# ENGG5781 Matrix Analysis and Computations Lecture 4: Positive Semidefinite Matrices and Variational Characterizations of Eigenvalues 

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## Lecture 4: Positive Semidefinite Matrices and Variational Characterizations of Eigenvalues

- positive semidefinite matrices
- application: subspace method for super-resolution spectral analysis
- application: Euclidean distance matrices
- variational characterizations of eigenvalues of real symmetric matrices
- matrix inequalities


## Hightlights

- a matrix $\mathbf{A} \in \mathbb{S}^{n}$ is said to be positive semidefinite (PSD) if

$$
\mathbf{x}^{T} \mathbf{A} \mathbf{x} \geq 0, \quad \text { for all } \mathbf{x} \in \mathbb{R}^{n}
$$

and positive definite (PD) if

$$
\mathbf{x}^{T} \mathbf{A} \mathbf{x}>0, \quad \text { for all } \mathbf{x} \in \mathbb{R}^{n} \text { with } \mathbf{x} \neq \mathbf{0}
$$

- a matrix $\mathbf{A} \in \mathbb{S}^{n}$ is PSD (resp. PD)
- if and only if its eigenvalues are all non-negative (resp. positive);
- if and only if it can be factored as $\mathbf{A}=\mathbf{B}^{T} \mathbf{B}$ for some $\mathbf{B} \in \mathbb{R}^{m \times n}$


## Highlights

- let $\mathbf{A} \in \mathbb{S}^{n}$, and let $\lambda_{1}(\mathbf{A}), \ldots, \lambda_{n}(\mathbf{A})$ be the eigenvalues of $\mathbf{A}$ with ordering

$$
\lambda_{\max }(\mathbf{A})=\lambda_{1}(\mathbf{A}) \geq \lambda_{2}(\mathbf{A}) \geq \cdots \geq \lambda_{n}(\mathbf{A})=\lambda_{\min }(\mathbf{A})
$$

where $\lambda_{\min }(\mathbf{A})$ and $\lambda_{\max }(\mathbf{A})$ denote the min. and max. eigenvalues of $\mathbf{A}$, resp.

- variational characterizations of $\lambda_{\min }(\mathbf{A})$ and $\lambda_{\max }(\mathbf{A})$ :

$$
\lambda_{\max }(\mathbf{A})=\max _{\mathbf{x} \in \mathbb{R}^{n},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x}, \quad \lambda_{\min }(\mathbf{A})=\min _{\mathbf{x} \in \mathbb{R}^{n},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x}
$$

- (Courant-Fischer) for $k \in\{1, \ldots, n\}$,

$$
\lambda_{k}(\mathbf{A})=\min _{\mathcal{S}_{n-k+1} \subseteq \mathbb{R}^{n}} \max _{\mathbf{x} \in \mathcal{S}_{n-k+1},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x}=\max _{\mathcal{S}_{k} \subseteq \mathbb{R}^{n}} \min _{\mathbf{x} \in \mathcal{S}_{k},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x}
$$

where $\mathcal{S}_{k}$ denotes a subspace of dimension $k$

- complex case: the same results apply; replace $\mathbb{R}$ by $\mathbb{C}, \mathbb{S}$ by $\mathbb{H}$, and " $T$ " by " $H$ "


## Quadratic Form

Let $\mathbf{A} \in \mathbb{S}^{n}$. For $\mathbf{x} \in \mathbb{R}^{n}$, the matrix product

$$
\mathbf{x}^{T} \mathbf{A} \mathbf{x}
$$

is called a quadratic form.

- some basic facts (try to verify):
$-\mathbf{x}^{T} \mathbf{A} \mathbf{x}=\sum_{i=1}^{n} \sum_{j=1}^{n} x_{i} x_{j} a_{i j}$
- it suffices to consider symmetric $\mathbf{A}$ since for general $\mathbf{A} \in \mathbb{R}^{n \times n}$,

$$
\mathbf{x}^{T} \mathbf{A} \mathbf{x}=\mathbf{x}^{T}\left[\frac{1}{2}\left(\mathbf{A}+\mathbf{A}^{T}\right)\right] \mathbf{x}
$$

- complex case:
* the quadratic form is defined as $\mathbf{x}^{H} \mathbf{A} \mathbf{x}$, where $\mathbf{x} \in \mathbb{C}^{n}$
* for $\mathbf{A} \in \mathbb{H}^{n}, \mathbf{x}^{H} \mathbf{A} \mathbf{x}$ is real for any $\mathbf{x} \in \mathbb{C}^{n}$


## Positive Semidefinite Matrices

A matrix $\mathbf{A} \in \mathbb{S}^{n}$ is said to be

- positive semidefinite (PSD) if $\mathbf{x}^{T} \mathbf{A} \mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^{n}$
- positive definite (PD) if $\mathbf{x}^{T} \mathbf{A} \mathbf{x}>0$ for all $\mathbf{x} \in \mathbb{R}^{n}$ with $\mathbf{x} \neq \mathbf{0}$
- indefinite if $\mathbf{A}$ is not PSD

Notation:

- $\mathbf{A} \succeq \mathbf{0}$ means that $\mathbf{A}$ is PSD
- $\mathbf{A} \succ \mathbf{0}$ means that $\mathbf{A}$ is PD
- $\mathbf{A} \nsucceq \mathbf{0}$ means that $\mathbf{A}$ is indefinite


## Example: Covariance Matrices

- let $\mathbf{y}_{0}, \mathbf{y}_{2}, \ldots \mathbf{y}_{T-1} \in \mathbb{R}^{n}$ be a sequence of multi-dimensional data samples
- examples: patches in image processing, multi-channel signals in signal processing, history of returns of assets in finance [Brodie-Daubechies-et al.'09],
- sample mean: $\hat{\boldsymbol{\mu}}_{y}=\frac{1}{T} \sum_{t=0}^{T-1} \mathbf{y}_{t}$
- sample covariance: $\hat{\mathbf{C}}_{y}=\frac{1}{T} \sum_{t=0}^{T-1}\left(\mathbf{y}_{t}-\hat{\boldsymbol{\mu}}_{y}\right)\left(\mathbf{y}_{t}-\hat{\boldsymbol{\mu}}_{y}\right)^{T}$
- a sample covariance is PSD: $\mathbf{x}^{T} \hat{\mathbf{C}}_{y} \mathbf{x}=\frac{1}{T} \sum_{t=0}^{T-1}\left|\left(\mathbf{y}_{t}-\hat{\boldsymbol{\mu}}_{y}\right)^{T} \mathbf{x}\right|^{2} \geq 0$
- the (statistical) covariance of $\mathbf{y}_{t}$ is also PSD
- to put into context, assume that $\mathbf{y}_{t}$ is a wide-sense stationary random process
- the covariance, defined as $\mathbf{C}_{y}=\mathrm{E}\left[\left(\mathbf{y}_{t}-\boldsymbol{\mu}_{y}\right)\left(\mathbf{y}_{t}-\boldsymbol{\mu}_{y}\right)^{T}\right]$ where $\boldsymbol{\mu}_{y}=\mathrm{E}\left[\mathbf{y}_{t}\right]$, can be shown to be PSD


## Example: Hessian

- let $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$ be a twice differentiable function
- the Hessian of $f$, denoted by $\nabla^{2} f(\mathbf{x}) \in \mathbb{S}^{n}$, is a matrix whose $(i, j)$ th entry is given by

$$
\left[\nabla^{2} f(\mathbf{x})\right]_{i, j}=\frac{\partial^{2} f}{\partial x_{i} \partial x_{j}}
$$

- Fact: $f$ is convex if and only if $\nabla^{2} f(\mathbf{x}) \succeq \mathbf{0}$ for all $\mathbf{x}$ in the problem domain
- example: consider the quadratic function

$$
f(\mathbf{x})=\frac{1}{2} \mathbf{x}^{T} \mathbf{R} \mathbf{x}+\mathbf{q}^{T} \mathbf{x}+c
$$

It can be verified that $\nabla^{2} f(\mathbf{x})=\mathbf{R}$. Thus, $f$ is convex if and only if $\mathbf{R} \succeq \mathbf{0}$

## Illustration of Quadratic Functions



## PSD Matrices and Eigenvalues

Theorem 4.1. Let $\mathbf{A} \in \mathbb{S}^{n}$, and let $\lambda_{1}, \ldots, \lambda_{n}$ be the eigenvalues of $\mathbf{A}$. We have

1. $\mathbf{A} \succeq \mathbf{0} \Longleftrightarrow \lambda_{i} \geq 0$ for $i=1, \ldots, n$
2. $\mathbf{A} \succ \mathbf{0} \Longleftrightarrow \lambda_{i}>0$ for $i=1, \ldots, n$

- proof: let $\mathbf{A}=\mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^{T}$ be the eigendecomposition of $\mathbf{A}$.

$$
\begin{aligned}
\mathbf{A} \succeq \mathbf{0} & \Longleftrightarrow \mathbf{x}^{T} \mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^{T} \mathbf{x} \geq 0, \quad \text { for all } \mathbf{x} \in \mathbb{R}^{n} \\
& \Longleftrightarrow \mathbf{z}^{T} \boldsymbol{\Lambda} \mathbf{z} \geq 0, \quad \text { for all } \mathbf{z} \in \mathcal{R}\left(\mathbf{V}^{T}\right)=\mathbb{R}^{n} \\
& \Longleftrightarrow \sum_{i=1}^{n} \lambda_{i}\left|z_{i}\right|^{2} \geq 0, \quad \text { for all } \mathbf{z} \in \mathbb{R}^{n} \\
& \Longleftrightarrow \lambda_{i} \geq 0 \text { for all } i
\end{aligned}
$$

The PD case is proven by the same manner.

## Example: Ellipsoid

- an ellipsoid of $\mathbb{R}^{n}$ is defined as

$$
\mathcal{E}=\left\{\mathbf{x} \in \mathbb{R}^{n} \mid \mathbf{x}^{T} \mathbf{P}^{-1} \mathbf{x} \leq 1\right\}
$$

for some PD $\mathbf{P} \in \mathbb{S}^{n}$


- let $\mathbf{P}=\mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^{T}$ be the eigendecomposition
- V determines the directions of the semi-axes
- $\lambda_{1}, \ldots, \lambda_{n}$ determine the lengths of the semi-axes


## Example: Multivariate Gaussian Distribution

- probability density function for a Gaussian-distributed vector $\mathbf{x} \in \mathbb{R}^{n}$ :

$$
p(\mathbf{x})=\frac{1}{(2 \pi)^{\frac{n}{2}}(\operatorname{det}(\boldsymbol{\Sigma}))^{\frac{1}{2}}} \exp \left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{T} \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)
$$

where $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are the mean and covariance of $\mathbf{x}$, resp.
$-\boldsymbol{\Sigma}$ is PD

- $\boldsymbol{\Sigma}$ determines how $\mathbf{x}$ is spread, by the same way as in ellipsoid


## Example: Multivariate Gaussian Distribution


(a) $\boldsymbol{\mu}=\mathbf{0}, \boldsymbol{\Sigma}=\left[\begin{array}{ll}1 & 0 \\ 0 & 1\end{array}\right]$.
(b) $\boldsymbol{\mu}=\mathbf{0}, \boldsymbol{\Sigma}=\left[\begin{array}{cc}1 & 0.8 \\ 0.8 & 1\end{array}\right]$.


## PSD Matrices and Square Root

Theorem 4.2. A matrix $\mathbf{A} \in \mathbb{S}^{n}$ is PSD if and only if it can be factored as

$$
\mathbf{A}=\mathbf{B}^{T} \mathbf{B}
$$

for some $\mathbf{B} \in \mathbb{R}^{m \times n}$ and for some positive integer $m$.

- proof:
- sufficiency: $\mathbf{A}=\mathbf{B}^{T} \mathbf{B} \Longrightarrow \mathbf{x}^{T} \mathbf{A} \mathbf{x}=\mathbf{x}^{T} \mathbf{B}^{T} \mathbf{B} \mathbf{x}=\|\mathbf{B x}\|_{2}^{2} \geq 0$ for all $\mathbf{x}$
- necessity: let $\boldsymbol{\Lambda}^{1 / 2}=\operatorname{Diag}\left(\lambda_{1}^{1 / 2}, \ldots, \lambda_{n}^{1 / 2}\right)$.

$$
\mathbf{A} \succeq \mathbf{0} \Longrightarrow \mathbf{A}=\left(\mathbf{V} \boldsymbol{\Lambda}^{1 / 2}\right)\left(\boldsymbol{\Lambda}^{1 / 2} \mathbf{V}^{T}\right), \text { with } \boldsymbol{\Lambda}^{1 / 2} \mathbf{V}^{T} \text { being real }
$$

## PSD Matrices and Square Root

- the factorization $\mathbf{A}=\mathbf{B}^{T} \mathbf{B}$ has non-unique factor $\mathbf{B}$
- for any orthogonal $\mathbf{U} \in \mathbb{R}^{n \times n}, \mathbf{B}=\mathbf{U} \boldsymbol{\Lambda}^{1 / 2} \mathbf{V}^{T}$ is a factor for $\mathbf{A}=\mathbf{B}^{T} \mathbf{B}$
- denote

$$
\mathbf{A}^{1 / 2}=\mathbf{V} \mathbf{\Lambda}^{1 / 2} \mathbf{V}^{T}
$$

$-\mathbf{B}=\mathbf{A}^{1 / 2}$ is a factor for $\mathbf{A}=\mathbf{B}^{T} \mathbf{B}$

- $\mathbf{A}^{1 / 2}$ is also a symmetric factor
- $\mathbf{A}^{1 / 2}$ is the unique $P S D$ factor for $\mathbf{A}=\mathbf{B}^{T} \mathbf{B}$ (how to prove it?)
- $\mathbf{A}^{1 / 2}$ is called the PSD square root of $\mathbf{A}$
- note: in general, a matrix $\mathbf{B} \in \mathbb{R}^{n \times n}$ is said to be a square root of another matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ if $\mathbf{A}=\mathbf{B}^{2}$


## Some Properties of PSD Matrices

- it can be directly seen from the definition that
- $\mathbf{A} \succeq \mathbf{0} \Longrightarrow a_{i i} \geq 0$ for all $i$
- $\mathbf{A} \succ \mathbf{0} \Longrightarrow a_{i i}>0$ for all $i$
- extension (also direct): partition $\mathbf{A}$ as

$$
\mathbf{A}=\left[\begin{array}{ll}
\mathbf{A}_{11} & \mathbf{A}_{12} \\
\mathbf{A}_{21} & \mathbf{A}_{22}
\end{array}\right]
$$

Then, $\mathbf{A} \succeq \mathbf{0} \Longrightarrow \mathbf{A}_{11} \succeq \mathbf{0}, \mathbf{A}_{22} \succeq \mathbf{0}$. Also, $\mathbf{A} \succ \mathbf{0} \Longrightarrow \mathbf{A}_{11} \succ \mathbf{0}, \mathbf{A}_{22} \succ \mathbf{0}$

- further extension:
- a principal submatrix of $\mathbf{A}$, denoted by $\mathbf{A}_{\mathcal{I}}$, where $\mathcal{I}=\left\{i_{1}, \ldots, i_{m}\right\} \subseteq$ $\{1, \ldots, n\}, m<n$, is a submatrix obtained by keeping only the rows and columns indicated by $\mathcal{I}$; i.e., $\left[\mathbf{A}_{\mathcal{I}}\right]_{j k}=a_{i_{j}, i_{k}}$ for all $j, k \in\{1, \ldots, m\}$
- if $\mathbf{A}$ is PSD (resp. PD), then any principal submatrix of $\mathbf{A}$ is PSD (resp. PD)


## Some Properties of PSD Matrices

Property 4.1. Let $\mathbf{A} \in \mathbb{S}^{n}, \mathbf{B} \in \mathbb{R}^{n \times m}$, and

$$
\mathbf{C}=\mathbf{B}^{T} \mathbf{A B}
$$

We have the following properties:

1. $\mathbf{A} \succeq \mathbf{0} \Longrightarrow \mathbf{C} \succeq \mathbf{0}$
2. suppose $\mathbf{A} \succ \mathbf{0}$. It holds that $\mathbf{C} \succ \mathbf{0} \Longleftrightarrow \mathbf{B}$ has full column rank
3. suppose $\mathbf{B}$ is nonsingular. It holds that $\mathbf{A} \succ \mathbf{0} \Longleftrightarrow \mathbf{C} \succ \mathbf{0}$, and that $\mathbf{A} \succeq \mathbf{0} \Longleftrightarrow$ $\mathbf{C} \succeq 0$.

- proof sketch: the 1st property is trivial. For the 2nd property, observe

$$
\begin{equation*}
\mathbf{C} \succ \mathbf{0} \Longleftrightarrow \mathbf{z}^{T} \mathbf{A} \mathbf{z}>\mathbf{0}, \forall \mathbf{z} \in \mathcal{R}(\mathbf{B}) \backslash\{\mathbf{0}\} . \tag{*}
\end{equation*}
$$

If $\mathbf{A} \succ \mathbf{0},(*)$ reduces to $\mathbf{C} \succ \mathbf{0} \Longleftrightarrow \mathbf{B x} \neq \mathbf{0}, \forall \mathbf{x} \neq \mathbf{0}$ (or $\mathbf{B}$ has full column rank). The 3rd property is proven by the similar manner.

## Properties for Symmetric Factorization

Property 4.2. Let $\mathbf{A} \in \mathbb{R}^{m \times k}$ and $\mathbf{B} \in \mathbb{R}^{k \times n}$, and suppose that $\mathbf{B}$ has full row rank. Then

$$
\mathcal{R}(\mathbf{A B})=\mathcal{R}(\mathbf{A})
$$

- proof:
- observe that $\operatorname{dim} \mathcal{R}(\mathbf{B})=\operatorname{rank}(\mathbf{B})=k$, which implies $\mathcal{R}(\mathbf{B})=\mathbb{R}^{k}$.
- we have $\mathcal{R}(\mathbf{A B})=\{\mathbf{y}=\mathbf{A} \mathbf{z} \mid \mathbf{z} \in \mathcal{R}(\mathbf{B})\}=\left\{\mathbf{y}=\mathbf{A} \mathbf{z} \mid \mathbf{z} \in \mathbb{R}^{k}\right\}=\mathcal{R}(\mathbf{A})$.
- corollary: let $\mathbf{R}$ be a PSD matrix. Suppose that we factor $\mathbf{R}$ as $\mathbf{R}=\mathbf{B B}^{T}$ for some full-column rank $\mathbf{B}$. Then, $\mathcal{R}(\mathbf{R})=\mathcal{R}(\mathbf{B})$.


## Properties for Symmetric Factorization

Property 4.3. Let $\mathbf{B} \in \mathbb{R}^{n \times k}, \mathbf{C} \in \mathbb{R}^{n \times k}$ be full-column rank matrices. It holds that

$$
\mathbf{B B}^{T}=\mathbf{C C}^{T} \Longleftrightarrow \mathbf{C}=\mathbf{B Q} \text { for some orthogonal } \mathbf{Q} \in \mathbb{R}^{k \times k}
$$

- proof: we consider " $\Longrightarrow$ " only, as " $\Longleftarrow$ " is trivial
- suppose $\mathbf{B B}^{T}=\mathbf{C C}^{T}$.
- from

$$
\mathbf{I}=\left(\mathbf{B}^{\dagger} \mathbf{B}\right)\left(\mathbf{B}^{\dagger} \mathbf{B}\right)^{T}=\mathbf{B}^{\dagger}\left(\mathbf{B B}^{T}\right)\left(\mathbf{B}^{\dagger}\right)^{T}=\mathbf{B}^{\dagger}\left(\mathbf{C} \mathbf{C}^{T}\right)\left(\mathbf{B}^{\dagger}\right)^{T}=\left(\mathbf{B}^{\dagger} \mathbf{C}\right)\left(\mathbf{B}^{\dagger} \mathbf{C}\right)^{T}
$$

we see that $\mathbf{B}^{\dagger} \mathbf{C}$ is orthogonal (note that $\mathbf{B}^{\dagger} \mathbf{C}$ is square).

- let $\mathbf{Q}=\mathbf{B}^{\dagger} \mathbf{C}$. We have $\mathbf{B Q}=\mathbf{B B}^{\dagger} \mathbf{C}=\mathbf{P}_{\mathbf{B}} \mathbf{C}$, or equivalently,

$$
\mathbf{B} \mathbf{q}_{i}=\Pi_{\mathcal{R}(\mathbf{B})}\left(\mathbf{c}_{i}\right), \quad i=1, \ldots, k
$$

- from Property 4.2 we see that $\mathcal{R}(\mathbf{B})=\mathcal{R}\left(\mathbf{B B}^{T}\right)=\mathcal{R}\left(\mathbf{C} \mathbf{C}^{T}\right)=\mathcal{R}(\mathbf{C})$. It follows that $\Pi_{\mathcal{R}(\mathbf{B})}\left(\mathbf{c}_{i}\right)=\mathbf{c}_{i}$ for all $i$.


## Application: Spectral Analysis

- consider the complex harmonic time-series

$$
y_{t}=\sum_{i=1}^{k} \alpha_{i} e^{j 2 \pi f_{i} t}+w_{t}, \quad t=0,1, \ldots, T-1
$$

where $\alpha_{i} \in \mathbb{C}$ is the amplitude-phase coefficient of the $i$ th sinusoid; $f_{i} \in\left[-\frac{1}{2}, \frac{1}{2}\right)$ is the frequency of the $i$ th sinusoid; $w_{t}$ is noise; $T$ is the observation time length

- Aim: estimate the frequencies $f_{1}, \ldots, f_{k}$ from $\left\{y_{t}\right\}_{t=0}^{T-1}$
- can be done by applying the Fourier transform
- the spectral resolution of Fourier-based methods is often limited by $T$
- our interest: study a subspace approach which can enable "super-resolution"
- suggested reading: [Stoica-Moses'97]


## Application: Spectral Analysis



An illustration of the Fourier spectrum. $T=64, k=5,\left\{f_{1}, \ldots, f_{k}\right\}=$ $\{-0.213,-0.1,-0.05,0.3,0.315\}$.

## Spectral Analysis via Subspace: Formulation

- let $z_{i}=e^{j 2 \pi f_{i}}$. Given a positive integer $d$, let

$$
\mathbf{y}_{t}=\left[\begin{array}{c}
y_{t} \\
y_{t+1} \\
\vdots \\
y_{t-d+1}
\end{array}\right]=\sum_{i=1}^{k} \alpha_{i}\left[\begin{array}{c}
z_{i}^{t} \\
z_{i}^{t+1} \\
\vdots \\
z_{i}^{t+d-1}
\end{array}\right]+\left[\begin{array}{c}
w_{t} \\
w_{t+1} \\
\vdots \\
w_{t+d-1}
\end{array}\right]=\sum_{i=1}^{k} \alpha_{i} \underbrace{\left[\begin{array}{c}
1 \\
z_{i} \\
\vdots \\
z_{i}^{d-1}
\end{array}\right]}_{=\mathbf{a}_{i}} z_{i}^{t}+\underbrace{\left[\begin{array}{c}
w_{t} \\
w_{t+1} \\
\vdots \\
w_{t-d+1}
\end{array}\right]}_{\mathbf{w}_{t}}
$$

- let $\mathbf{Y}=\left[\mathbf{y}_{0}, \mathbf{y}_{1}, \ldots, \mathbf{y}_{T_{d}-1}\right]$ where $T_{d}=T-d+1$. We can write

$$
\mathbf{Y}=\mathbf{A D S}+\mathbf{W}
$$

where $\mathbf{A}=\left[\mathbf{a}_{1}, \ldots, \mathbf{a}_{k}\right], \mathbf{D}=\operatorname{Diag}\left(\alpha_{1}, \ldots, \alpha_{k}\right), \mathbf{W}=\left[\mathbf{w}_{1}, \ldots, \mathbf{w}_{T_{d}-1}\right]$,

$$
\mathbf{S}=\left[\begin{array}{ccccc}
1 & z_{1} & z_{1}^{2} & \ldots & z_{1}^{T_{d}-1} \\
1 & z_{2} & z_{2}^{2} & \ldots & z_{2}^{T_{d}-1} \\
\vdots & & & & \vdots \\
1 & z_{k} & z_{k}^{2} & \ldots & z_{k}^{T_{d}-1}
\end{array}\right]
$$

## Spectral Analysis via Subspace: Formulation

- let $\mathbf{R}_{y}=\frac{1}{T_{d}} \sum_{t=0}^{T_{d}-1} \mathbf{y}_{t} \mathbf{y}_{t}^{H}=\frac{1}{T_{d}} \mathbf{Y} \mathbf{Y}^{H}$ be the correlation matrix of $\mathbf{y}_{t}$. We have

$$
\mathbf{R}_{y}=\mathbf{A} \underbrace{\left(\frac{1}{T_{d}} \mathbf{D S S}^{H} \mathbf{D}^{H}\right)}_{=\boldsymbol{\Phi}} \mathbf{A}^{H}+\frac{1}{T_{d}} \mathbf{A} \mathbf{D} \mathbf{S} \mathbf{W}^{H}+\frac{1}{T_{d}} \mathbf{W} \mathbf{S}^{H} \mathbf{D}^{H} \mathbf{A}^{H}+\frac{1}{T_{d}} \mathbf{W} \mathbf{W}^{H}
$$

- (this requires knowledge of random processes) assume that $w_{t}$ is a temporally white circular Gaussian process with mean zero and variance $\sigma^{2}$. Then, as $T_{d} \rightarrow \infty$,

$$
\frac{1}{T_{d}} \mathbf{S} \mathbf{W}^{H} \rightarrow \mathbf{0}, \quad \frac{1}{T_{d}} \mathbf{W} \mathbf{W}^{H} \rightarrow \sigma^{2} \mathbf{I}
$$

## Spectral Analysis via Subspace: Formulation

- let us summarize
- Model: the correlation matrix $\mathbf{R}_{y}=\frac{1}{T_{d}} \mathbf{Y} \mathbf{Y}^{H}$ is modeled as

$$
\mathbf{R}_{y}=\mathbf{A} \boldsymbol{\Phi} \mathbf{A}^{H}+\sigma^{2} \mathbf{I}
$$

where $\sigma^{2}>0$ is the noise power; $\mathbf{\Phi}=\frac{1}{T_{d}} \mathbf{D S S} \mathbf{S}^{H} \mathbf{D}^{H} ; \mathbf{D}=\operatorname{Diag}\left(\alpha_{1}, \ldots, \alpha_{k}\right)$;

$$
\mathbf{A}=\left[\begin{array}{cccc}
1 & 1 & \ldots & 1 \\
z_{1} & z_{2} & & z_{k} \\
\vdots & \vdots & & \vdots \\
z_{1}^{d-1} & z_{2}^{d-1} & \ldots & z_{k}^{d-1}
\end{array}\right] \in \mathbb{C}^{d \times k}, \mathbf{S}=\left[\begin{array}{ccccc}
1 & z_{1} & z_{1}^{2} & \ldots & z_{1}^{T_{d}-1} \\
1 & z_{2} & z_{2}^{2} & \ldots & z_{2}^{T_{d}-1} \\
\vdots & & & & \vdots \\
1 & z_{k} & z_{k}^{2} & \ldots & z_{k}^{T_{d}-1}
\end{array}\right] \in \mathbb{C}^{k \times T_{d}}
$$

$$
\text { with } z_{i}=e^{j 2 \pi f_{i}}
$$

- observation: A and $\mathbf{S}$ are both Vandemonde


## Spectral Analysis via Subspace: Subspace Properties

- Assumptions: i) $\alpha_{i} \neq 0$ for all $i$, ii) $f_{i} \neq f_{j}$ for all $i \neq j$, iii) $d>k$, iv) $T_{d} \geq k$
- results:
- A has full column rank, $\mathbf{S}$ has full row rank
- $\boldsymbol{\Phi}$ is positive definite (and thus nonsingular)
* proof: $\mathbf{x}^{H} \mathbf{D S S} \mathbf{S}^{H} \mathbf{D}^{H} \mathbf{x}=\left\|\mathbf{S}^{H} \mathbf{D}^{H} \mathbf{x}\right\|_{2}^{2}$, and $\mathbf{S}^{H} \mathbf{D}^{H} \mathbf{x}=\mathbf{0}$ if and only if $\mathbf{S}^{H}$ does not have full column rank
- $\mathcal{R}\left(\mathbf{A} \mathbf{\Phi} \mathbf{A}^{H}\right)=\mathcal{R}(\mathbf{A})$, by Property 4.2
$-\operatorname{rank}\left(\mathbf{A} \boldsymbol{\Phi} \mathbf{A}^{H}\right)=\operatorname{rank}(\mathbf{A})=k$, thus $\mathbf{A} \boldsymbol{\Phi} \mathbf{A}^{H}$ has $k$ nonzero eigenvalues


## Spectral Analysis via Subspace: Subspace Properties

- consider the eigendecomposition of $\mathbf{A} \boldsymbol{\Phi} \mathbf{A}^{H}$. Let $\mathbf{A} \boldsymbol{\Phi} \mathbf{A}^{H}=\mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^{H}$ and assume $\lambda_{1} \geq \lambda_{2} \geq \ldots \geq \lambda_{d}$.
- since $\lambda_{i}>0$ for $i=1, \ldots, k$ and $\lambda_{i}=0$ for $i=k+1, \ldots, d$,

$$
\mathbf{A} \boldsymbol{\Phi} \mathbf{A}^{H}=\left[\begin{array}{ll}
\mathbf{V}_{1} & \mathbf{V}_{2}
\end{array}\right]\left[\begin{array}{cc}
\boldsymbol{\Lambda}_{1} & \mathbf{0} \\
\mathbf{0} & \mathbf{0}
\end{array}\right]\left[\begin{array}{c}
\mathbf{V}_{1}^{H} \\
\mathbf{V}_{2}^{H}
\end{array}\right]=\mathbf{V}_{1} \boldsymbol{\Lambda}_{1} \mathbf{V}_{1}^{H}
$$

where $\mathbf{V}_{1}=\left[\mathbf{v}_{1}, \ldots, \mathbf{v}_{k}\right] \in \mathbb{C}^{d \times k}, \mathbf{V}_{2}=\left[\mathbf{v}_{k+1}, \ldots, \mathbf{v}_{d}\right] \in \mathbb{C}^{d \times(d-k)}, \boldsymbol{\Lambda}_{1}=$ $\operatorname{Diag}\left(\lambda_{1}, \ldots, \lambda_{k}\right)$.

- result: $\mathcal{R}\left(\mathbf{A} \mathbf{\Phi} \mathbf{A}^{H}\right)=\mathcal{R}\left(\mathbf{V}_{1}\right), \mathcal{R}\left(\mathbf{A} \mathbf{\Phi} \mathbf{A}^{H}\right)^{\perp}=\mathcal{R}\left(\mathbf{V}_{2}\right)$


## Spectral Analysis via Subspace: Subspace Properties

- consider the eigendecomposition of $\mathbf{R}_{y}$. Observe

$$
\mathbf{R}_{y}=\left[\begin{array}{ll}
\mathbf{V}_{1} & \mathbf{V}_{2}
\end{array}\right]\left[\begin{array}{cc}
\boldsymbol{\Lambda}_{1}+\sigma^{2} \mathbf{I} & \mathbf{0} \\
\mathbf{0} & \sigma^{2} \mathbf{I}
\end{array}\right]\left[\begin{array}{c}
\mathbf{V}_{1}^{H} \\
\mathbf{V}_{2}^{H}
\end{array}\right]
$$

- results:
- $\mathbf{V}\left(\boldsymbol{\Lambda}+\sigma^{2} \mathbf{I}\right) \mathbf{V}^{H}$ is the eigendecomposition of $\mathbf{R}_{y}$
- $\mathbf{V}_{1}$ can be obtained from $\mathbf{R}_{y}$ by finding the eigenvectors associated with the first $k$ largest eigenvalues of $\mathbf{R}_{y}$


## Spectral Analysis via Subspace: Subspace Properties

- let us summarize
- compute the eigenvector matrix $\mathbf{V} \in \mathbb{C}^{d \times d}$ of $\mathbf{R}_{y}$. Partition $\mathbf{V}=\left[\mathbf{V}_{1}, \mathbf{V}_{2}\right]$ where $\mathbf{V}_{1} \in \mathbb{C}^{n \times k}$ corresponds the first $k$ largest eigenvalues. Then,

$$
\mathcal{R}\left(\mathbf{V}_{1}\right)=\mathcal{R}(\mathbf{A}), \quad \mathcal{R}\left(\mathbf{V}_{2}\right)=\mathcal{R}(\mathbf{A})^{\perp}
$$

- Idea of subspace methods: let

$$
\mathbf{a}(z)=\left[\begin{array}{c}
1 \\
z \\
\vdots \\
z^{d-1}
\end{array}\right] .
$$

Find any $f \in\left[-\frac{1}{2}, \frac{1}{2}\right)$ that satisfies $\mathbf{a}\left(e^{j 2 \pi f}\right) \in \mathcal{R}(\mathbf{A})$.

## Spectral Analysis via Subspace: Subspace Properties

- Question: it is true that $f \in\left\{f_{1}, \ldots f_{k}\right\}$ implies $\mathbf{a}\left(e^{j 2 \pi f}\right) \in \mathcal{R}(\mathbf{A})$. But is it also true that $\mathbf{a}\left(e^{j 2 \pi f}\right) \in \mathcal{R}(\mathbf{A})$ implies $f \in\left\{f_{1}, \ldots f_{k}\right\}$ ?
- The answer is yes if $d>k$. The following matrix result gives the answer.

Theorem 4.3. Let $\mathbf{A} \in \mathbb{C}^{d \times k}$ any Vandemonde matrix with distinct roots $z_{1}, \ldots, z_{k}$ and with $d \geq k+1$. Then it holds that

$$
z \in\left\{z_{1}, \ldots, z_{k}\right\} \quad \Longleftrightarrow \quad \mathbf{a}(z) \in \mathcal{R}(\mathbf{A})
$$

## Spectral Analysis via Subspace: Subspace Properties

- proof of Theorem 4.3: " $\Longrightarrow$ " is trivial, and we consider " $\Longleftarrow$ "
- suppose there exists $\bar{z} \notin\left\{z_{1}, \ldots, z_{k}\right\}$ such that $\mathbf{a}(\bar{z}) \in \mathcal{R}(\mathbf{A})$.
- let $\tilde{\mathbf{A}}=[\mathbf{a}(\bar{z}) \mathbf{A}] \in \mathbb{C}^{d \times(k+1)}$.
$-\mathbf{a}(\bar{z}) \in \mathcal{R}(\mathbf{A})$ implies that $\tilde{\mathbf{A}}$ has linearly dependent columns
- however, $\tilde{\mathbf{A}}$ is Vandemonde with distinct roots $\bar{z}, z_{1}, \ldots, z_{k}$, and for $d \geq k+1$ $\tilde{\mathbf{A}}$ must have linearly independent columns-a contradiction


## Spectral Analysis via Subspace: Algorithm

- there are many subspace methods, and multiple signal classification (MUSIC) is most well-known
- MUSIC uses the fact that $\mathbf{a}\left(e^{\boldsymbol{j} 2 \pi f}\right) \in \mathcal{R}(\mathbf{A}) \Longleftrightarrow \mathbf{V}_{2}^{H} \mathbf{a}\left(e^{\boldsymbol{j} 2 \pi f}\right)=\mathbf{0}$

$$
\begin{aligned}
& \text { Algorithm: MUSIC } \\
& \text { input: the correlation matrix } \mathbf{R}_{y} \in \mathbb{C}^{d \times d} \text { and the model order } k<d \\
& \text { Perform eigendecomposition } \mathbf{R}_{y}=\mathbf{V} \mathbf{\Lambda} \mathbf{V}^{H} \text { with } \lambda_{1} \geq \lambda_{2} \geq \ldots \geq \lambda_{d} \\
& \text { Let } \mathbf{V}_{2}=\left[\mathbf{v}_{k+1}, \ldots, \mathbf{v}_{d}\right] \text {, and compute } \\
& \qquad S(f)=\frac{1}{\left\|\mathbf{V}_{2}^{H} \mathbf{a}\left(e^{\boldsymbol{j} 2 \pi f}\right)\right\|_{2}^{2}} \\
& \text { for } f \in\left[-\frac{1}{2}, \frac{1}{2}\right) \text { (done by discretization). } \\
& \text { output: } S(f)
\end{aligned}
$$

## Spectral Analysis via Subspace: Algorithm

MUSIC Spectrum


An illustration of the MUSIC spectrum. $T=64, k=5, \quad\left\{f_{1}, \ldots, f_{k}\right\}=$ $\{-0.213,-0.1,-0.05,0.3,0.315\}$.

## Application: Euclidean Distance Matrices

- let $\mathbf{x}_{1}, \ldots, \mathbf{x}_{n} \in \mathbb{R}^{d}$ be a collection of points, and let $\mathbf{X}=\left[\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right]$
- let $d_{i j}=\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|_{2}$ be the Euclidean distance between points $i$ and $j$
- Problem: given $d_{i j}$ 's for all $i, j \in\{1, \ldots, n\}$, recover $\mathbf{X}$
- this problem is called the Euclidean distance matrix (EDM) problem
- applications: sensor network localization (SNL), molecule conformation, ....
- suggested reading: [Dokmanić-Parhizkar-et al.'15]


## EDM Applications


(a) SNL. (b) Molecular transformation. Source: [Dokmanić-Parhizkar-et al.'15]

## EDM: Formulation

- let $\mathbf{R} \in \mathbb{R}^{n \times n}$ be matrix whose entries are $r_{i j}=d_{i j}^{2}$ for all $i, j$
- from

$$
r_{i j}=d_{i j}^{2}=\left\|\mathbf{x}_{i}\right\|_{2}^{2}-2 \mathbf{x}_{i}^{T} \mathbf{x}_{j}+\left\|\mathbf{x}_{j}\right\|_{2}^{2}
$$

we see that $\mathbf{R}$ can be written as

$$
\begin{equation*}
\mathbf{R}=\mathbf{1}\left(\operatorname{diag}\left(\mathbf{X}^{T} \mathbf{X}\right)\right)^{T}-2 \mathbf{X}^{T} \mathbf{X}+\left(\operatorname{diag}\left(\mathbf{X}^{T} \mathbf{X}\right)\right) \mathbf{1}^{T} \tag{*}
\end{equation*}
$$

where the notation diag means that $\operatorname{diag}(\mathbf{Y})=\left[y_{11}, \ldots, y_{n n}\right]^{T}$ for any square $\mathbf{Y}$

- observation: ( $*$ ) also holds if we replace $\mathbf{X}$ by
$-\tilde{\mathbf{X}}=\left[\mathbf{x}_{1}+\mathbf{b}, \ldots, \mathbf{x}_{n}+\mathbf{b}\right]$ for any $\mathbf{b} \in \mathbb{R}^{d}\left(d_{i j}=\left\|\tilde{\mathbf{x}}_{i}-\tilde{\mathbf{x}}_{j}\right\|_{2}\right.$ is also true $)$
$-\tilde{\mathbf{X}}=\mathbf{Q X}$ for any orthogonal $\mathbf{Q}\left(\tilde{\mathbf{X}}^{T} \tilde{\mathbf{X}}=\mathbf{X}^{T} \mathbf{X}\right)$
- implication: recovery of $\mathbf{X}$ from $\mathbf{R}$ is subjected to translations and rotations/reflections
- in SNL we can use anchors to fix this issue


## EDM: Formulation

- assume $\mathbf{x}_{1}=\mathbf{0}$ w.l.o.g. Then,

$$
\mathbf{r}_{1}=\left[\begin{array}{c}
\left\|\mathbf{x}_{1}-\mathbf{x}_{1}\right\|_{2}^{2} \\
\left\|\mathbf{x}_{2}-\mathbf{x}_{1}\right\|_{2}^{2} \\
\vdots \\
\left\|\mathbf{x}_{n}-\mathbf{x}_{1}\right\|_{2}^{2}
\end{array}\right]=\left[\begin{array}{c}
0 \\
\left\|\mathbf{x}_{2}\right\|_{2}^{2} \\
\vdots \\
\left\|\mathbf{x}_{n}\right\|_{2}^{2}
\end{array}\right], \quad \operatorname{diag}\left(\mathbf{X}^{T} \mathbf{X}\right)=\left[\begin{array}{c}
\left\|\mathbf{x}_{1}\right\|_{2}^{2} \\
\left\|\mathbf{x}_{2}\right\|_{2}^{2} \\
\vdots \\
\left\|\mathbf{x}_{n}\right\|_{2}^{2}
\end{array}\right]=\mathbf{r}_{1}
$$

- construct from $\mathbf{R}$ the following matrix

$$
\mathbf{G}=-\frac{1}{2}\left(\mathbf{R}-\mathbf{1} \mathbf{r}_{1}^{T}-\mathbf{r}_{1} \mathbf{1}^{T}\right) .
$$

We have

$$
\mathbf{G}=\mathbf{X}^{T} \mathbf{X}
$$

- idea: do a symmetric factorization for $\mathbf{G}$ to try to recover $\mathbf{X}$


## EDM: Method

- assumption: $\mathbf{X}$ has full row rank
- $\mathbf{G}$ is $\operatorname{PSD}$ and has $\operatorname{rank}(\mathbf{G})=d$
- denote the eigendecomposition of $\mathbf{G}$ as $\mathbf{G}=\mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^{T}$. Assuming $\lambda_{1} \geq \ldots \geq \lambda_{n}$, it takes the form

$$
\mathbf{G}=\left[\begin{array}{ll}
\mathbf{V}_{1} & \mathbf{V}_{2}
\end{array}\right]\left[\begin{array}{cc}
\boldsymbol{\Lambda}_{1} & \mathbf{0} \\
\mathbf{0} & \mathbf{0}
\end{array}\right]\left[\begin{array}{c}
\mathbf{V}_{1}^{T} \\
\mathbf{V}_{2}^{T}
\end{array}\right]=\left(\boldsymbol{\Lambda}^{1 / 2} \mathbf{V}_{1}^{T}\right)^{T}\left(\boldsymbol{\Lambda}^{1 / 2} \mathbf{V}_{1}^{T}\right)
$$

where $\mathbf{V}_{1} \in \mathbb{R}^{n \times d}, \boldsymbol{\Lambda}_{1}=\operatorname{Diag}\left(\lambda_{1}, \ldots, \lambda_{d}\right)$

- EDM solution: take $\hat{\mathbf{X}}=\boldsymbol{\Lambda}^{1 / 2} \mathbf{V}_{1}^{T}$ as an estimate of $\mathbf{X}$
- recovery guarantee: by Property 4.3, we have $\hat{\mathbf{X}}=\mathbf{Q X}$ for some orthogonal $\mathbf{Q}$


## EDM: Further Discussion

- in applications such as SNL, not all pairwise distances $d_{i j}$ 's are available
- or, there are missing entries with $\mathbf{R}$
- possible solution: apply low-rank matrix completion to try to recover the full $\mathbf{R}$
- to use low-rank matrix completion, we need to know a rank bound on $\mathbf{R}$
- by the result $\operatorname{rank}(\mathbf{A}+\mathbf{B}) \leq \operatorname{rank}(\mathbf{A})+\operatorname{rank}(\mathbf{B})$, we get

$$
\begin{aligned}
\operatorname{rank}(\mathbf{R}) & \leq \operatorname{rank}\left(\mathbf{1}\left(\operatorname{diag}\left(\mathbf{X}^{T} \mathbf{X}\right)\right)^{T}\right)+\operatorname{rank}\left(-2 \mathbf{X}^{T} \mathbf{X}\right)+\operatorname{rank}\left(\left(\operatorname{diag}\left(\mathbf{X}^{T} \mathbf{X}\right)\right) \mathbf{1}^{T}\right) \\
& \leq 1+d+1=d+2
\end{aligned}
$$

- other issues: noisy distance measurements, resolving the orthogonal rotation problem with $\hat{\mathbf{X}}$. See the suggested reference [Dokmanić-Parhizkar-et al.'15].


## Variational Characterizations of Eigenvalues of Real Symmetric Matrices

Notation and Conventions:

- $\lambda_{1}(\mathbf{A}), \ldots, \lambda_{n}(\mathbf{A})$ denote the eigenvalues of a given $\mathbf{A} \in \mathbb{S}^{n}$ with ordering

$$
\lambda_{\max }(\mathbf{A})=\lambda_{1}(\mathbf{A}) \geq \lambda_{2}(\mathbf{A}) \geq \ldots \geq \lambda_{n}(\mathbf{A})=\lambda_{\min }(\mathbf{A})
$$

where $\lambda_{\min }(\mathbf{A})$ and $\lambda_{\max }(\mathbf{A})$ denote the smallest and largest eigenvalues, resp.

- if not specified, $\lambda_{1}, \ldots, \lambda_{n}$ will be used to denote the eigenvalues of $\mathbf{A} \in \mathbb{S}^{n}$; they also follow the ordering

$$
\lambda_{\max }=\lambda_{1} \geq \lambda_{2} \geq \ldots \geq \lambda_{n}=\lambda_{\min }
$$

Also, $\mathbf{V} \boldsymbol{\Lambda} \mathbf{V}^{T}$ will be used to denote the eigendecomposition of $\mathbf{A} \in \mathbb{S}^{n}$

## Variational Characterizations of Eigenvalues

- let $\mathbf{A} \in \mathbb{S}^{n}$.
- for any $\mathbf{x} \in \mathbb{R}^{n}$ with $\mathbf{x} \neq \mathbf{0}$, the ratio

$$
\frac{\mathbf{x}^{T} \mathbf{A} \mathbf{x}}{\mathbf{x}^{T} \mathbf{x}}
$$

is called the Rayleigh quotient.

- our interest: quadratic optimization such as

$$
\begin{aligned}
& \max _{\mathbf{x} \in \mathbb{R}^{n}, \mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^{T} \mathbf{A} \mathbf{x}}{\mathbf{x}^{T} \mathbf{x}}=\max _{\mathbf{x} \in \mathbb{R}^{n},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x} \\
& \min _{\mathbf{x} \in \mathbb{R}^{n}, \mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^{T} \mathbf{A} \mathbf{x}}{\mathbf{x}^{T} \mathbf{x}}=\min _{\mathbf{x} \in \mathbb{R}^{n},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x}
\end{aligned}
$$

## Variational Characterizations of Eigenvalues: Rayleigh-Ritz

Theorem 4.4 (Rayleigh-Ritz). Let $\mathbf{A} \in \mathbb{S}^{n}$. It holds that

$$
\begin{gathered}
\lambda_{\min }\|\mathbf{x}\|_{2}^{2} \leq \mathbf{x}^{T} \mathbf{A} \mathbf{x} \leq \lambda_{\max }\|\mathbf{x}\|_{2}^{2} \\
\lambda_{\min }=\min _{\mathbf{x} \in \mathbb{R}^{n},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x}, \quad \lambda_{\max }=\max _{\mathbf{x} \in \mathbb{R}^{n},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x}
\end{gathered}
$$

- proof:
- by a change of variable $\mathbf{y}=\mathbf{V}^{T} \mathbf{x}$, we have

$$
\mathbf{x}^{T} \mathbf{A} \mathbf{x}=\mathbf{y}^{T} \boldsymbol{\Lambda} \mathbf{y}=\sum_{i=1}^{n} \lambda_{i}\left|y_{i}\right|^{2} \leq \lambda_{1} \sum_{i=1}^{n}\left|y_{i}\right|^{2}=\lambda_{1}\left\|\mathbf{V}^{T} \mathbf{x}\right\|_{2}^{2}=\lambda_{1}\|\mathbf{x}\|_{2}^{2}
$$

- we thus have $\max _{\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A x} \leq \lambda_{1}$
- since $\mathbf{v}_{1}^{T} \mathbf{A} \mathbf{v}_{1}=\lambda_{1}$, the above equality is attained
- the results $\mathbf{x}^{T} \mathbf{A} \mathbf{x} \geq \lambda_{n}\|\mathbf{x}\|_{2}^{2}$ and $\min _{\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x}=\lambda_{n}$ are proven by the same way


## Variational Characterizations of Eigenvalues: Courant-Fischer

Question: how about $\lambda_{k}$ for any $k \in\{1, \ldots, n\}$ ? Do we have a similar variational characterization as that in the Rayleigh-Ritz 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

$$
\begin{aligned}
\lambda_{k} & =\min _{\mathcal{S}_{n-k+1} \subseteq \mathbb{R}^{n}} \max _{\mathbf{x} \in \mathcal{S}_{n-k+1},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x} \\
& =\max _{\mathcal{S}_{k} \subseteq \mathbb{R}^{n}} \min _{\mathbf{x} \in \mathcal{S}_{k},\|\mathbf{x}\|_{2}=1} \mathbf{x}^{T} \mathbf{A} \mathbf{x}
\end{aligned}
$$

- proof: see the accompanying note


## Variational Characterizations of Eigenvalues: More Results

The Courant-Fischer theorem and its variants lead to a rich collection of eigenvalue inequalities: For $\mathbf{A}, \mathbf{B} \in \mathbb{S}^{n}, \mathbf{z} \in \mathbb{R}^{n}$,

- (Weyl) $\lambda_{k}(\mathbf{A})+\lambda_{n}(\mathbf{B}) \leq \lambda_{k}(\mathbf{A}+\mathbf{B}) \leq \lambda_{k}(\mathbf{A})+\lambda_{1}(\mathbf{B}), k=1, \ldots, n$
- (interlacing) $\lambda_{k+1}(\mathbf{A}) \leq \lambda_{k}\left(\mathbf{A} \pm \mathbf{z z}^{T}\right) \leq \lambda_{k-1}(\mathbf{A})$ for appropriate $k$
- if $\operatorname{rank}(\mathbf{B}) \leq r$, then $\lambda_{k+r}(\mathbf{A}) \leq \lambda_{k}(\mathbf{A}+\mathbf{B}) \leq \lambda_{k-r}(\mathbf{A})$ for appropriate $k$
- (Weyl) $\lambda_{j+k-1}(\mathbf{A}+\mathbf{B}) \leq \lambda_{j}(\mathbf{A})+\lambda_{k}(\mathbf{B})$ for appropriate $j, k$
- for any semi-orthogonal $\mathbf{U} \in \mathbb{R}^{n \times r}, \lambda_{k+n-r}(\mathbf{A}) \leq \lambda_{k}\left(\mathbf{U}^{T} \mathbf{A} \mathbf{U}\right) \leq \lambda_{k}(\mathbf{A})$ for appropriate $k$
- many more...


## Variational Characterizations of Eigenvalues: More Results

An extension of the variational characterization to a sum of eigenvalues:

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

$$
\sum_{i=1}^{r} \lambda_{i}=\max _{\substack{\mathbf{U} \in \mathbb{R}^{n \times r} \\\left\|\mathbf{u}_{i}\right\|_{2}=1 \\ \forall i, \mathbf{u}_{i}^{T} \mathbf{u}_{j}=0}} \sum_{i=i \neq j}^{r} \mathbf{u}_{i}^{T} \mathbf{A} \mathbf{u}_{i}=\max _{\substack{\mathbf{U} \in \mathbb{R}^{n \times r} \\ \mathbf{U}^{T} \mathbf{U}=\mathbf{I}}} \operatorname{tr}\left(\mathbf{U}^{T} \mathbf{A} \mathbf{U}\right)
$$

- can be proved by the eigenvalue inequality $\lambda_{k}\left(\mathbf{U}^{T} \mathbf{A U}\right) \leq \lambda_{k}(\mathbf{A})$


## Variational Characterizations of Eigenvalues: More Results

Some more results (the proofs require more than just the Courant-Fischer theorem):

- (von Neumann) Let $\mathbf{A}, \mathbf{B} \in \mathbb{S}^{n}$. It holds that

$$
\operatorname{tr}(\mathbf{A B}) \leq \sum_{i=1}^{n} \lambda_{i}(\mathbf{A}) \lambda_{i}(\mathbf{B})
$$

- (Lidskii) Let $\mathbf{A}, \mathbf{B} \in \mathbb{S}^{n}$. For any $1 \leq i_{1} \leq i_{2} \leq \cdots \leq i_{k}$,

$$
\sum_{j=1}^{k} \lambda_{i_{j}}(\mathbf{A}+\mathbf{B}) \leq \sum_{j=1}^{k} \lambda_{i_{j}}(\mathbf{A})+\sum_{j=1}^{k} \lambda_{j}(\mathbf{B}) .
$$

## PSD Matrix Inequalities

- the notion of PSD matrices can be used to define inequalities for matrices
- PSD matrix inequalities are frequently used in topics like semidefinite programming
- definition:
$-\mathbf{A} \succeq \mathbf{B}$ means that $\mathbf{A}-\mathbf{B}$ is PSD
$-\mathbf{A} \succ \mathbf{B}$ means that $\mathbf{A}-\mathbf{B}$ is PD
- $\mathbf{A} \nsucceq \mathbf{B}$ means that $\mathbf{A}-\mathbf{B}$ is indefinite
- results that immediately follow from the definition: let $\mathbf{A}, \mathbf{B}, \mathbf{C} \in \mathbb{S}^{n}$.
- $\mathbf{A} \succeq \mathbf{0}, \alpha \geq 0($ resp. $\mathbf{A} \succ \mathbf{0}, \alpha>0) \Longrightarrow \alpha \mathbf{A} \succeq \mathbf{0}($ resp. $\alpha \mathbf{A} \succ \mathbf{0})$
- $\mathbf{A}, \mathbf{B} \succeq \mathbf{0}$ (resp. $\mathbf{A} \succeq \mathbf{0}, \mathbf{B} \succ \mathbf{0}) \Longrightarrow \mathbf{A}+\mathbf{B} \succeq \mathbf{0}$ (resp. $\mathbf{A}+\mathbf{B} \succ \mathbf{0}$ )
$-\mathbf{A} \succeq \mathbf{B}, \mathbf{B} \succeq \mathbf{C}($ resp. $\mathbf{A} \succeq \mathbf{B}, \mathbf{B} \succ \mathbf{C}) \Longrightarrow \mathbf{A} \succeq \mathbf{C}($ resp. $\mathbf{A} \succ \mathbf{C})$
- $\mathbf{A} \nsucceq \mathbf{B}$ does not imply $\mathbf{B} \succeq \mathbf{A}$


## PSD Matrix Inequalities

- more results: let $\mathbf{A}, \mathbf{B} \in \mathbb{S}^{n}$.
- $\mathbf{A} \succeq \mathbf{B} \Longrightarrow \lambda_{k}(\mathbf{A}) \geq \lambda_{k}(\mathbf{B})$ for all $k$; the converse is not always true
$-\mathbf{A} \succeq \mathbf{I}($ resp. $\mathbf{A} \succ \mathbf{I}) \Longleftrightarrow \lambda_{k}(\mathbf{A}) \geq 1$ for all $k\left(\right.$ resp. $\lambda_{k}(\mathbf{A})>1$ for all $\left.k\right)$
$-\mathbf{I} \succeq \mathbf{A}($ resp. $\mathbf{I} \succ \mathbf{A}) \Longleftrightarrow \lambda_{k}(\mathbf{A}) \leq 1$ for all $k\left(\right.$ resp. $\lambda_{k}(\mathbf{A})<1$ for all $k$ )
- if $\mathbf{A}, \mathbf{B} \succ \mathbf{0}$ then $\mathbf{A} \succeq \mathbf{B} \Longleftrightarrow \mathbf{B}^{-1} \succeq \mathbf{A}^{-1}$
- some results as consequences of the above results:
- for $\mathbf{A} \succeq \mathbf{B} \succeq \mathbf{0}, \operatorname{det}(\mathbf{A}) \geq \operatorname{det}(\mathbf{B})$
- for $\mathbf{A} \succeq \mathbf{B}, \operatorname{tr}(\mathbf{A}) \geq \operatorname{tr}(\mathbf{B})$
- for $\mathbf{A} \succeq \mathbf{B} \succ \mathbf{0}, \operatorname{tr}\left(\mathbf{A}^{-1}\right) \leq \operatorname{tr}\left(\mathbf{B}^{-1}\right)$


## PSD Matrix Inequalities

- the Schur complement: let

$$
\mathbf{X}=\left[\begin{array}{cc}
\mathbf{A} & \mathbf{B} \\
\mathbf{B}^{T} & \mathbf{C}
\end{array}\right]
$$

where $\mathbf{A} \in \mathbb{S}^{m}, \mathbf{B} \in \mathbb{R}^{m \times n}, \mathbf{C} \in \mathbb{S}^{n}$ with $\mathbf{C} \succ \mathbf{0}$. Let

$$
\mathbf{S}=\mathbf{A}-\mathbf{B C}^{-1} \mathbf{B}^{T}
$$

which is called the Schur complement. We have

$$
\mathbf{X} \succeq \mathbf{0}(\text { resp. } \mathbf{X} \succ \mathbf{0}) \quad \Longleftrightarrow \quad \mathbf{S} \succeq \mathbf{0}(\text { resp. } \mathbf{S} \succ \mathbf{0})
$$

- example: let $\mathbf{C}$ be PD. By the Schur complement,

$$
1-\mathbf{b}^{T} \mathbf{C}^{-1} \mathbf{b} \geq 0 \Longleftrightarrow \mathbf{C}-\mathbf{b b}^{T} \succeq \mathbf{0}
$$

## References

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