# **SI231** Matrix Analysis and Computations Topic 6: Positive Semidefinite Matrices

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#### **Topic 6: Positive Semidefinite Matrices**

• positive semidefinite matrices

• matrix inequalities

• application: subspace method for super-resolution spectral analysis

• application: Euclidean distance matrices

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#### **Hightlights**

ullet 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  $\mathbf{x} \in \mathbb{R}^n$ ;

and positive definite (PD) if

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

- ullet 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  $\mathbf{B} \in \mathbb{R}^{m \times n}$
- in this lecture, we will deal with the real-symmetric matrices—the Hermitian case follows along the same lines

#### **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):

$$-\mathbf{x}^{T}\mathbf{A}\mathbf{x} = \sum_{i=1}^{n} \sum_{j=1}^{n} x_{i}x_{j}a_{ij} = \sum_{i=1}^{n} a_{ii}x_{i}^{2} + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} 2a_{ij}x_{i}x_{j}$$

- $\mathbf{x}^T \mathbf{A} \mathbf{x} = \sum_{i=1}^n a_{ii} x_i^2 + \sum_{i=1}^{n-1} \sum_{j=i+1}^n (a_{ij} + a_{ji}) x_i x_j$  for general  $\mathbf{A} \in \mathbb{R}^{n \times n}$ , there may exist  $\mathbf{A}_1$  and  $\mathbf{A}_2$  s.t.  $\mathbf{x}^T \mathbf{A}_1 \mathbf{x} = \mathbf{x}^T \mathbf{A}_2 \mathbf{x}$ 
  - \* it suffices to consider unique symmetric  ${f A}$  for general  ${f A} \in \mathbb{R}^{n imes n}$  since

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

- complex case:
  - \* the (complex) 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 both A and -A are not PSD

#### Notation:

- $A \succeq 0$  means that A is PSD
- A > 0 means that A is PD
- ullet  $\mathbf{A} \not\succeq \mathbf{0}$  means that  $\mathbf{A}$  is indefinite
- if A is PD, then it is also PSD
- ullet a quadratic form is called PSD (resp. PD) if old A is PSD (resp. PD)
- ullet The concepts negative semidefinite and negative definite may be defined by reversing the inequalities or, equivalently, by saying  $-\mathbf{A}$  is PSD or PD, respectively.

#### **Example: Covariance Matrices**

- let  $\mathbf{y}_0, \mathbf{y}_2, \dots \mathbf{y}_{T-1} \in \mathbb{R}^n$  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],
     ...
- ullet sample mean:  $\hat{oldsymbol{\mu}}_y = rac{1}{T} \sum_{t=0}^{T-1} \mathbf{y}_t$
- ullet sample covariance:  $\hat{\mathbf{C}}_y = \frac{1}{T} \sum_{t=0}^{T-1} (\mathbf{y}_t \hat{\boldsymbol{\mu}}_y) (\mathbf{y}_t \hat{\boldsymbol{\mu}}_y)^T$
- a sample covariance is PSD:  $\mathbf{x}^T \hat{\mathbf{C}}_y \mathbf{x} = \frac{1}{T} \sum_{t=0}^{T-1} |(\mathbf{y}_t \hat{\boldsymbol{\mu}}_y)^T \mathbf{x}|^2 \ge 0$
- ullet 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  $\mathbf{C}_y = \mathrm{E}[(\mathbf{y}_t \boldsymbol{\mu}_y)(\mathbf{y}_t \boldsymbol{\mu}_y)^T]$  where  $\boldsymbol{\mu}_y = \mathrm{E}[\mathbf{y}_t]$ , can be shown to be PSD

# **Example: Hessian**

- let  $f: \mathbb{R}^n \to \mathbb{R}$  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

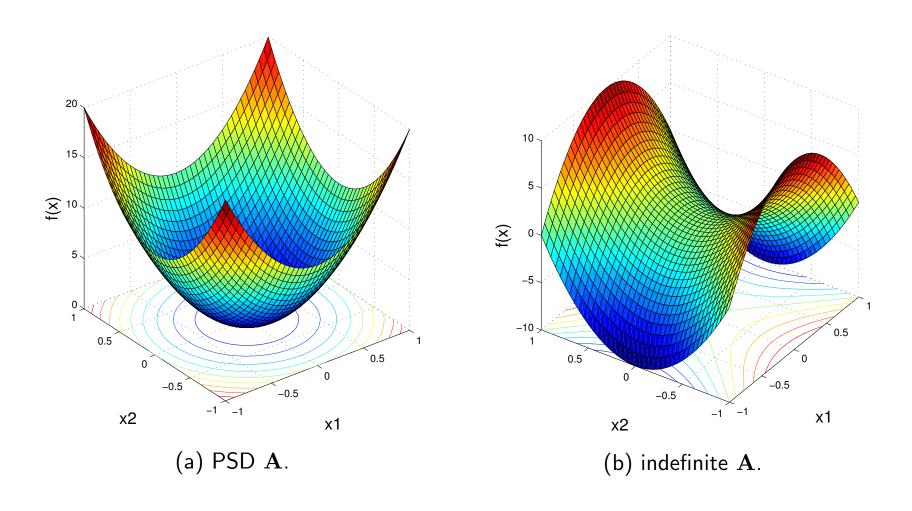
$$\left[\nabla^2 f(\mathbf{x})\right]_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

- 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**



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# **Properties of PSD Matrices: Eigenvalues**

**Theorem 5.1.** Let  $\mathbf{A} \in \mathbb{S}^n$ , and let  $\lambda_1, \ldots, \lambda_n$  be the eigenvalues of  $\mathbf{A}$ . We have

1. 
$$\mathbf{A} \succeq \mathbf{0} \iff \lambda_i \geq 0 \text{ for } i = 1, \dots, n$$

2. 
$$\mathbf{A} \succ \mathbf{0} \iff \lambda_i > 0 \text{ for } i = 1, \dots, n$$

• proof: let  $A = V\Lambda V^T$  be the eigendecomposition of A.

$$\mathbf{A} \succeq \mathbf{0} \iff \mathbf{x}^T \mathbf{V} \mathbf{\Lambda} \mathbf{V}^T \mathbf{x} \ge 0, \quad \text{for all } \mathbf{x} \in \mathbb{R}^n$$

$$\iff \mathbf{z}^T \mathbf{\Lambda} \mathbf{z} \ge 0, \quad \text{for all } \mathbf{z} \in \mathcal{R}(\mathbf{V}^T) = \mathbb{R}^n$$

$$\iff \sum_{i=1}^n \lambda_i |z_i|^2 \ge 0, \quad \text{for all } \mathbf{z} \in \mathbb{R}^n$$

$$\iff \lambda_i \ge 0 \text{ for all } i$$

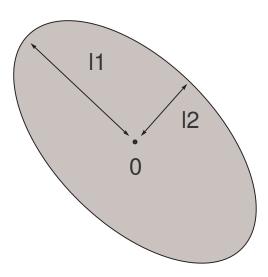
The PD case is proven by the same manner.

#### **Example: Ellipsoid**

ullet an ellipsoid of  $\mathbb{R}^n$  centered at  $oldsymbol{0}$  is defined as

$$\mathcal{E} = \{ \mathbf{x} \in \mathbb{R}^n \mid \mathbf{x}^T \mathbf{P}^{-1} \mathbf{x} \le 1 \},$$

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



- ullet let  $\mathbf{P} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^T$  be the eigendecomposition
  - V determines the directions of the semi-axes
  - $\lambda_1,\ldots,\lambda_n$  determine the lengths of the semi-axes

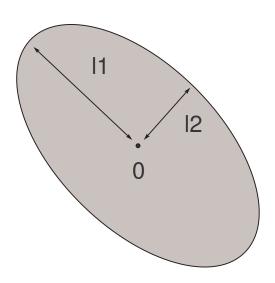
$$-\ell_i = \lambda_i^{\frac{1}{2}} \mathbf{v}_i$$

#### **Example: Ellipsoid**

ullet an ellipsoid of  $\mathbb{R}^n$  centered at  $oldsymbol{0}$  is defined as

$$\mathcal{E} = \{ \mathbf{x} \in \mathbb{R}^n \mid \mathbf{x}^T \mathbf{P}^{-1} \mathbf{x} \le 1 \},$$

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



• note:

- in direction  $\mathbf{v}_1$ ,  $\mathbf{x}^T \mathbf{P}^{-1} \mathbf{x}$  is large, hence ellipsoid is fat in direction  $\mathbf{v}_1$ 

- in direction  $\mathbf{v}_n$ ,  $\mathbf{x}^T \mathbf{P}^{-1} \mathbf{x}$  is small, hence ellipsoid is thin in direction  $\mathbf{v}_n$ 

-  $\sqrt{\lambda_1/\lambda_n}$  gives maximum eccentricity

•  $\tilde{\mathcal{E}} = \{ \mathbf{x} \in \mathbb{R}^n \mid \mathbf{x}^T \mathbf{Q}^{-1} \mathbf{x} \leq 1 \}$ , for some PD  $\mathbf{Q} \in \mathbb{S}^n$ , the  $\mathcal{E} \supseteq \tilde{\mathcal{E}} \iff \mathbf{P} \succeq \mathbf{Q}$ 

# **Example: Multivariate Gaussian Distribution**

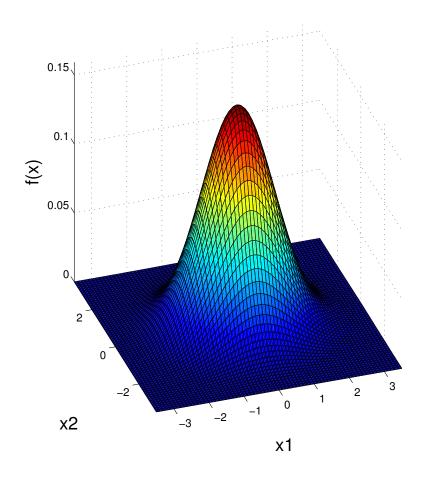
• probability density function for a Gaussian-distributed vector  $\mathbf{x} \in \mathbb{R}^n$ :

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

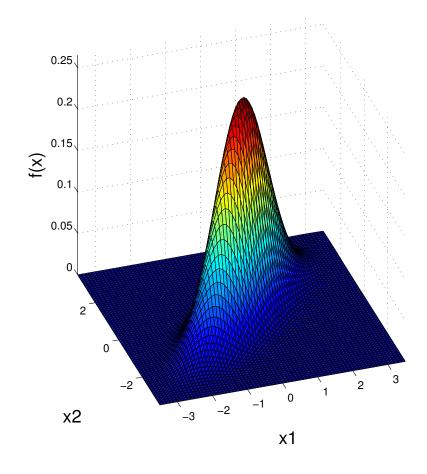
where  $\mu$  and  $\Sigma$  are the mean and covariance of x, resp.

- $-\Sigma$  is PD
- $-\Sigma$  determines how x is spread, by the same way as in ellipsoid

# **Example: Multivariate Gaussian Distribution**



(a) 
$$oldsymbol{\mu} = oldsymbol{0}, \, oldsymbol{\Sigma} = egin{bmatrix} 1 & 0 \ 0 & 1 \end{bmatrix}$$
.



(b) 
$$oldsymbol{\mu}=0$$
,  $oldsymbol{\Sigma}=egin{bmatrix}1&0.8\0.8&1\end{bmatrix}$ .

#### **Properties of PSD Matrices**

- it can be directly seen from the definition that
  - $\mathbf{A} \succeq \mathbf{0} \Longrightarrow a_{ii} \geq 0$  for all i
  - $\mathbf{A} \succ \mathbf{0} \Longrightarrow a_{ii} > 0$  for all i
- A is PSD,  $\mathbf{x}^T \mathbf{A} \mathbf{x} = 0 \iff \mathbf{A} \mathbf{x} = 0$  for a  $\mathbf{x}$ . (A is PD  $\iff \mathbf{A}$  is nonsingular.)
- extension (also direct): partition A as

$$\mathbf{A} = egin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}.$$

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  $\mathcal{I} = \{i_1, \ldots, i_m\} \subseteq \{1, \ldots, n\}$ , m < n, is a submatrix obtained by keeping only the rows and columns indicated by  $\mathcal{I}$ ; i.e.,  $[\mathbf{A}_{\mathcal{I}}]_{jk} = a_{i_j,i_k}$  for all  $j,k \in \{1,\ldots,m\}$
  - if A is PSD (resp. PD), then any principal submatrix of A is PSD (resp. PD)

#### **Properties of PSD Matrices**

**Property 5.1.** Let  $\mathbf{A} \in \mathbb{S}^n$ ,  $\mathbf{B} \in \mathbb{R}^{n \times m}$ , and

$$C = B^T A B$$
.

We have the following properties:

- 1.  $\mathbf{A}\succeq\mathbf{0}\Longrightarrow\mathbf{C}\succeq\mathbf{0}$  (specially,  $\mathbf{A}\succ\mathbf{0}\Longrightarrow\mathbf{C}\succeq\mathbf{0}$ )
- 2. suppose  $A \succ 0$ . It holds that  $C \succ 0 \iff B$  has full column rank
- 3. suppose  ${\bf B}$  is nonsingular. It holds that  ${\bf A}\succ {\bf 0}\Longleftrightarrow {\bf C}\succ {\bf 0}$ , and that  ${\bf A}\succeq {\bf 0}\Longleftrightarrow {\bf C}\succ {\bf 0}$ .
- proof sketch: the 1st property is trivial. For the 2nd property, observe

$$\mathbf{C} \succ \mathbf{0} \iff \mathbf{z}^T \mathbf{A} \mathbf{z} > \mathbf{0}, \ \forall \ \mathbf{z} \in \mathcal{R}(\mathbf{B}) \setminus \{\mathbf{0}\}.$$
 (\*)

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

# **Properties of PSD Matrices: Symmetric Factorization**

**Theorem 5.2.** 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  $\mathbf{B} \in \mathbb{R}^{m \times n}$ .

- proof:
  - sufficiency:  $\mathbf{A} = \mathbf{B}^T \mathbf{B} \Longrightarrow \mathbf{x}^T \mathbf{A} \mathbf{x} = \mathbf{x}^T \mathbf{B}^T \mathbf{B} \mathbf{x} = \|\mathbf{B} \mathbf{x}\|_2^2 \ge 0$  for all  $\mathbf{x}$
  - necessity: let  $\Lambda^{1/2} = \operatorname{Diag}(\lambda_1^{1/2}, \dots, \lambda_n^{1/2})$  with  $\lambda_i \geq 0$ .

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

- corollary:  $Ax = 0 \iff Bx = 0$ , so  $\mathcal{N}(A) = \mathcal{N}(B)$  and rank(A) = rank(B)
- corollary:  $\mathbf{A} \in \mathbb{R}^{n \times n}$  is PSD with  $rank(\mathbf{A}) = r$  if and only if there exists a  $\mathbf{B}$  with  $rank(\mathbf{B}) = r$  such that  $\mathbf{A} = \mathbf{B}^T \mathbf{B}$ .
- corollary:  $\mathbf{A} \in \mathbb{R}^{n \times n}$  is PD if and only if there exists a nonsingular  $\mathbf{B} \in \mathbb{R}^{n \times n}$  such that  $\mathbf{A} = \mathbf{B}^T \mathbf{B}$ .
  - While **B** is not unique, there exists one and only one upper-triangular matrix **R** with  $r_{ii} > 0$  s.t.  $\mathbf{A} = \mathbf{R}^T \mathbf{R}$ , which is the Cholesky factorization of **A**.
  - A has an LU (or LDL) factorization with all pivots being positive.

# **Properties of PSD Matrices: Symmetric Factorization**

- ullet the factorization  ${f A}={f B}^T{f B}$  has non-unique factor  ${f B}$ 
  - for any orthogonal  $\mathbf{U} \in \mathbb{R}^{n \times n}$ ,  $\mathbf{B} = \mathbf{U} \mathbf{\Lambda}^{1/2} \mathbf{V}^T$  is a factor for  $\mathbf{A} = \mathbf{B}^T \mathbf{B}$
  - for any orthogonal  $\mathbf{U} \in \mathbb{R}^{n \times n}$ ,  $\mathbf{B} = \mathbf{U}\mathbf{R}$  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  $\mathbf{A} = \mathbf{B}^T \mathbf{B}$
- ${f A}^{1/2}$  is also a symmetric factor
- $\mathbf{A}^{1/2}$  is the *unique PSD* factor for  $\mathbf{A} = \mathbf{B}^T \mathbf{B}$
- ullet  ${f A}^{1/2}$  is called the PSD square root of  ${f A}$ 
  - 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  $\mathbf{A} = \mathbf{B}^2$

#### **Properties for Symmetric Factorization**

**Property 5.2.** 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

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

- proof:
  - observe that  $\dim \mathcal{R}(\mathbf{B}) = \operatorname{rank}(\mathbf{B}) = k$ , which implies  $\mathcal{R}(\mathbf{B}) = \mathbb{R}^k$ .
  - we have  $\mathcal{R}(\mathbf{AB}) = \{ \mathbf{y} = \mathbf{Az} \mid \mathbf{z} \in \mathcal{R}(\mathbf{B}) \} = \{ \mathbf{y} = \mathbf{Az} \mid \mathbf{z} \in \mathbb{R}^k \} = \mathcal{R}(\mathbf{A}).$
- corollary: if  $\mathbf{R}$  is a PSD matrix with factorization  $\mathbf{R} = \mathbf{B}\mathbf{B}^T$  for some full-column rank  $\mathbf{B}$ , then  $\mathcal{R}(\mathbf{R}) = \mathcal{R}(\mathbf{B})$ .

#### **Properties for Symmetric Factorization**

**Property 5.3.** 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

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

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

$$\mathbf{I} = (\mathbf{B}^{\dagger}\mathbf{B})(\mathbf{B}^{\dagger}\mathbf{B})^{T} = \mathbf{B}^{\dagger}(\mathbf{B}\mathbf{B}^{T})(\mathbf{B}^{\dagger})^{T} = \mathbf{B}^{\dagger}(\mathbf{C}\mathbf{C}^{T})(\mathbf{B}^{\dagger})^{T} = (\mathbf{B}^{\dagger}\mathbf{C})(\mathbf{B}^{\dagger}\mathbf{C})^{T},$$
 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  $\mathbf{B}\mathbf{Q}=\mathbf{B}\mathbf{B}^{\dagger}\mathbf{C}=\mathbf{P_{B}C}$ , or equivalently,

$$\mathbf{B}\mathbf{q}_i = \Pi_{\mathcal{R}(\mathbf{B})}(\mathbf{c}_i), \quad i = 1, \dots, k.$$

- from Property 5.2 we see that  $\mathcal{R}(\mathbf{B}) = \mathcal{R}(\mathbf{B}\mathbf{B}^T) = \mathcal{R}(\mathbf{C}\mathbf{C}^T) = \mathcal{R}(\mathbf{C})$ . It follows that  $\Pi_{\mathcal{R}(\mathbf{B})}(\mathbf{c}_i) = \mathbf{c}_i$  for all i.

#### **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 (SDP)
- definition:
  - $-\mathbf{A}\succeq\mathbf{B}$  means that  $\mathbf{A}-\mathbf{B}$  is PSD
  - $A \succ B$  means that A B is PD
  - $\mathbf{A} \not\succeq \mathbf{B}$  means that  $\mathbf{A} \mathbf{B}$  is indefinite
- results that immediately follow from the definition: let  $\mathbf{A}, \mathbf{B}, \mathbf{C} \in \mathbb{S}^n$ .
  - $\mathbf{A} \succeq \mathbf{0}, \alpha \geq 0 \text{ (resp. } \mathbf{A} \succ \mathbf{0}, \alpha > 0) \Longrightarrow \alpha \mathbf{A} \succeq \mathbf{0} \text{ (resp. } \alpha \mathbf{A} \succ \mathbf{0})$
  - $\mathbf{-}\ \mathbf{A},\mathbf{B}\succeq\mathbf{0}\ (\mathsf{resp.}\ \mathbf{A}\succeq\mathbf{0},\mathbf{B}\succ\mathbf{0})\Longrightarrow\mathbf{A}+\mathbf{B}\succeq\mathbf{0}\ (\mathsf{resp.}\ \mathbf{A}+\mathbf{B}\succ\mathbf{0})$
  - $\mathbf{-A}\succeq\mathbf{B},\mathbf{B}\succeq\mathbf{C}\ (\mathsf{resp}.\ \mathbf{A}\succeq\mathbf{B},\mathbf{B}\succ\mathbf{C})\Longrightarrow\mathbf{A}\succeq\mathbf{C}\ (\mathsf{resp}.\ \mathbf{A}\succ\mathbf{C})$
  - $\mathbf{A} \not\succeq \mathbf{B}$  does not imply  $\mathbf{B} \succeq \mathbf{A}$

#### **PSD** Matrix Inequalities

- more results: let  $A, B \in \mathbb{S}^n$ .
  - $-\mathbf{A} \succeq \mathbf{B} \Longrightarrow \lambda_k(\mathbf{A}) \geq \lambda_k(\mathbf{B})$  for all k; the converse is not always true
  - $-\mathbf{A} \succeq \mathbf{I}$  (resp.  $\mathbf{A} \succ \mathbf{I}$ )  $\iff \lambda_k(\mathbf{A}) \ge 1$  for all k (resp.  $\lambda_k(\mathbf{A}) > 1$  for all k)
  - $\mathbf{I} \succeq \mathbf{A}$  (resp.  $\mathbf{I} \succ \mathbf{A}$ )  $\iff \lambda_k(\mathbf{A}) \leq 1$  for all k (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  $\mathbf{A} \succeq \mathbf{B} \succeq \mathbf{0}$ ,  $\det(\mathbf{A}) \ge \det(\mathbf{B})$
  - for  $\mathbf{A} \succeq \mathbf{B}$ ,  $\operatorname{tr}(\mathbf{A}) \ge \operatorname{tr}(\mathbf{B})$
  - for  $\mathbf{A} \succeq \mathbf{B} \succ \mathbf{0}$ ,  $\operatorname{tr}(\mathbf{A}^{-1}) \leq \operatorname{tr}(\mathbf{B}^{-1})$

#### **PSD** Matrix Inequalities

• the Schur complement: let

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

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

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

which is called the Schur complement of C.

We have

$$\mathbf{X}\succeq\mathbf{0} \ (\mathsf{resp.}\ \mathbf{X}\succ\mathbf{0}) \iff \mathbf{S}_{C}\succeq\mathbf{0} \ (\mathsf{resp.}\ \mathbf{S}_{C}\succ\mathbf{0})$$

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

$$1 - \mathbf{b}^T \mathbf{C}^{-1} \mathbf{b} > 0 \iff \mathbf{C} - \mathbf{b} \mathbf{b}^T \succeq \mathbf{0}$$

(prove by yourself)

#### **Application: Spectral Analysis**

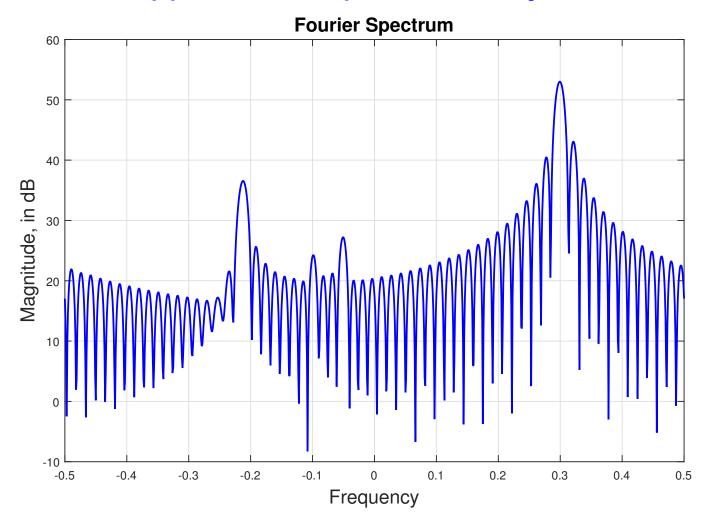
consider the complex harmonic time-series

$$y_t = \sum_{i=1}^k \alpha_i e^{j2\pi f_i t} + w_t, \quad t = 0, 1, \dots, T - 1$$

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  $\{y_t\}_{t=0}^{T-1}$ 
  - can be done by applying the Fourier transform
  - the spectral resolution of Fourier-based methods is often limited by  ${\cal T}$
- 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.  $T=64,\ k=5,\ \{f_1,\ldots,f_k\}=\{-0.213,-0.1,-0.05,0.3,0.315\}.$ 

#### Spectral Analysis via Subspace: Formulation

• let  $z_i = e^{j2\pi f_i}$ . Given a positive integer d, let

$$\mathbf{y}_{t} = \begin{bmatrix} y_{t} \\ y_{t+1} \\ \vdots \\ y_{t+d-1} \end{bmatrix} = \sum_{i=1}^{k} \alpha_{i} \begin{bmatrix} z_{i}^{t} \\ z_{i}^{t+1} \\ \vdots \\ z_{i}^{t+d-1} \end{bmatrix} + \begin{bmatrix} w_{t} \\ w_{t+1} \\ \vdots \\ w_{t+d-1} \end{bmatrix} = \sum_{i=1}^{k} \alpha_{i} \underbrace{\begin{bmatrix} 1 \\ z_{i} \\ \vdots \\ z_{d-1}^{d-1} \end{bmatrix}}_{\mathbf{a}_{t}} z_{i}^{t} + \underbrace{\begin{bmatrix} w_{t} \\ w_{t+1} \\ \vdots \\ w_{t-d+1} \end{bmatrix}}_{\mathbf{w}_{t}}$$

• let  $\mathbf{Y} = [\mathbf{y}_0, \mathbf{y}_1, \dots, \mathbf{y}_{T_d-1}]$  where  $T_d = T - d + 1$ . We can write

$$Y = ADS + W,$$

where  $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_k]$ ,  $\mathbf{D} = \mathrm{Diag}(\alpha_1, \dots, \alpha_k)$ ,  $\mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_{T_d-1}]$ ,

$$\mathbf{S} = egin{bmatrix} 1 & z_1 & z_1^2 & \dots & z_1^{T_d-1} \ 1 & z_2 & z_2^2 & \dots & z_2^{T_d-1} \ dots & & dots \ 1 & z_k & z_k^2 & \dots & z_k^{T_d-1} \end{bmatrix}$$

# 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

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

• (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  $T_d \to \infty$ ,

$$\frac{1}{T_d} \mathbf{S} \mathbf{W}^H \to \mathbf{0}, \qquad \frac{1}{T_d} \mathbf{W} \mathbf{W}^H \to \sigma^2 \mathbf{I}$$

# Spectral Analysis via Subspace: Formulation

- let us summarize
- ullet Model: the correlation matrix  ${f R}_y=rac{1}{T_d}{f Y}{f Y}^H$  is modeled as

$$\mathbf{R}_y = \mathbf{A}\mathbf{\Phi}\mathbf{A}^H + \sigma^2 \mathbf{I}$$

where  $\sigma^2 > 0$  is the noise power;  $\mathbf{\Phi} = \frac{1}{T_d} \mathbf{D} \mathbf{S} \mathbf{S}^H \mathbf{D}^H$ ;  $\mathbf{D} = \mathrm{Diag}(\alpha_1, \dots, \alpha_k)$ ;

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ z_1 & z_2 & & z_k \\ \vdots & \vdots & & \vdots \\ z_1^{d-1} & z_2^{d-1} & \dots & z_k^{d-1} \end{bmatrix} \in \mathbb{C}^{d \times k}, \ \mathbf{S} = \begin{bmatrix} 1 & z_1 & z_1^2 & \dots & z_1^{T_d-1} \\ 1 & z_2 & z_2^2 & \dots & z_2^{T_d-1} \\ \vdots & & & \vdots \\ 1 & z_k & z_k^2 & \dots & z_k^{T_d-1} \end{bmatrix} \in \mathbb{C}^{k \times T_d},$$

with  $z_i = e^{\mathbf{j}2\pi f_i}$ 

• observation: A and S are both Vandemonde

- 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:
  - $-\mathbf{A}$  has full column rank,  $\mathbf{S}$  has full row rank
  - $-\Phi$  is positive definite (and thus nonsingular)
    - \* proof:  $\mathbf{x}^H \mathbf{D} \mathbf{S} \mathbf{S}^H \mathbf{D}^H \mathbf{x} = \|\mathbf{S}^H \mathbf{D}^H \mathbf{x}\|_2^2$ , and  $\mathbf{S}^H \mathbf{D}^H \mathbf{x} = \mathbf{0}$  if and only if  $\mathbf{S}^H$  does not have full column rank
  - $\mathcal{R}(\mathbf{A}\mathbf{\Phi}\mathbf{A}^H) = \mathcal{R}(\mathbf{A})$ , by Property 5.2
  - $-\operatorname{rank}(\mathbf{A}\mathbf{\Phi}\mathbf{A}^H)=\operatorname{rank}(\mathbf{A})=k$ , thus  $\mathbf{A}\mathbf{\Phi}\mathbf{A}^H$  has k nonzero eigenvalues

- consider the eigendecomposition of  $\mathbf{A}\Phi\mathbf{A}^H$ . Let  $\mathbf{A}\Phi\mathbf{A}^H=\mathbf{V}\Lambda\mathbf{V}^H$  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  $i = k + 1, \ldots, d$ ,

$$\mathbf{A}\mathbf{\Phi}\mathbf{A}^H = egin{bmatrix} \mathbf{V}_1 & \mathbf{V}_2 \end{bmatrix} egin{bmatrix} oldsymbol{\Lambda}_1 & oldsymbol{0} \ oldsymbol{0} & oldsymbol{0} \end{bmatrix} egin{bmatrix} \mathbf{V}_1^H \ \mathbf{V}_2^H \end{bmatrix} = \mathbf{V}_1 oldsymbol{\Lambda}_1 \mathbf{V}_1^H$$

where  $\mathbf{V}_1 = [\mathbf{v}_1, \dots, \mathbf{v}_k] \in \mathbb{C}^{d \times k}$ ,  $\mathbf{V}_2 = [\mathbf{v}_{k+1}, \dots, \mathbf{v}_d] \in \mathbb{C}^{d \times (d-k)}$ ,  $\mathbf{\Lambda}_1 = \mathrm{Diag}(\lambda_1, \dots, \lambda_k)$ .

- result:  $\mathcal{R}(\mathbf{A}\mathbf{\Phi}\mathbf{A}^H) = \mathcal{R}(\mathbf{V}_1)$ ,  $\mathcal{R}(\mathbf{A}\mathbf{\Phi}\mathbf{A}^H)^{\perp} = \mathcal{R}(\mathbf{V}_2)$ 

 $\bullet$  consider the eigendecomposition of  $\mathbf{R}_y$ . Observe

$$\mathbf{R}_y = egin{bmatrix} \mathbf{V}_1 & \mathbf{V}_2 \end{bmatrix} egin{bmatrix} \mathbf{\Lambda}_1 + \sigma^2 \mathbf{I} & \mathbf{0} \ \mathbf{0} & \sigma^2 \mathbf{I} \end{bmatrix} egin{bmatrix} \mathbf{V}_1^H \ \mathbf{V}_2^H \end{bmatrix}$$

#### • results:

- $\mathbf{V}(\mathbf{\Lambda} + \sigma^2 \mathbf{I})\mathbf{V}^H$  is the eigendecomposition of  $\mathbf{R}_y$
- ${f V}_1$  can be obtained from  ${f R}_y$  by finding the eigenvectors associated with the first k largest eigenvalues of  ${f R}_y$

- let us summarize
- compute the eigenvector matrix  $\mathbf{V} \in \mathbb{C}^{d \times d}$  of  $\mathbf{R}_y$ . Partition  $\mathbf{V} = [\mathbf{V}_1, \mathbf{V}_2]$  where  $\mathbf{V}_1 \in \mathbb{C}^{n \times k}$  corresponds the first k largest eigenvalues. Then,

$$\mathcal{R}(\mathbf{V}_1) = \mathcal{R}(\mathbf{A}), \qquad \mathcal{R}(\mathbf{V}_2) = \mathcal{R}(\mathbf{A})^{\perp}$$

Idea of subspace methods: let

$$\mathbf{a}(z) = \begin{bmatrix} 1 \\ z \\ \vdots \\ z^{d-1} \end{bmatrix}.$$

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

- Question: it is true that  $f \in \{f_1, \dots f_k\}$  implies  $\mathbf{a}(e^{\mathbf{j}2\pi f}) \in \mathcal{R}(\mathbf{A})$ . But is it also true that  $\mathbf{a}(e^{\mathbf{j}2\pi f}) \in \mathcal{R}(\mathbf{A})$  implies  $f \in \{f_1, \dots f_k\}$ ?
- The answer is yes if d > k. The following matrix result gives the answer.

**Theorem 5.3.** 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

$$z \in \{z_1, \dots, z_k\} \iff \mathbf{a}(z) \in \mathcal{R}(\mathbf{A}).$$

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- proof of Theorem 5.3: " $\Longrightarrow$ " is trivial, and we consider " $\Longleftrightarrow$ "
  - suppose there exists  $\bar{z} \notin \{z_1, \dots, z_k\}$  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

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# Spectral Analysis via Subspace: Algorithm

- there are many subspace methods, and multiple signal classification (MUSIC) is most well-known
- ullet MUSIC uses the fact that  $\mathbf{a}(e^{\mathbf{j}2\pi f}) \in \mathcal{R}(\mathbf{A}) \Longleftrightarrow \mathbf{V}_2^H \mathbf{a}(e^{\mathbf{j}2\pi f}) = \mathbf{0}$

**Algorithm:** MUSIC

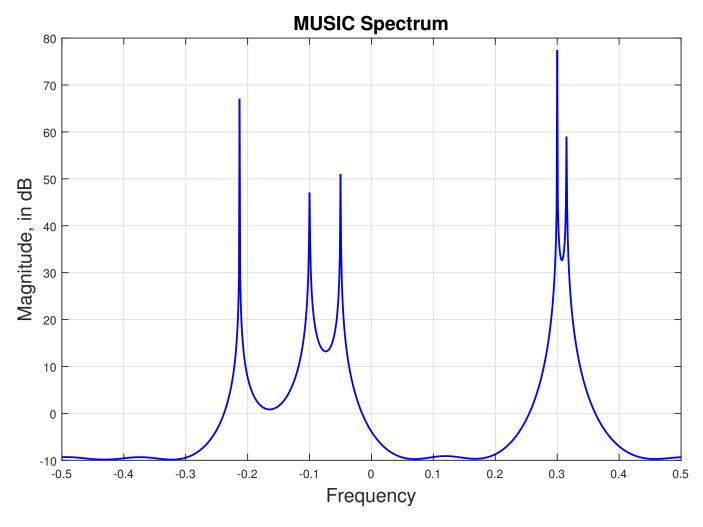
**input:** the correlation matrix  $\mathbf{R}_y \in \mathbb{C}^{d \times d}$  and the model order k < d Perform eigendecomposition  $\mathbf{R}_y = \mathbf{V} \Lambda \mathbf{V}^H$  with  $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$ . Let  $\mathbf{V}_2 = [\ \mathbf{v}_{k+1}, \ldots, \mathbf{v}_d\ ]$ , and compute

$$S(f) = \frac{1}{\|\mathbf{V}_2^H \mathbf{a}(e^{\mathbf{j}2\pi f})\|_2^2}$$

for  $f \in \left[-\frac{1}{2}, \frac{1}{2}\right)$  (done by discretization).

output:  $\bar{S}(\bar{f})$ 

#### **Spectral Analysis via Subspace: Algorithm**

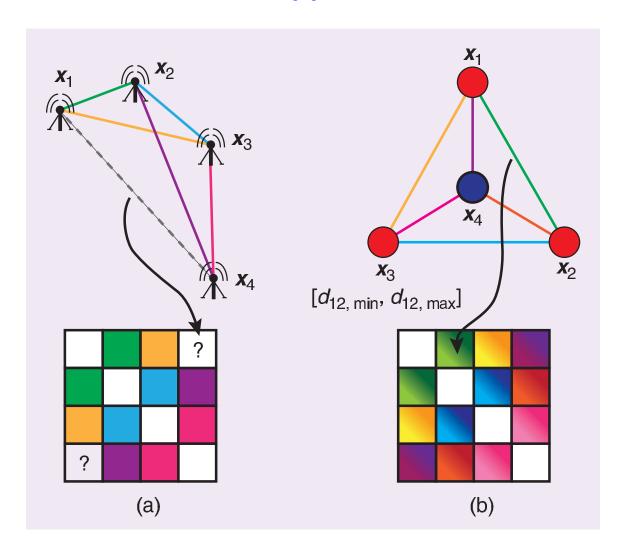


An illustration of the MUSIC spectrum.  $T=64,\ k=5,\ \{f_1,\ldots,f_k\}=\{-0.213,-0.1,-0.05,0.3,0.315\}.$ 

#### **Application: Euclidean Distance Matrices**

- ullet let  $\mathbf{x}_1,\ldots,\mathbf{x}_n\in\mathbb{R}^d$  be a collection of points, and let  $\mathbf{X}=[\ \mathbf{x}_1,\ldots,\mathbf{x}_n\ ]$
- let  $d_{ij} = \|\mathbf{x}_i \mathbf{x}_j\|_2$  be the Euclidean distance between points i and j
- Problem: given  $d_{ij}$ 's for all  $i, j \in \{1, ..., n\}$ , recover X
  - this problem is called the Euclidean distance matrix (EDM) problem
- applications: sensor network localization (SNL), molecular conformation, ....
- suggested reading: [Dokmanić-Parhizkar-et al.'15]

# **EDM Applications**



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

#### **EDM: Formulation**

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

$$r_{ij} = d_{ij}^2 = \|\mathbf{x}_i\|_2^2 - 2\mathbf{x}_i^T\mathbf{x}_j + \|\mathbf{x}_j\|_2^2,$$

we see that  ${f R}$  can be written as

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

where the notation diag means that  $diag(\mathbf{Y}) = [y_{11}, \dots, y_{nn}]^T$  for any square  $\mathbf{Y}$ 

- observation: (\*) also holds if we replace X by
  - $ilde{\mathbf{X}} = [\mathbf{x}_1 + \mathbf{b}, \dots, \mathbf{x}_n + \mathbf{b}]$  for any  $\mathbf{b} \in \mathbb{R}^d$   $(d_{ij} = \| ilde{\mathbf{x}}_i ilde{\mathbf{x}}_j\|_2$  is also true)
  - $\tilde{\mathbf{X}} = \mathbf{Q}\mathbf{X}$  for any orthogonal  $\mathbf{Q}$   $(\tilde{\mathbf{X}}^T\tilde{\mathbf{X}} = \mathbf{X}^T\mathbf{X})$
- ullet implication: recovery of  ${f X}$  from  ${f R}$  is subjected to translations and rotations/reflections
  - in SNL we can use anchors to fix this issue

#### **EDM: Formulation**

ullet assume  ${f x}_1={f 0}$  w.l.o.g. Then,

$$\mathbf{r}_{1} = \begin{bmatrix} \|\mathbf{x}_{1} - \mathbf{x}_{1}\|_{2}^{2} \\ \|\mathbf{x}_{2} - \mathbf{x}_{1}\|_{2}^{2} \\ \vdots \\ \|\mathbf{x}_{n} - \mathbf{x}_{1}\|_{2}^{2} \end{bmatrix} = \begin{bmatrix} 0 \\ \|\mathbf{x}_{2}\|_{2}^{2} \\ \vdots \\ \|\mathbf{x}_{n}\|_{2}^{2} \end{bmatrix}, \quad \operatorname{diag}(\mathbf{X}^{T}\mathbf{X}) = \begin{bmatrix} \|\mathbf{x}_{1}\|_{2}^{2} \\ \|\mathbf{x}_{2}\|_{2}^{2} \\ \vdots \\ \|\mathbf{x}_{n}\|_{2}^{2} \end{bmatrix} = \mathbf{r}_{1}$$

ullet construct from  ${f R}$  the following matrix

$$\mathbf{G} = -\frac{1}{2}(\mathbf{R} - \mathbf{1}\mathbf{r}_1^T - \mathbf{r}_1\mathbf{1}^T).$$

We have

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

ullet idea: do a symmetric factorization for G to try to recover X

#### **EDM: Method**

- assumption: X has full row rank
- **G** is PSD and has  $rank(\mathbf{G}) = d$
- denote the eigendecomposition of G as  $G = V\Lambda V^T$ . Assuming  $\lambda_1 \geq \ldots \geq \lambda_n$ , it takes the form

$$\mathbf{G} = \begin{bmatrix} \mathbf{V}_1 & \mathbf{V}_2 \end{bmatrix} \begin{bmatrix} \mathbf{\Lambda}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{V}_1^T \\ \mathbf{V}_2^T \end{bmatrix} = (\mathbf{\Lambda}_1^{1/2} \mathbf{V}_1^T)^T (\mathbf{\Lambda}_1^{1/2} \mathbf{V}_1^T)$$

where  $\mathbf{V}_1 \in \mathbb{R}^{n \times d}$ ,  $\mathbf{\Lambda}_1 = \mathrm{Diag}(\lambda_1, \ldots, \lambda_d)$ 

- ullet EDM solution: take  $\hat{\mathbf{X}} = \mathbf{\Lambda}^{1/2} \mathbf{V}_1^T$  as an estimate of  $\mathbf{X}$
- ullet recovery guarantee: by Property 5.3, we have  $\hat{\mathbf{X}} = \mathbf{Q}\mathbf{X}$  for some orthogonal  $\mathbf{Q}$

#### **EDM: Further Discussion**

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

$$rank(\mathbf{R}) \le rank(\mathbf{1}(\operatorname{diag}(\mathbf{X}^T\mathbf{X}))^T) + rank(-2\mathbf{X}^T\mathbf{X}) + rank((\operatorname{diag}(\mathbf{X}^T\mathbf{X}))\mathbf{1}^T)$$

$$\le 1 + d + 1 = d + 2$$

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

#### References

[Brodie-Daubechies-et al.'09] J. Brodie, I. Daubechies, C. De Mol, D. Giannone, and I. Loris, "Sparse and stable Markowitz portfolios," *Proceedings of the National Academy of Sciences*, vol. 106, no. 30, pp. 12267–12272, 2009.

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