

Proposition 3.11. *Let A and $A+V$ be two self-adjoint matrices where the spectra of A and $A+V$ are equal, and the multiplicities of the respective eigenvalues are also equal. Then the spectral shift function is identically 0.*

Proof. We begin with the forward direction. Let $\{\lambda_i\}_{i=1}^n = \{\mu_j\}_{j=1}^n$ where $\lambda_1 = \mu_1, \lambda_2 = \mu_2, \ldots, \lambda_n = \mu_n$. Given this, we can see that $\text{Card}\{i \mid \lambda_i < x\} = \text{Card}\{j \mid \mu_j < x\}\ \forall x \in \mathbb{R}$. Since this is the case, we know that $\xi(x) = \text{Card}\{i \mid \lambda_i < x\} - \text{Card}\{j \mid \mu_j < x\} = 0\ \forall x \in \mathbb{R}$.

Now we do the other direction. Let $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$ and $\mu_1 \le \mu_2 \le \ldots \le \mu_n$ be the eigenvalues of A and $A+V$ respectively. Suppose $\xi(x) = 0$ for all $\forall x \in \mathbb{R}$. Then $\text{Card}\{i \mid \lambda_i < x\} = \text{Card}\{j \mid \mu_j < x\}$ for all $\forall x \in \mathbb{R}$. Suppose $\exists k$ such that $\lambda_k \neq \mu_k$, and assume without loss of generality that $\lambda_k < \mu_k$. In particular, we know $\text{Card}\{i \mid \lambda_i < \lambda_k\} = \text{Card}\{j \mid \mu_j < \lambda_k\}$. Since $\lambda_k < \mu_k$, $\exists \epsilon \in \mathbb{R}$ such that $\lambda_k + \epsilon < \mu_k$ too. Then $\text{Card}\{i \mid \lambda_i < \lambda_k + \epsilon\} > \text{Card}\{i \mid \lambda_i < \lambda_k\}$, while $\text{Card}\{j \mid \mu_j < \lambda_k + \epsilon\} = \text{Card}\{j \mid \mu_j < \lambda_k\}$. From that we see $\text{Card}\{i \mid \lambda_i < \lambda_k + \epsilon\} > \text{Card}\{i \mid \lambda_i < \lambda_k\} = \text{Card}\{j \mid \mu_j < \lambda_k\} = \text{Card}\{j \mid \mu_j < \lambda_k + \epsilon\}$. This gives us $\text{Card}\{i \mid \lambda_i < \lambda_k + \epsilon\} > \text{Card}\{j \mid \mu_j < \lambda_k + \epsilon\}$, which means for $x = \lambda_k + \epsilon$, $\xi(x) \neq 0$. This is a contradiction of our assumption, so it must be that $\{\lambda_i\}_{i=1}^n = \{\mu_j\}_{j=1}^n$ where $\lambda_1 = \mu_1, \lambda_2 = \mu_2, \ldots, \lambda_n = \mu_n$. □

4. The Second Order Spectral Shift Function

The second order spectral shift function is a considerably more complicated object. The second order spectral shift function is useful when $\xi(x)$ is 0 in the finite dimensional case, or when $\xi(x)$ is undefined in the infinite dimensional case. All of the examples in this paper are for finite dimensional operators that we have represented with matrices. One can interpret the second order spectral shift function as how much the eigenvalues change when they are perturbed. The second order spectral shift function is used in *Koplienko's Trace Formula.*

$$tr\left[f(A+V) - f(A) - \frac{d}{dx}\left(f(A+xV)\right)|_{x=0}\right] = \int_{\mathbb{R}} f''(x)\eta(x)dx \tag{18}$$

References to *Koplienko's Trace Formula* can be found in [4].

The second order spectral shift function can also be represented in terms of the first order spectral shift function with a proof appearing in [4]. The following representation is typically used as the definition of η.

Definition 4.1. *The second order spectral shift function is defined as*

$$\eta(x) := tr(\chi_{(-\infty,x)}(A)V) - \int_{-\infty}^{x} \xi(\lambda)d\lambda. \tag{19}$$

One equivalent form of $\eta(x)$ is given below.

Proposition 4.2. *The second order spectral shift function can be defined as*

$$\eta(x) = tr((xI - A - V)(\chi_{(-\infty,x)}(A+V) - \chi_{(-\infty,x)}(A))). \tag{20}$$

The second equivalent form of $\eta(x)$ is the easiest one to use for calculations. The following proposition was derived in Lemma 5.2 in *Trace Inequalities and Spectral Shift*, appearing in Operators and Matrices, Volume 3 [4], and was communicated to the author by A. Skripka.

Proposition 4.3. *The second order spectral shift function can be defined as the sum*

$$\eta(x) = \sum_{k,j=1}^{n} |\mu_k - x| \cdot |\langle f_j, g_k\rangle|^2 \cdot \chi_{[\mu_k,\lambda_j]}(x), \tag{21}$$

where $\chi_{[\mu_k,\lambda_j]}(x)$ *denotes* $\chi_{[\lambda_j,\mu_k]}(x)$ *if* $\lambda_j < \mu_k$*. In this equation,* $\{f_j\}_{j=1}^n$ *are the orthonormal eigenvectors of* A*,* $\{g_k\}_{k=1}^n$ *are the orthonormal eigenvectors of* $A+V$*,* $\{\lambda_j\}_{j=1}^n$ *are the eigenvalues of* A*,* $\{\mu_k\}_{k=1}^n$ *are the eigenvalues of* $A+V$*, and* $|\langle f_j, g_k\rangle|$ *is the absolute value of the dot product of two eigenvectors.*

Proof. We begin by noting that $\chi_{(-\infty,x)}(A+V)$ and $\chi_{(-\infty,x)}(A)$ are the orthogonal projections we encountered in (14), so we can use equation (3) to write

$$\chi_{(-\infty,x)}(A+V) - \chi_{(-\infty,x)}(A) = \chi_{(-\infty,x)}(A+V)\chi_{[x,\infty)}(A) - \chi_{[x,\infty)}(A+V)\chi_{(-\infty,x)}(A).$$

Substituting this into (20) gives us

$$\operatorname{tr}((xI - A - V)(\chi_{(-\infty,x)}(A+V)\chi_{[x,\infty)}(A) - \chi_{[x,\infty)}(A)\chi_{(-\infty,x)}(A+V)).$$

The trace function is cyclic, (11), and it can be written as a dot product, (9), so

$$\begin{aligned}
&\operatorname{tr}((xI - A - V)\chi_{(-\infty,x)}(A+V)\chi_{[x,\infty)}(A)) \\
&\qquad = \operatorname{tr}(\chi_{[x,\infty)}(A)(xI - A - V)\chi_{(-\infty,x)}(A+V)) \\
&\qquad = \sum_{\lambda_j > x} \left\langle (xI - A - V)\chi_{(-\infty,x)}(A+V) f_j, f_j \right\rangle .
\end{aligned}$$

Using equations (6) and (7) we can write

$$\begin{aligned}
&(xI - A - V)\chi_{(-\infty,x)}(A+V) \\
&\qquad = (xI)\chi_{(-\infty,x)}(A+V) - (A+V)\chi_{(-\infty,x)}(A+V) \\
&\qquad = (xI)\sum_{k=1}^n \chi_{(-\infty,x)}(\mu_k) S_2 E_{kk} S_2^{-1} - (A+V)\sum_{k=1}^n \chi_{(-\infty,x)}(\mu_k) S_2 E_{kk} S_2^{-1} \\
&\qquad = \sum_{k=1}^n x\chi_{(-\infty,x)}(\mu_k) S_2 E_{kk} S_2^{-1} - \sum_{k=1}^n \mu_k \chi_{(-\infty,x)}(\mu_k) S_2 E_{kk} S_2^{-1} \\
&\qquad = \sum_{\mu_k < x} x S_2 E_{kk} S_2^{-1} - \sum_{\mu_k < x} \mu_k S_2 E_{kk} S_2^{-1} \\
&\qquad = \sum_{\mu_k < x} (x - \mu_k) S_2 E_{kk} S_2^{-1} \\
&\qquad = \sum_{\mu_k < x} (x - \mu_k) \langle \cdot, g_k \rangle g_k
\end{aligned}$$

The operator $\sum_{\mu_k < x} \langle \cdot, g_k \rangle g_k$ should be thought of as being applied to a vector. With that in mind, we can immediately see

$$\begin{aligned}
&(xI - A - V)\chi_{(-\infty,x)}(A+V) f_j \\
&\qquad = \sum_{\mu_k < x} (x - \mu_k) \langle f_j, g_k \rangle g_k.
\end{aligned}$$

Using properties of the dot product gives us

$$\sum_{\lambda_j > x} \left\langle (xI - A - V)\chi_{(-\infty,x)}(A+V)f_j, f_j \right\rangle$$
$$= \sum_{\lambda_j > x} \sum_{\mu_k < x} (x - \mu_k) \langle f_j, g_k \rangle \langle g_k, f_j \rangle$$
$$= \sum_{\lambda_j > x} \sum_{\mu_k < x} (x - \mu_k) | \langle f_j, g_k \rangle |^2.$$
$$= \sum_{\mu_k < x < \lambda_j} |x - \mu_k| | \langle f_j, g_k \rangle |^2.$$

Thus,

$$\text{tr}((xI - A - V)\chi_{(-\infty,x)}(A+V)\chi_{[x,\infty)}(A))$$
$$= \sum_{\mu_k < x < \lambda_j} |x - \mu_k| | \langle f_j, g_k \rangle |^2.$$

Similarly,

$$\text{tr}((A + V - xI)\chi_{[x,\infty)}(A+V)\chi_{(-\infty,x)}(A))$$
$$= \sum_{\lambda_j < x} \left\langle (A + V - xI)\chi_{[x,\infty)}(A+V)f_j, f_j \right\rangle$$
$$= \sum_{\lambda_j < x} \sum_{\mu_k > x} (\mu_k - x) \langle f_j, g_k \rangle \langle g_k, f_j \rangle$$
$$= \sum_{\lambda_j < x} \sum_{\mu_k > x} (\mu_k - x) | \langle f_j, g_k \rangle |^2$$
$$= \sum_{\lambda_j < x < \mu_k} |x - \mu_k| | \langle f_j, g_k \rangle |^2.$$

Finally,

$$\text{tr}((xI - A - V)(\chi_{(-\infty,x)}(A+V)\chi_{[x,\infty)}(A) - \chi_{(-\infty,x)}(A)\chi_{[x,\infty)}(A+V))$$

$$= \text{tr}((xI - A - V)\chi_{(-\infty,x)}(A+V)\chi_{[x,\infty)}(A)) + \text{tr}((A + V - xI)\chi_{[x,\infty)}(A+V)\chi_{(-\infty,x)}(A))$$
$$= \sum_{\mu_k < x < \lambda_j} |x - \mu_k| | \langle f_j, g_k \rangle |^2 + \sum_{\lambda_j < x < \mu_k} |x - \mu_k| | \langle f_j, g_k \rangle |^2$$
$$= \sum_{k,j=1}^{n} |\mu_k - x| \cdot | \langle f_j, g_k \rangle |^2 \cdot \chi_{[\mu_k, \lambda_j]}(x).$$

□

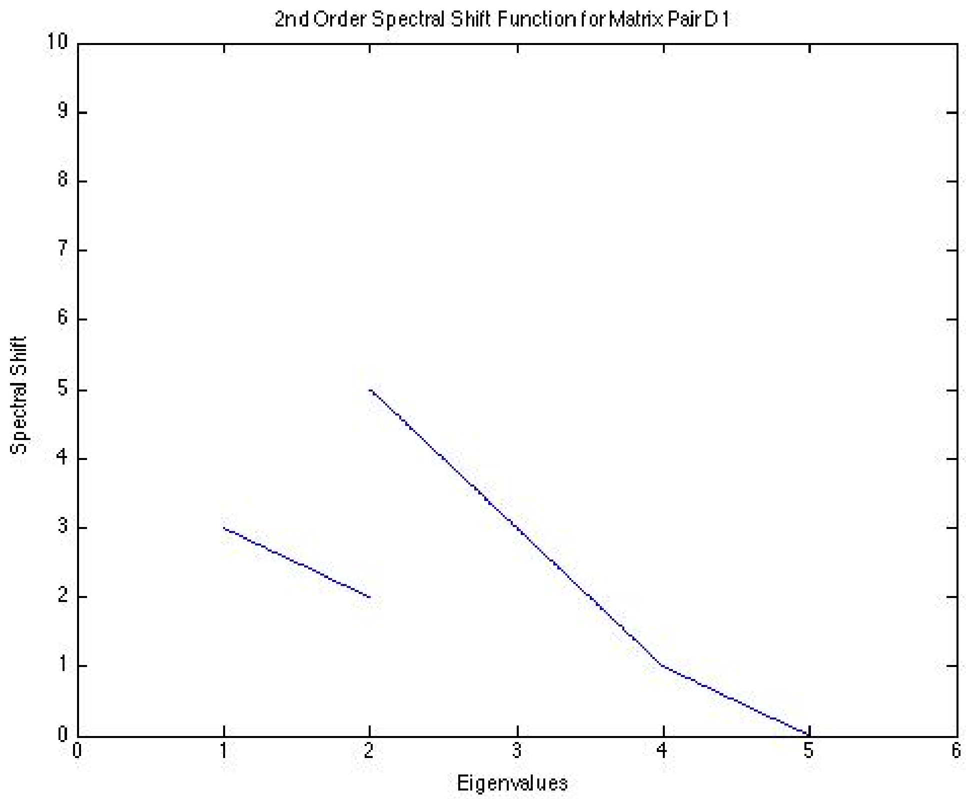
It is clear from the representation of $\eta(x)$ given in (21) that $\eta(x) \geq 0$. In the graphs that follow, note that $\eta(x)$ is a piece-wise linear function. Like $\xi(x)$, $\eta(x)$ can only be nonzero on the interval $[a, b]$, where $a = min\{\lambda_i, \mu_j\}_{i,j=1}^{n}$ and $b = max\{\lambda_i, \mu_j\}_{i,j=1}^{n}$.

Example 4.4. **Diagonal Pair D1**

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \quad A+V = \begin{bmatrix} 4 & 0 \\ 0 & 5 \end{bmatrix}$$

$$\sigma(A) = \{1,2\} \quad \sigma(A+V) = \{4,5\}$$

$$U_A = U_{A+V} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \eta(t) = \begin{cases} 4-t, & \text{if } t \in [1,2) \\ 9-2t, & \text{if } t \in [2,4] \\ 5-t, & \text{if } t \in (4,5] \\ 0, & \text{otherwise} \end{cases}$$



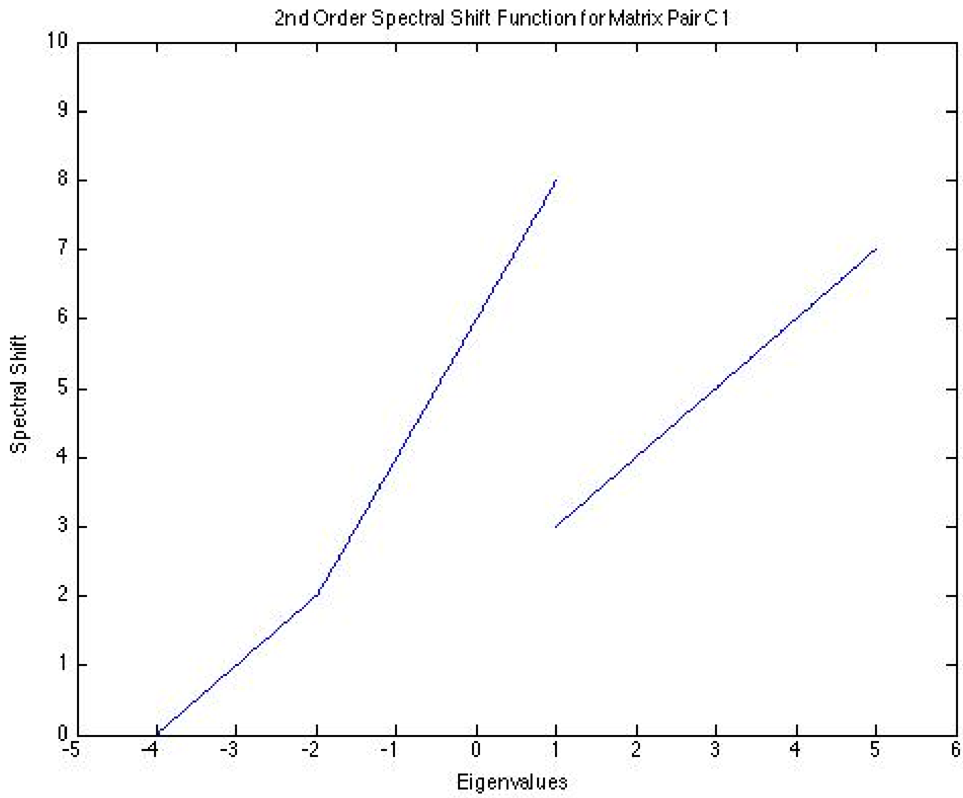
Example 4.5. **Commuting Pair C1**

$$A = \begin{bmatrix} 3 & 2i \\ -2i & 3 \end{bmatrix} \quad A + V = \begin{bmatrix} -3 & i \\ -i & -3 \end{bmatrix}$$

$$\sigma(A) = \{1, 5\} \quad \sigma(A + V) = \{-4, -2\}$$

$$U_A = U_{A+V} = \frac{1}{\sqrt{2}} \begin{bmatrix} -i & i \\ 1 & 1 \end{bmatrix}$$

$$\eta(t) = \begin{cases} 4 + t, & \text{if } t \in (-4, -2] \\ 6 + 2t, & \text{if } t \in (-2, 1] \\ 2 + t, & \text{if } t \in (1, 5] \\ 0, & \text{otherwise} \end{cases}$$



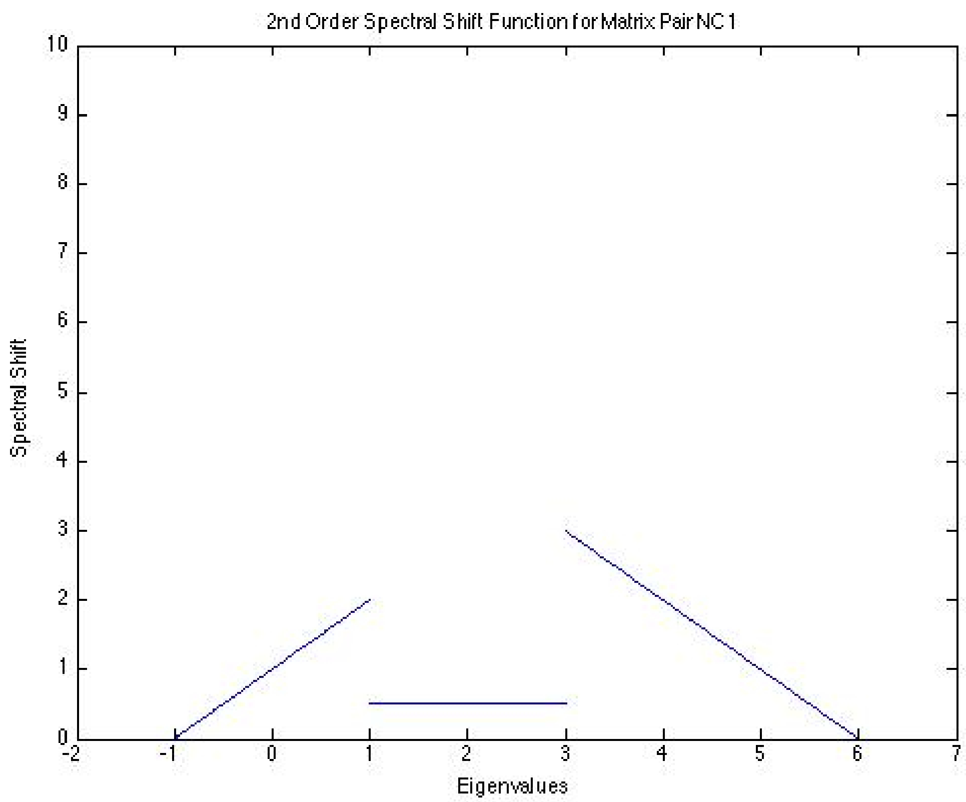
Example 4.6. **Noncommuting Pair NC1**

$$A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \quad A + V = \begin{bmatrix} 1 & 3+i \\ 3-i & 4 \end{bmatrix}$$

$$\sigma(A) = \{1, 3\} \quad \sigma(A+V) = \{-1, 6\}$$

$$U_A = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \quad U_{A+V} = \begin{bmatrix} \frac{-5}{\sqrt{35}} & \frac{2}{\sqrt{14}} \\ \frac{3-i}{\sqrt{35}} & \frac{3-i}{\sqrt{14}} \end{bmatrix}$$

$$\eta(t) = \begin{cases} 1+t, & \text{if } t \in [-1, 1] \\ \frac{1}{2}, & \text{if } t \in (1, 3) \\ 6-t, & \text{if } t \in [3, 6] \\ 0, & \text{otherwise} \end{cases}$$

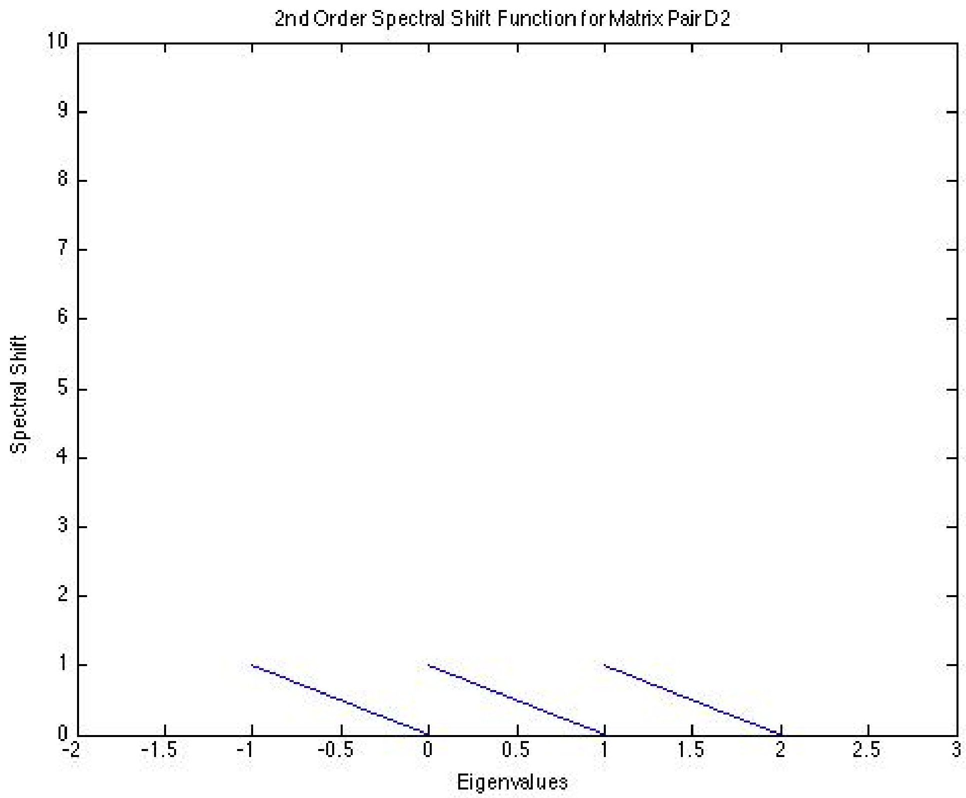


Example 4.7. **Diagonal Pair D2**

$$A = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad A + V = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

$$\sigma(A) = \{-1, 0, 1\} \quad \sigma(A + V) = \{0, 1, 2\}$$

$$U_A = U_{A+V} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \eta(t) = \begin{cases} -t, & \text{if } t \in [-1, 0) \\ 1 - t, & \text{if } t \in [0, 1) \\ 2 - t, & \text{if } t \in [1, 2] \\ 0, & \text{otherwise} \end{cases}$$

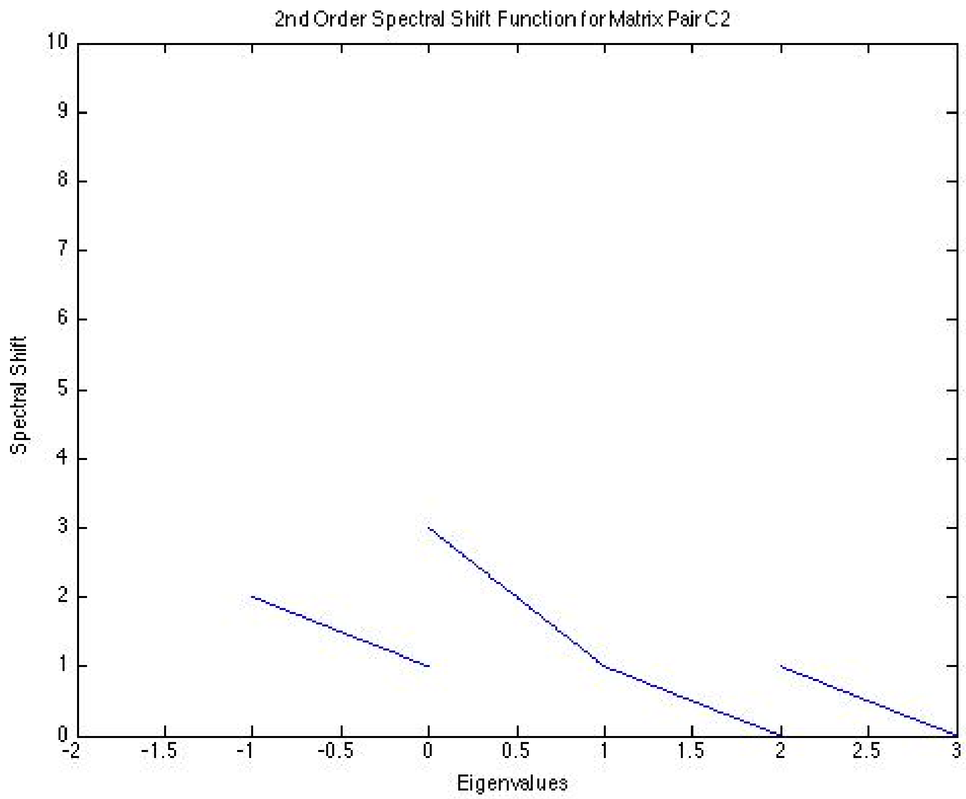


Example 4.8. **Commuting Pair C2**

$$A = \begin{bmatrix} 1 & i & 0 \\ -i & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix} \quad A + V = \begin{bmatrix} 2 & i & 0 \\ -i & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

$$\sigma(A) = \{-1, 0, 2\} \quad \sigma(A + V) = \{1, 2, 3\}$$

$$U_A = U_{A+V} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & i \\ 0 & i & 1 \\ \sqrt{2} & 0 & 0 \end{bmatrix} \qquad \eta(t) = \begin{cases} 1 - t, & \text{if } t \in [-1, 0) \\ 3 - 2t, & \text{if } t \in [0, 1] \\ 2 - t, & \text{if } t \in (1, 2] \\ 3 - t, & \text{if } t \in (2, 3] \\ 0, & \text{otherwise} \end{cases}$$



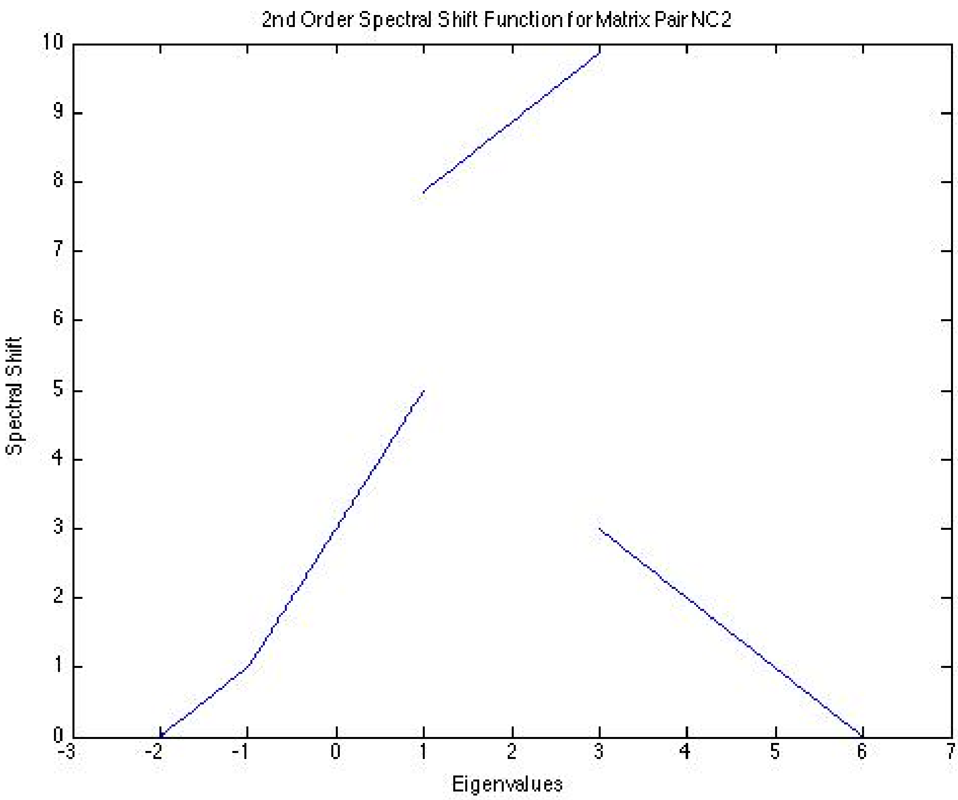
Example 4.9. **Noncommuting Pair NC2**

$$A = \begin{bmatrix} 2 & 0 & -i \\ 0 & 3 & 0 \\ i & 0 & 2 \end{bmatrix} \quad A+V = \begin{bmatrix} 3 & 2-i & -3i \\ 2+i & 0 & 1-i \\ 3i & 1+i & 0 \end{bmatrix}$$

$$\sigma(A) = \{1, 3\} \quad \sigma(A+V) = \{-2, -1, 6\}$$

$$U_A = \frac{1}{\sqrt{2}} \begin{bmatrix} i & 0 & -i \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \end{bmatrix} \quad U_{A+V} = \begin{bmatrix} -0.378 & 0.0371 - 0.7783i & 0.1581 + 0.4743i \\ 0.387 + 0.7659 & 0.2224 - 0.3336i & -0.3162 + 0.1581i \\ 0.378 & 0.4818 & 0.7906 \end{bmatrix}$$

$$\eta(t) = \begin{cases} 2+t, & \text{if } t \in [-2,-1) \\ 3+2t, & \text{if } t \in [-1,1] \\ 0.9999 + 6.8571t, & \text{if } t \in (1,3] \\ 6-t, & \text{if } t \in (3,6] \\ 0, & \text{otherwise} \end{cases}$$



As with the first order spectral shift function, it can be insightful to ask when $\eta(x)$ is zero everywhere. We can see from the examples that follow, wherein $\xi(x)$ is identically 0 and $\eta(x)$ is identically 0, that this occurs when the matrices A and $A+V$ both commute and have the same eigenvalues with the same multiplicities. Since they commute, they have the same set of eigenvectors and can have the same diagonalizing matrices. Furthermore, if $\eta(x) = 0$, then $\xi(x) = 0$. This implication does not go the other way. If the matrices do not commute, but do have the same eigenvalues with the same multiplicities, then $\eta(x)$ seems to be a piece-wise constant function. Examples of this behavior are also included.

Proposition 4.10. *If two self-adjoint matrices have the same spectra of eigenvalues with the same multiplicities and the same eigenvectors, then* $\eta(x) = 0\ \forall x \in \mathbb{R}$.

Proof. Suppose that A and $A+V$ have the same eigenvalues with the same multiplicities and with the same eigenvectors. Let $\{\lambda_i\}_{i=1}^n = \{\mu_j\}_{j=1}^n$ where $\lambda_1 = \mu_1, \lambda_2 = \mu_2, \ldots, \lambda_n = \mu_n$. We know that the diagonalizing matrices have columns composed of orthonormal eigenvectors, so the dot product of any two of them that are not equal is 0. This means that any terms with $|\langle f_i, f_j\rangle|^2$ where $j \neq i$ will become 0 in the sum $\sum_i \sum_j |\lambda_i - x| \cdot |\langle f_i, f_j\rangle|^2 \cdot \chi_{[\lambda_i,\lambda_i]}(x)$. This leaves us with the terms where $j = i$. Since all the eigenvalues are equal and have the same multiplicities, when $j = i$, $\chi_{[\lambda_i,\lambda_i]}(x) = \chi_{\{\lambda_i\}}(x)$. In other words, the only time that $\chi_{\{\lambda_i\}}(x) \neq 0$, is when $x = \lambda_i$. However when $x = \lambda_i$, $|\lambda_i - x| = 0$. Thus the terms in the sum$\sum_i \sum_j |\lambda_i - x| \cdot |\langle f_i, f_j\rangle|^2 \cdot \chi_{[\lambda_i,\lambda_i]}(x)$ where $j = i$ are also 0. In conclusion, $\eta(x) = 0$. □

Conjecture 4.11. *If* $\eta(x) = 0\ \forall x \in \mathbb{R}$ *for two self-adjoint matrices, then* $\xi(x) = 0\ \forall x \in \mathbb{R}$ *for those matrices too.*

It may be possible to prove 4.10 in the other direction using 4.11.

Conjecture 4.12. *If* $\xi(x) = 0$ *and* $\eta(x) = 0\ \forall x \in \mathbb{R}$ *for two self-adjoint matrices, then those two self-adjoint matrices have the same spectra of eigenvalues with the same multiplicities and the same eigenvectors.*

Additionally, it may be possible to prove under what conditions $\eta(x)$ is a piece-wise constant function.

Conjecture 4.13. *If two self-adjoint matrices have the same spectra of eigenvalues with the same multiplicities, but not the same eigenvectors, then* $\xi(x) = 0$ *and* $\eta(x)$ *is a piece-wise constant function* $\forall x \in \mathbb{R}$.

Example 4.14. **Diagonal Pair, Eigenvalues Permuted, XD2**

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \quad A + V = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\sigma(A) = \sigma(A + V) = \{1, 2\}$$

$$U_A = U_{A+V} = \mathrm{I}$$

$$\eta(t) = 0$$

Example 4.15. **Commuting Pair, Eigenvalues Permuted, XPC1**

$$A = \tfrac{1}{3} \begin{bmatrix} 4 & -\sqrt{2} \\ -\sqrt{2} & 5 \end{bmatrix} \quad A + V = \tfrac{1}{3} \begin{bmatrix} 5 & -\sqrt{2} \\ -\sqrt{2} & 4 \end{bmatrix}$$

$$\sigma(A) = \sigma(A + V) = \{1, 2\}$$

$$D_A = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \quad D_{A+V} = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}$$

$$U_A = U_{A+V} = \tfrac{1}{\sqrt{2}} \begin{bmatrix} \frac{1-i}{\sqrt{3}} & \frac{-i}{\sqrt{3}} \\ \frac{1-i}{\sqrt{6}} & \frac{2i}{\sqrt{6}} \end{bmatrix}$$

$$\eta(t) = 0$$

Example 4.16. **Noncommuting Pair, Eigenvalues Not Permuted, XNC1**

$$A = \tfrac{1}{3} \begin{bmatrix} 4 & -\sqrt{2} \\ -\sqrt{2} & 5 \end{bmatrix} \quad A + V = \tfrac{1}{25} \begin{bmatrix} 34 & 12i \\ -12i & 41 \end{bmatrix}$$

$$\sigma(A) = \sigma(A + V) = \{1, 2\}$$

$$D_A = D_{A+V} = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$

$$U_A = \tfrac{1}{\sqrt{2}} \begin{bmatrix} \frac{1-i}{\sqrt{3}} & \frac{-i}{\sqrt{3}} \\ \frac{1-i}{\sqrt{6}} & \frac{2i}{\sqrt{6}} \end{bmatrix} \quad U_{A+V} = \tfrac{1}{2} \begin{bmatrix} 1-i & 1+i \\ 1+1 & 1-i \end{bmatrix}$$

$$\eta(t) = \begin{cases} \frac{1}{2}, & \text{if } t \in [1, 2] \\ 0, & \text{otherwise} \end{cases}$$

Example 4.17. **Noncommuting Pair, Eigenvalues Permuted, XPNC1**

$$A = \frac{1}{3}\begin{bmatrix} 4 & -\sqrt{2} \\ -\sqrt{2} & 5 \end{bmatrix} \quad A + V = \frac{1}{2}\begin{bmatrix} 3 & -i \\ i & 3 \end{bmatrix}$$

$$\sigma(A) = \sigma(A + V) = \{1, 2\}$$

$$D_A = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \quad D_{A+V} = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}$$

$$U_A = \frac{1}{\sqrt{2}}\begin{bmatrix} \frac{1-i}{\sqrt{3}} & \frac{-i}{\sqrt{3}} \\ \frac{1-i}{\sqrt{6}} & \frac{2i}{\sqrt{6}} \end{bmatrix} \quad U_{A+V} = \frac{1}{2}\begin{bmatrix} 1-i & 1+i \\ 1+1 & 1-i \end{bmatrix}$$

$$\eta(t) = \begin{cases} \frac{1}{2}, & \text{if } t \in [1, 2] \\ 0, & \text{otherwise} \end{cases}$$

Example 4.18. **Commuting Pair, Eigenvalues Permuted, XPC2**

$$A = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -2 & 0 \\ -1 & 0 & 0 \end{bmatrix} \quad A + V = \begin{bmatrix} \frac{-1}{2} & 0 & \frac{-3}{2} \\ 0 & -1 & 0 \\ \frac{-3}{2} & 0 & \frac{-1}{2} \end{bmatrix}$$

$$\sigma(A) = \sigma(A + V) = \{-2, -1, 1\}$$

$$D_A = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad D_{A+V} = \begin{bmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$U_A = U_{A+V} = \frac{1}{\sqrt{2}}\begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1-i}{2} \\ 0 & -i & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1+i}{2} \end{bmatrix}$$

$$\eta(t) = 0$$

Example 4.19. **Noncommuting Pair, Eigenvalues Not Permuted, XNC2**

$$A = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -2 & 0 \\ -1 & 0 & 0 \end{bmatrix} \quad A + V = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & -1+i \\ 0 & -1-i & 0 \end{bmatrix}$$

$$\sigma(A) = \sigma(A + V) = \{-2, -1, 1\}$$

$$D_A = D_{A+V} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$U_A = \frac{1}{\sqrt{2}}\begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1-i}{2} \\ 0 & -i & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1+i}{2} \end{bmatrix} \quad U_{A+V} = \begin{bmatrix} 0 & \frac{-1-i}{\sqrt{6}} & \frac{2}{\sqrt{6}} \\ 1 & 0 & 0 \\ 0 & \frac{1+i}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{bmatrix}$$

$$\eta(t) = \begin{cases} 3, & \text{if } t \in [-2, -1) \\ 2, & \text{if } t \in [-1, 1] \\ 0, & \text{otherwise} \end{cases}$$

Example 4.20. **Noncommuting Pair, Eigenvalues Permuted, XPNC2**

$$A = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -2 & 0 \\ -1 & 0 & 0 \end{bmatrix} \quad A + V = \begin{bmatrix} -1 & 0 & -\sqrt{2} \\ 0 & -1 & 0 \\ -\sqrt{2} & 0 & 0 \end{bmatrix}$$

$$\sigma(A) = \sigma(A+V) = \{-2, -1, 1\}$$

$$D_A = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad D_{A+V} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

$$U_A = \frac{1}{\sqrt{2}} \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1-i}{2} \\ 0 & -i & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1+i}{2} \end{bmatrix} \quad U_{A+V} = \begin{bmatrix} 0 & \frac{-1-i}{\sqrt{6}} & \frac{2}{\sqrt{6}} \\ 1 & 0 & 0 \\ 0 & \frac{1+i}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{bmatrix}$$

$$\eta(t) = \begin{cases} 3, & \text{if } t \in [-2, -1) \\ 2, & \text{if } t \in [-1, 1] \\ 0, & \text{otherwise} \end{cases}$$

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