ENGG 5781: Matrix Analysis and Computations **2016-17 Second Term**

Lecture 4: Positive Semidefinite Matrices and Variational Characterizations of Eigenvalues

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The focus of this note is to give a more in-depth description of variational characterizations of eigenvalues of real symmetric matrices. I will also provide the proof of some results concerning the PSD matrix inequalities in the main lecture slides.

Our notations is as follows. The eigenvalues of a given matrix $\mathbf{A} \in \mathbb{S}^n$ are denoted by $\lambda_1(\mathbf{A}), \ldots, \lambda_n(\mathbf{A})$, and they are assumed to be arranged such that

$$\lambda_{\max}(\mathbf{A}) = \lambda_1(\mathbf{A}) \geq \lambda_2(\mathbf{A}) \geq \ldots \geq \lambda_n(\mathbf{A}) = \lambda_{\min}(\mathbf{A}),$$

where we also denote $\lambda_{\min}(\mathbf{A})$ and $\lambda_{\max}(\mathbf{A})$ as the smallest and largest eigenvalues of $\mathbf{A}$, respectively. If not specified, we will simply denote $\lambda_1, \ldots, \lambda_n$, with $\lambda_1 \geq \ldots \geq \lambda_n$, as the eigenvalues of $\mathbf{A} \in \mathbb{S}^n$. Also, we will denote $\mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^T$ as the eigendecomposition of $\mathbf{A}$ without explicit mentioning.

1 Variational Charcterizations of Eigenvalues of Real Symmetric Matrices

For a general $\mathbf{A} \in \mathbb{R}^{n \times n}$, we may only characterize its eigenvalues as the roots of the characteristic polynomial $p(\lambda) = \det(\mathbf{A} - \lambda\mathbf{I})$. However, for a real symmetric $\mathbf{A}$, we can alternatively characterize the eigenvalues as solutions to certain quadratic optimization problems. As we will see, such variational characterizations of the eigenvalues lead to a number of interesting matrix analysis results.

1.1 Rayleigh Quotient Maximization and Minimization

Let $\mathbf{A} \in \mathbb{S}^n$, and consider the following optimization problems

$$\max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{x}}, \tag{1}$$

$$\min_{\mathbf{x} \in \mathbb{R}^n, \mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{x}}, \tag{2}$$

Note that the ratio $\mathbf{x}^T\mathbf{A}\mathbf{x}/\mathbf{x}^T\mathbf{x}$ is called a *Rayleigh quotient*. Rayleigh quotients are invariant to $\|\mathbf{x}\|_2^2$; one can see that

$$\frac{(\alpha\mathbf{x})^T\mathbf{A}(\alpha\mathbf{x})}{(\alpha\mathbf{x})^T(\alpha\mathbf{x})} = \frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{x}},$$

for any $\alpha \neq 0$ and $\mathbf{x} \neq \mathbf{0}$. Without loss of generality, let us assume $\|\mathbf{x}\|_2 = 1$ and rewrite problems (1) and (2) as

$$\max_{\mathbf{x} \in \mathbb{R}^n, \mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \max_{\mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\|_2 = 1} \mathbf{x}^T\mathbf{A}\mathbf{x},$$

$$\min_{\mathbf{x} \in \mathbb{R}^n, \mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \min_{\mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\|_2 = 1} \mathbf{x}^T\mathbf{A}\mathbf{x},$$

respectively. The solutions to problems (1) and (2) are described in the following theorem.

Theorem 4.4 (Rayleigh-Ritz) *For any* $\mathbf{A} \in \mathbb{S}^n$*, it holds that*

$$\lambda_{\min}\|\mathbf{x}\|_2^2 \leq \mathbf{x}^T\mathbf{A}\mathbf{x} \leq \lambda_{\max}\|\mathbf{x}\|_2^2, \tag{3}$$

$$\lambda_{\max} = \max_{\mathbf{x}\in\mathbb{R}^n, \|\mathbf{x}\|_2=1} \mathbf{x}^T\mathbf{A}\mathbf{x}, \tag{4}$$

$$\lambda_{\min} = \min_{\mathbf{x}\in\mathbb{R}^n, \|\mathbf{x}\|_2=1} \mathbf{x}^T\mathbf{A}\mathbf{x}. \tag{5}$$

Proof: This theorem is a direct consequence of eigendecomposition for real symmetric matrices. By letting $\mathbf{y} = \mathbf{V}^T\mathbf{x}$, the term $\mathbf{x}^T\mathbf{A}\mathbf{x}$ can be expressed as

$$\mathbf{x}^T\mathbf{A}\mathbf{x} = \mathbf{y}^T\mathbf{\Lambda}\mathbf{y} = \sum_{i=1}^n \lambda_i|y_i|^2.$$

Since

$$\lambda_n \sum_{i=1}^n |y_i|^2 \leq \sum_{i=1}^n \lambda_i|y_i|^2 \leq \lambda_1 \sum_{i=1}^n |y_i|^2$$

and $\|\mathbf{y}\|_2^2 = \|\mathbf{V}^T\mathbf{x}\|_2^2 = \|\mathbf{x}\|_2^2$ for any orthogonal $\mathbf{V}$, we have (3). It follows that

$$\mathbf{x}^T\mathbf{A}\mathbf{x} \leq \lambda_{\max}, \quad \text{for all } \mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\|_2 = 1, \tag{6}$$

$$\mathbf{x}^T\mathbf{A}\mathbf{x} \geq \lambda_{\min}, \quad \text{for all } \mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\|_2 = 1. \tag{7}$$

It can be verified that the equalities in (6) and (7) are attained when $\mathbf{x} = \mathbf{v}_1$ and $\mathbf{x} = \mathbf{v}_n$, respectively. Thus, we also have shown (4) and (5). ■

1.2 The Courant-Fischer Minimax Theorem

The Rayleigh-Ritz theorem gives an alternative characterization of the smallest and largest eigenvalues of a real symmetric matrix. The next question is whether we provide a similar characterization for *any* eigenvalue. To give some insight, consider the following problem

$$\max_{\substack{\mathbf{x}\in\text{span}\{\mathbf{v}_2,\ldots,\mathbf{v}_n\} \\ \|\mathbf{x}\|_2=1}} \mathbf{x}^T\mathbf{A}\mathbf{x},$$

Following the same proof as in the Rayleigh-Ritz theorem, it can be shown that

$$\lambda_2 = \max_{\substack{\mathbf{x}\in\text{span}\{\mathbf{v}_2,\ldots,\mathbf{v}_n\} \\ \|\mathbf{x}\|_2=1}} \mathbf{x}^T\mathbf{A}\mathbf{x};$$

(please try). Also, the above problem can be alternatively expressed as

$$\lambda_2 = \max_{\substack{\mathbf{x}\in\text{span}\{\mathbf{v}_1\}^\perp \\ \|\mathbf{x}\|_2=1}} \mathbf{x}^T\mathbf{A}\mathbf{x}. \tag{8}$$

However, the above eigenvalue characterization does not look very attractive as its feasible set depends on the principal eigenvector. Let us consider another problem

$$\max_{\substack{\mathbf{x}\in\mathbb{R}^n, \|\mathbf{x}\|_2=1 \\ \mathbf{w}^T\mathbf{x}=0}} \mathbf{x}^T\mathbf{A}\mathbf{x},$$

where $\mathbf{w} \in \mathbb{R}^n$ is given. By letting $\mathbf{y} = \mathbf{V}^T\mathbf{x}$ again, we can derive a lower bound

$$\begin{aligned}
\max_{\substack{\mathbf{x}\in\mathbb{R}^n, \|\mathbf{x}\|_2=1 \\ \mathbf{w}^T\mathbf{x}=0}} \mathbf{x}^T\mathbf{A}\mathbf{x} &= \max_{\substack{\mathbf{y}\in\mathbb{R}^n, \|\mathbf{y}\|_2=1 \\ (\mathbf{V}^T\mathbf{w})^T\mathbf{y}=0}} \mathbf{y}^T\mathbf{\Lambda}\mathbf{y} \\
&\geq \max_{\substack{\mathbf{y}\in\mathbb{R}^n, \|\mathbf{y}\|_2=1 \\ (\mathbf{V}^T\mathbf{w})^T\mathbf{y}=0 \\ y_3=y_4=\ldots=y_n=0}} \mathbf{y}^T\mathbf{\Lambda}\mathbf{y} \\
&= \max_{\substack{\mathbf{y}\in\text{span}\{\mathbf{V}^T\mathbf{w}, \mathbf{e}_3, \ldots, \mathbf{e}_n\}^\perp \\ \|\mathbf{y}\|_2=1}} \mathbf{y}^T\mathbf{\Lambda}\mathbf{y}.
\end{aligned} \tag{9}$$

Here, there is a subtle issue that we should pay some attention—Eq. (9) is invalid if the subspace $\text{span}\{\mathbf{V}^T\mathbf{w}, \mathbf{e}_3, \ldots, \mathbf{e}_n\}^\perp$ equals $\{\mathbf{0}\}$. Or, we need to make sure that there exists a nonzero vector $\mathbf{y}$ in $\text{span}\{\mathbf{V}^T\mathbf{w}, \mathbf{e}_3, \ldots, \mathbf{e}_n\}^\perp$, for otherwise problem (9) is infeasible. But since

$$\dim(\text{span}\{\mathbf{V}^T\mathbf{w}, \mathbf{e}_3, \ldots, \mathbf{e}_n\}^\perp) = n - \dim(\text{span}\{\mathbf{V}^T\mathbf{w}, \mathbf{e}_3, \ldots, \mathbf{e}_n\}) \geq n - (n-1) = 1,$$

there always exists a nonzero vector $\mathbf{y} \in \text{span}\{\mathbf{V}^T\mathbf{w}, \mathbf{e}_3, \ldots, \mathbf{e}_n\}^\perp$. From (9), we further get

$$\max_{\substack{\mathbf{y}\in\text{span}\{\mathbf{V}^T\mathbf{w}, \mathbf{e}_3, \ldots, \mathbf{e}_n\}^\perp \\ \|\mathbf{y}\|_2=1}} \mathbf{y}^T\mathbf{\Lambda}\mathbf{y} = \max_{\substack{\mathbf{y}\in\text{span}\{\mathbf{V}^T\mathbf{w}, \mathbf{e}_3, \ldots, \mathbf{e}_n\}^\perp \\ \|\mathbf{y}\|_2=1}} \sum_{i=1}^{2} \lambda_i |y_i|^2 \geq \lambda_2. \tag{10}$$

Combining (9)–(10), we have the following inequality

$$\max_{\substack{\mathbf{x}\in\mathbb{R}^n, \|\mathbf{x}\|_2=1 \\ \mathbf{w}^T\mathbf{x}=0}} \mathbf{x}^T\mathbf{A}\mathbf{x} \geq \lambda_2.$$

Moreover, we notice that the equality above is attained if we choose $\mathbf{w} = \mathbf{v}_1$; specifically this is the consequence of (8). Hence, we have a variational characterization of λ_2 as follows

$$\lambda_2 = \min_{\mathbf{w}\in\mathbb{R}^n} \max_{\substack{\mathbf{x}\in\mathbb{R}^n, \|\mathbf{x}\|_2=1 \\ \mathbf{w}^T\mathbf{x}=0}} \mathbf{x}^T\mathbf{A}\mathbf{x}.$$

The example showcased above is an instance of a more general variational characterization result called the *Courant-Fischer theorem.*

Theorem 4.5 (Courant-Fischer) *Let $\mathbf{A} \in \mathbb{S}^n$, and let $\mathcal{S}_k$ denote any subspace of $\mathbb{R}^n$ and of dimension k. For any $k \in \{1, \ldots, n\}$, it holds that*

$$\lambda_k = \min_{\mathcal{S}_{n-k+1}\subseteq\mathbb{R}^n} \max_{\mathbf{x}\in\mathcal{S}_{n-k+1}, \|\mathbf{x}\|_2=1} \mathbf{x}^T\mathbf{A}\mathbf{x}, \tag{11}$$

$$\lambda_k = \max_{\mathcal{S}_k\subseteq\mathbb{R}^n} \min_{\mathbf{x}\in\mathcal{S}_k, \|\mathbf{x}\|_2=1} \mathbf{x}^T\mathbf{A}\mathbf{x}. \tag{12}$$

Proof: We will show (11) only as the proof of (12) is similar to that of (11) (or take the proof of (12) as a self-practice problem). First, we show that

$$\min_{\mathcal{S}_{n-k+1}\subseteq\mathbb{R}^n} \max_{\mathbf{x}\in\mathcal{S}_{n-k+1}, \|\mathbf{x}\|_2=1} \mathbf{x}^T\mathbf{A}\mathbf{x} \leq \lambda_k. \tag{13}$$

It can be verified that

$$\lambda_k = \max_{\substack{\mathbf{x}\in\text{span}\{\mathbf{v}_k,\ldots,\mathbf{v}_n\}\\ \|\mathbf{x}\|_2=1}} \mathbf{x}^T\mathbf{A}\mathbf{x}.$$

Also, since $\dim(\text{span}\{\mathbf{v}_k,\ldots,\mathbf{v}_n\}) = n-k+1$, which means that $\text{span}\{\mathbf{v}_k,\ldots,\mathbf{v}_n\}$ is feasible to the outer maximization problem on the left-hand side of (13), we obtain (13).

Second, we show that

$$\min_{\mathcal{S}_{n-k+1}\subseteq\mathbb{R}^n} \max_{\mathbf{x}\in\mathcal{S}_{n-k+1},\|\mathbf{x}\|_2=1} \mathbf{x}^T\mathbf{A}\mathbf{x} \geq \lambda_k, \tag{14}$$

and thereby completes the proof. Let

$$\begin{aligned}\mathcal{V} &= \{\mathbf{y} = \mathbf{V}^T\mathbf{x} \mid \mathbf{x}\in\mathcal{S}_{n-k+1}\},\\ \mathcal{W} &= \{\mathbf{y}\in\mathbb{R}^n \mid y_{k+1} = \ldots = y_n = 0\} = \text{span}\{\mathbf{e}_1,\ldots,\mathbf{e}_k\}.\end{aligned}$$

It can be shown that $\dim\mathcal{V} = n-k+1$ for any $\mathcal{S}_{n-k+1}$ and $\dim\mathcal{W} = k$. Also, we will need the following subspace property:

Property 4.4 *Let $\mathcal{S}_1,\mathcal{S}_2$ be subspaces of $\mathbb{R}^n$. If $\dim\mathcal{S}_1+\dim\mathcal{S}_2 > n$, then the intersecting subspace $\mathcal{S}_1\cap\mathcal{S}_2$ must not equal $\{\mathbf{0}\}$ (or have $\dim(\mathcal{S}_1\cap\mathcal{S}_2)\geq 1$).*

Proof of Property 4.4: One can prove this property from the subspace result $\dim\mathcal{S}_1+\dim\mathcal{S}_2-\dim(\mathcal{S}_1\cap\mathcal{S}_2) = \dim(\mathcal{S}_1+\mathcal{S}_2)$. Specifically, we have

$$\dim(\mathcal{S}_1\cap\mathcal{S}_2) = \dim\mathcal{S}_1+\dim\mathcal{S}_2-\dim(\mathcal{S}_1+\mathcal{S}_2) \geq \dim\mathcal{S}_1+\dim\mathcal{S}_2-n.$$

Hence, if $\dim\mathcal{S}_1+\dim\mathcal{S}_2\geq n+1$, the intersecting subspace $\mathcal{S}_1\cap\mathcal{S}_2$ must have dimension no less than one and consequently must not equal $\{\mathbf{0}\}$.

I also show you an alternative proof that does not require the result $\dim\mathcal{S}_1+\dim\mathcal{S}_2-\dim(\mathcal{S}_1\cap\mathcal{S}_2) = \dim(\mathcal{S}_1+\mathcal{S}_2)$. Suppose that $\mathcal{S}_1\cap\mathcal{S}_2 = \{\mathbf{0}\}$, but $\dim\mathcal{S}_1+\dim\mathcal{S}_2\geq n+1$. Let $k = \dim\mathcal{S}_1$, $l = \dim\mathcal{S}_2$, and let $\{\mathbf{a}_1,\ldots,\mathbf{a}_k\}$ and $\{\mathbf{b}_1,\ldots,\mathbf{b}_l\}$ be bases of $\mathcal{S}_1$ and $\mathcal{S}_2$, respectively. The condition $\mathcal{S}_1\cap\mathcal{S}_2 = \{\mathbf{0}\}$ implies that

$$\sum_{i=1}^k \alpha_i\mathbf{a}_i = \sum_{i=1}^l \beta_i\mathbf{b}_i \quad \text{for some } \boldsymbol{\alpha},\boldsymbol{\beta} \quad \Longrightarrow \boldsymbol{\alpha} = \mathbf{0}, \boldsymbol{\beta} = \mathbf{0}. \tag{15}$$

On the other hand, for $k+l\geq n+1$, the vector set $\{\mathbf{a}_1,\ldots,\mathbf{a}_k,\mathbf{b}_1,\ldots,\mathbf{b}_l\}$ must be linearly dependent. This implies that there must exist $\boldsymbol{\alpha},\boldsymbol{\beta}$, with either $\boldsymbol{\alpha}\neq\mathbf{0}$ or $\boldsymbol{\beta}\neq\mathbf{0}$, such that the left-hand side of (15) holds. This contradicts with the implication in (15). ■

By Property 4.4, the intersecting subspace $\mathcal{V}\cap\mathcal{W}$ must contain a nonzero vector for any $\mathcal{S}_{n-k+1}$. Subsequently, we have

$$\begin{aligned}\min_{\mathcal{S}_{n-k+1}\subseteq\mathbb{R}^n} \max_{\mathbf{x}\in\mathcal{S}_{n-k+1},\|\mathbf{x}\|_2=1} \mathbf{x}^T\mathbf{A}\mathbf{x} &= \min_{\mathcal{V}\subseteq\mathbb{R}^n} \max_{\mathbf{y}\in\mathcal{V},\|\mathbf{y}\|_2=1} \mathbf{y}^T\boldsymbol{\Lambda}\mathbf{y}\\ &\geq \min_{\mathcal{V}\subseteq\mathbb{R}^n} \max_{\substack{\mathbf{y}\in\mathcal{V}\cap\mathcal{W}\\ \|\mathbf{y}\|_2=1}} \mathbf{y}^T\boldsymbol{\Lambda}\mathbf{y}\\ &= \min_{\mathcal{V}\subseteq\mathbb{R}^n} \max_{\substack{\mathbf{y}\in\mathcal{V}\cap\mathcal{W}\\ \|\mathbf{y}\|_2=1}} \sum_{i=k}^n \lambda_i|y_i|^2\\ &\geq \lambda_k,\end{aligned}$$

and the proof is complete. ■

1.3 Implications of the Courant-Fischer Theorem

The Courant-Fischer theorem and its proof insight have led a collection of elegant results for eigenvalue inequalities, and here we describe some of them. Let $\mathbf{A}, \mathbf{B} \in \mathbb{S}^n$, $\mathbf{z} \in \mathbb{R}^n$. We have the following results:

(a) (Weyl) $\lambda_k(\mathbf{A}) + \lambda_n(\mathbf{B}) \leq \lambda_k(\mathbf{A} + \mathbf{B}) \leq \lambda_k(\mathbf{A}) + \lambda_1(\mathbf{B})$ for $k = 1, \ldots, n$;

(b) (interlacing) $\lambda_{k+1}(\mathbf{A}) \leq \lambda_k(\mathbf{A} \pm \mathbf{z}\mathbf{z}^T)$ for $k = 1, \ldots, n-1$, and $\lambda_k(\mathbf{A} \pm \mathbf{z}\mathbf{z}^T) \leq \lambda_{k-1}(\mathbf{A})$ for $k = 2, \ldots, n$;

(c) if $\text{rank}(\mathbf{B}) \leq r$, then $\lambda_{k+r}(\mathbf{A}) \leq \lambda_k(\mathbf{A} + \mathbf{B})$ for $k = 1, \ldots, n-r$ and $\lambda_k(\mathbf{A} + \mathbf{B}) \leq \lambda_{k-r}(\mathbf{A})$ for $k = r+1, \ldots, n$;

(d) (Weyl) $\lambda_{j+k-1}(\mathbf{A} + \mathbf{B}) \leq \lambda_j(\mathbf{A}) + \lambda_k(\mathbf{B})$ for $j, k \in \{1, \ldots, n\}$ with $j + k \leq n + 1$;

(e) for any $\mathcal{I} = \{i_1, \ldots, i_r\} \subseteq \{1, \ldots, n\}$, $\lambda_{k+n-r}(\mathbf{A}) \leq \lambda_k(\mathbf{A}_{\mathcal{I}}) \leq \lambda_k(\mathbf{A})$ for $k = 1, \ldots, r$.

(f) for any semi-orthogonal $\mathbf{U} \in \mathbb{R}^{n \times r}$, $\lambda_{k+n-r}(\mathbf{A}) \leq \lambda_k(\mathbf{U}^T\mathbf{A}\mathbf{U}) \leq \lambda_k(\mathbf{A})$ for $k = 1, \ldots, r$.

The details of the proof of the above results are left as self-practice problems for you, and here are some hints: Result (a) is obtained by applying (3) to (11). Result (b) is shown via the Courier-Fischer theorem; specifically we have

$$
\begin{aligned}
\lambda_k(\mathbf{A} \pm \mathbf{z}\mathbf{z}^T) &= \min_{\mathcal{S}_{n-k+1} \subseteq \mathbb{R}^n} \ \max_{\mathbf{x} \in \mathcal{S}_{n-k+1}, \|\mathbf{x}\|_2 = 1} \mathbf{x}^T(\mathbf{A} \pm \mathbf{z}\mathbf{z}^T)\mathbf{x} \\
&\geq \min_{\mathcal{S}_{n-k+1} \subseteq \mathbb{R}^n} \ \max_{\mathbf{x} \in \mathcal{S}_{n-k+1} \cap \mathcal{R}(\mathbf{z})^\perp, \|\mathbf{x}\|_2 = 1} \mathbf{x}^T\mathbf{A}\mathbf{x} \\
&\geq \min_{\substack{\mathcal{S}_r \subseteq \mathbb{R}^n \\ n-k \leq r}} \ \max_{\mathbf{x} \in \mathcal{S}_r, \|\mathbf{x}\|_2 = 1} \mathbf{x}^T\mathbf{A}\mathbf{x} \\
&= \lambda_{k+1}(\mathbf{A}),
\end{aligned}
$$

where the second inequality is obtained by showing that $\dim(\mathcal{S}_{n-k+1} \cap \mathcal{R}(\mathbf{z})^\perp) \geq n - k$ (use the result $\dim \mathcal{S}_1 + \dim \mathcal{S}_2 - \dim(\mathcal{S}_1 \cap \mathcal{S}_2) = \dim(\mathcal{S}_1 + \mathcal{S}_2)$). Result (c) is shown by applying Result (b) and using the fact that a matrix $\mathbf{B} \in \mathbb{S}^n$ with $\text{rank}(\mathbf{B}) \leq r$ can be written as a sum of r outer products $\mathbf{B} = \sum_{i=1}^r \mu_i \mathbf{u}_i\mathbf{u}_i^T$. Result (d) is proven by applying Result (c). For Result (e), consider the case of $\mathcal{I} = \{1, \ldots, r\}$ for ease of exposition of ideas. We have

$$
\begin{aligned}
\lambda_k(\mathbf{A}) &\geq \min_{\mathcal{S}_{n-k+1} \subseteq \mathbb{R}^n} \ \max_{\substack{\mathbf{x} \in \mathcal{S}_{n-k+1} \cap \text{span}\{\mathbf{e}_1, \ldots, \mathbf{e}_r\} \\ \|\mathbf{x}\|_2 = 1}} \mathbf{x}^T\mathbf{A}\mathbf{x} \\
&\geq \min_{\substack{\mathcal{S}_l \subseteq \mathbb{R}^r \\ r-k+1 \leq l}} \ \max_{\mathbf{y} \in \mathcal{S}_l, \ \|\mathbf{y}\|_2 = 1} \mathbf{y}^T\mathbf{A}_{\mathcal{I}}\mathbf{y} \\
&= \lambda_k(\mathbf{A}_{\mathcal{I}}),
\end{aligned}
$$

where one needs to show that $\dim(\mathcal{S}_{n-k+1} \cap \text{span}\{\mathbf{e}_1, \ldots, \mathbf{e}_r\}) \geq r - k + 1$; some care also needs to be taken as we change the vector dimension in the second equation above. Result (f) is a consequence of Result (e).

1.4 Maximization of a Sum of Rayleigh Quotients

In the previous subsections we consider maximization or minimization of a Rayleigh quotient. Here we are interested in a problem concerning a sum of Rayleigh quotients:

$$\max_{\substack{\mathbf{U}\in\mathbb{R}^{n\times r}\\ \mathbf{u}_i\neq\mathbf{0}\ \forall i,\ \mathbf{u}_i^T\mathbf{u}_j=0\ \forall i\neq j}} \sum_{i=1}^{r}\frac{\mathbf{u}_i^T\mathbf{A}\mathbf{u}_i}{\mathbf{u}_i^T\mathbf{u}_i}, \tag{16}$$

where we want the vectors $\mathbf{u}_1,\dots\mathbf{u}_r$ of the Rayleigh quotients to be orthogonal to each other. This problem finds applications in matrix factorization and PCA, as we will see in the next lecture. As in the previous treatment for Rayleigh quotients, we can rewrite problem (16) as

$$\begin{aligned}\max_{\substack{\mathbf{U}\in\mathbb{R}^{n\times r}\\ \mathbf{u}_i\neq\mathbf{0}\ \forall i,\ \mathbf{u}_i^T\mathbf{u}_j=0\ \forall i\neq j}} \sum_{i=1}^{r}\frac{\mathbf{u}_i^T\mathbf{A}\mathbf{u}_i}{\mathbf{u}_i^T\mathbf{u}_i} &= \max_{\substack{\mathbf{U}\in\mathbb{R}^{n\times r}\\ \|\mathbf{u}_i\|_2=1\ \forall i,\ \mathbf{u}_i^T\mathbf{u}_j=0\ \forall i\neq j}} \sum_{i=1}^{r}\mathbf{u}_i^T\mathbf{A}\mathbf{u}_i \\ &= \max_{\substack{\mathbf{U}\in\mathbb{R}^{n\times r}\\ \mathbf{U}^T\mathbf{U}=\mathbf{I}}} \operatorname{tr}(\mathbf{U}^T\mathbf{A}\mathbf{U}), \end{aligned}\tag{17}$$

The following result describes an equivalence relation between problem (17) and eigenvalues.

Theorem 4.6 *Let $\mathbf{A}\in\mathbb{S}^n$. It holds that*

$$\sum_{i=1}^{r}\lambda_i = \max_{\substack{\mathbf{U}\in\mathbb{R}^{n\times r}\\ \mathbf{U}^T\mathbf{U}=\mathbf{I}}} \operatorname{tr}(\mathbf{U}^T\mathbf{A}\mathbf{U}). \tag{18}$$

Proof: This theorem can be easily shown by Result (f) in Section 1.3. Specifically, for any semi-orthogonal $\mathbf{U}\in\mathbb{R}^{n\times r}$ we have

$$\operatorname{tr}(\mathbf{U}^T\mathbf{A}\mathbf{U}) = \sum_{i=1}^{r}\lambda_i(\mathbf{U}^T\mathbf{A}\mathbf{U}) \leq \sum_{i=1}^{r}\lambda_i(\mathbf{A}), \tag{19}$$

where the inequality is owing to Result (f) in Section 1.3. Since the equality in (19) is attained by $\mathbf{U} = [\ \mathbf{v}_1,\dots,\mathbf{v}_r]$, we obtain the desired result.

To enrich your understanding of this topic, I also show you an alternative proof which does not use Result (f) in Section 1.3. In essence, the main challenge lies in showing (19). Consider the following problem

$$\max_{\substack{\mathbf{U}\in\mathbb{R}^{n\times r}\\ \mathbf{U}^T\mathbf{U}=\mathbf{I}}} \operatorname{tr}(\mathbf{U}^T\boldsymbol{\Lambda}\mathbf{U}).$$

It can be shown that the above problem is equivalent to the problem on the right-hand side of (18). Now, observe that

$$\operatorname{tr}(\mathbf{U}^T\boldsymbol{\Lambda}\mathbf{U}) = \operatorname{tr}(\mathbf{U}\mathbf{U}^T\boldsymbol{\Lambda}) = \sum_{i=1}^{n}[\mathbf{U}\mathbf{U}^T]_{ii}\lambda_i,$$

and that for any semi-orthogonal $\mathbf{U}\in\mathbb{R}^{n\times r}$ we have

$$[\mathbf{U}\mathbf{U}^T]_{ii} = \mathbf{e}_i^T\mathbf{U}_i\mathbf{U}_i^T\mathbf{e}_i = \|\mathbf{U}_i^T\mathbf{e}_i\|_2^2 \leq \|\mathbf{e}_i\|_2^2 = 1,$$

$$\sum_{i=1}^{n}[\mathbf{U}\mathbf{U}^T]_{ii} = \operatorname{tr}(\mathbf{U}\mathbf{U}^T) = \operatorname{tr}(\mathbf{U}^T\mathbf{U}) = r.$$

This leads us to consider a relaxation

$$\max_{\mathbf{U}\in\mathbb{R}^{n\times r},\ \mathbf{U}^T\mathbf{U}=\mathbf{I}} \operatorname{tr}(\mathbf{U}^T\mathbf{\Lambda}\mathbf{U}) \leq \begin{array}{rl} \max\limits_{\mathbf{x}\in\mathbb{R}^n} & \sum\limits_{i=1}^n x_i\lambda_i \\ \text{s.t.} & 0 \leq x_i \leq 1,\ i=1,\dots,n \\ & \sum\limits_{i=1}^n x_i = r \end{array}$$

In particular, we replace every $[\mathbf{U}\mathbf{U}^T]_{ii}$ by x_i. One can easily see that the optimal value of the problem on the right-hand side of the above equation is $\sum_{i=1}^r \lambda_i$. Hence, we have shown (19). ■

2 Matrix Inequalities

In this section the aim is to give the proof of some of the results we mentioned in PSD matrix inequalities in the main lecture slides. To be specific, let $\mathbf{A},\mathbf{B}\in\mathbb{S}^n$ and recall the following results.

(a) $\mathbf{A}\succeq\mathbf{B}$ implies $\lambda_k(\mathbf{A})\geq\lambda_k(\mathbf{B})$ for $k=1,\dots,n$.

(b) $\mathbf{A}\succeq\mathbf{I}$ is equivalent to $\lambda_k(\mathbf{A})\geq 1$ for $k=1,\dots,n$. Also, $\mathbf{A}\succ\mathbf{I}$ is equivalent to $\lambda_k(\mathbf{A})>1$ for $k=1,\dots,n$.

(c) $\mathbf{I}\succeq\mathbf{A}$ is equivalent to $\lambda_k(\mathbf{A})\leq 1$ for $k=1,\dots,n$. Also, $\mathbf{I}\succ\mathbf{A}$ is equivalent to $\lambda_k(\mathbf{A})<1$ for $k=1,\dots,n$.

(d) If $\mathbf{A},\mathbf{B}\succ\mathbf{0}$ then $\mathbf{A}\succeq\mathbf{B}$ is equivalent to $\mathbf{B}^{-1}\succeq\mathbf{A}^{-1}$.

(e) (The Schur complement) Let

$$\mathbf{X}=\begin{bmatrix}\mathbf{A} & \mathbf{B}\\ \mathbf{B}^T & \mathbf{C}\end{bmatrix},$$

where $\mathbf{A}\in\mathbb{S}^m$, $\mathbf{B}\in\mathbb{R}^{m\times n}$, $\mathbf{C}\in\mathbb{S}^n$ with $\mathbf{C}\succ\mathbf{0}$, and denote $\mathbf{S}=\mathbf{A}-\mathbf{B}\mathbf{C}^{-1}\mathbf{B}^T$. It holds that

$$\mathbf{X}\succeq\mathbf{0} \quad\Longleftrightarrow\quad \mathbf{S}\succeq\mathbf{0}$$

Also, we have $\mathbf{X}\succ\mathbf{0}\Longleftrightarrow\mathbf{S}\succ\mathbf{0}$.

The proof is as follows.

Proof of (a): Suppose $\mathbf{A}\succeq\mathbf{B}$. We have, for any $k\in\{1,\dots,n\}$,

$$\lambda_k(\mathbf{A})=\lambda_k(\mathbf{B}+\mathbf{A}-\mathbf{B})\geq\lambda_k(\mathbf{B})+\lambda_n(\mathbf{A}-\mathbf{B})\geq\lambda_k(\mathbf{B}).$$

where the first inequality is due to Weyl's inequality, and the second inequality is because $\mathbf{A}-\mathbf{B}$ is PSD.

Proof of (b): Consider the matrix $\mathbf{A}-\mathbf{I}$. Since $\mathbf{A}-\mathbf{I}=\mathbf{V}(\mathbf{\Lambda}-\mathbf{I})\mathbf{V}^T$, the eigenvalues of $\mathbf{A}-\mathbf{I}$ are $\lambda_1-1,\dots,\lambda_n-1$. It follows that $\mathbf{A}-\mathbf{I}$ is PSD if and only if $\lambda_k-1\geq 0$ for all k, and that $\mathbf{A}-\mathbf{I}$ is PD if and only if $\lambda_k-1>0$ for all k.

Proof of (c): The proof is the same as that of (b) and is omitted for brevity.

Proof of (d): Since $\mathbf{A}$ is PD, its square root $\mathbf{A}^{1/2}$ is invertible. We have

$$\mathbf{A} - \mathbf{B} \succeq \mathbf{0} \iff \mathbf{A}^{1/2}(\mathbf{I} - \mathbf{A}^{-1/2}\mathbf{B}\mathbf{A}^{-1/2})\mathbf{A}^{1/2} \succeq \mathbf{0} \iff \mathbf{I} - \mathbf{A}^{-1/2}\mathbf{B}\mathbf{A}^{-1/2} \succeq \mathbf{0} \tag{20}$$

where Theorem 4.3 has been used to obtain the second equivalence. Let $\mathbf{C} = \mathbf{A}^{-1/2}\mathbf{B}\mathbf{A}^{-1/2}$, and denote its eigendecomposition as $\mathbf{C} = \mathbf{Q}\mathbf{D}\mathbf{Q}^T$ where $\mathbf{D} = \mathrm{Diag}(d_1, \ldots, d_n)$. Since $\mathbf{B}$ is PD and $\mathbf{A}^{1/2}$ is invertible, by Theorem 4.3 $\mathbf{C}$ is PD; hence, we have $d_k > 0$ for all k. From the right-hand side of (20) we further show the following equivalence

$$\begin{aligned}
\mathbf{I} - \mathbf{C} \succeq \mathbf{0} &\iff 1 \geq d_k,\ k = 1, \ldots, n \\
&\iff \frac{1}{d_k} \geq 1,\ k = 1, \ldots, n \\
&\iff \mathbf{D}^{-1} \succeq \mathbf{I} \\
&\iff \mathbf{Q}(\mathbf{D}^{-1} - \mathbf{I})\mathbf{Q}^T \succeq \mathbf{0} \\
&\iff \mathbf{C}^{-1} - \mathbf{I} \succeq \mathbf{0} \\
&\iff \mathbf{A}^{1/2}\mathbf{B}^{-1}\mathbf{A}^{1/2} - \mathbf{I} \succeq \mathbf{0} \\
&\iff \mathbf{B}^{-1} - \mathbf{A}^{-1} \succeq \mathbf{0},
\end{aligned}$$

where we have applied Theorem 4.3 multiple times and Results (b)–(c).

Proof of (e): Let

$$\mathbf{Y} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{C}^{-1}\mathbf{B}^T & \mathbf{I} \end{bmatrix}.$$

One can verify that

$$\mathbf{Y}^T\mathbf{X}\mathbf{Y} = \begin{bmatrix} \mathbf{A} - \mathbf{B}\mathbf{C}^{-1}\mathbf{B}^T & \mathbf{0} \\ \mathbf{0} & \mathbf{C} \end{bmatrix}.$$

Also, $\mathbf{Y}$ is nonsingular; from the block triangular structure of $\mathbf{Y}$ we see that $\det(\mathbf{Y}) = 1$. Hence, by Theorem 4.3, $\mathbf{X}$ is PSD if and only if $\mathbf{Y}^T\mathbf{X}\mathbf{Y} \succeq \mathbf{0}$. The condition $\mathbf{Y}^T\mathbf{X}\mathbf{Y} \succeq \mathbf{0}$ is equivalent to $\mathbf{A} - \mathbf{B}\mathbf{C}^{-1}\mathbf{B} \succeq \mathbf{0}$ and $\mathbf{C} \succeq \mathbf{0}$, and hence we have shown the desired result for the PSD case. The PD case is shown by the same manner.