Dimensionality Reduction Part 2: MDS

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Dimensionality Reduction

- Linear methods
  - PCA (Principal Component Analysis)
  - **cMDS** (Classical Multidimensional Scaling)
- Non-linear methods
  - KPCA (Kernel PCA)
  - **mMDS** (Metric MDS)
  - Isomap
  - LLE (Locally Linear Embedding)
  - Laplacian Eigenmap
  - t-SNE (t-distributed Stochastic Neighbor Embedding)
  - UMAP (Uniform Manifold Approximation and Projection)

Multidimensional Scaling (MDS)

- Classical MDS (cMDS)
  - Reconstruct coordinates from **Euclidean distance** matrix
- Metric MDS (mMDS)
  - Redefined cMDS problem with loss function defined on any metric
- Non-metric MDS (nMDS)
  - When only an ordering on the distances is known
- Generalized (kernel) classical MDS

Classical MDS (cMDS)

- Reconstruct a set of points given their **Euclidean distances**
- Given $n \times n$ distance matrix $D = (d_{ij})$, reconstruct coordinates $x_1, \dots, x_n \in \mathbb{R}^m$ with $\|x_i - x_j\| = d_{ij}$
  - The solution $X = [x_1 \quad \cdots \quad x_n]^{\mathrm{T}} \in \mathbb{R}^{n \times m}$ is not unique due to infinitely many translations, rotations, and reflections
  - A centered solution $X = (x_{ij})$ (i.e. $\forall k, 1 \leq k \leq m, \sum_i x_{ik} = 0$) can be found using cMDS
    - Note that solution is still not unique

cMDS idea

- Given $D = (d_{ij})$, first note that Euclidean distance d_{ij} is related to $X = (x_{ij})$ through

$$(d_{ij})^2 = (x_i - x_j)^{\mathrm{T}}(x_i - x_j) = x_i^{\mathrm{T}} x_i + x_j^{\mathrm{T}} x_j - 2x_i^{\mathrm{T}} x_j$$

- On the other hand, for X where $\forall k, 1 \leq k \leq m,$ $\sum_i x_{ik} = 0$, we can show that

$$A = -2XX^{\mathrm{T}}$$

  where $A = (d_{ij}^2)$
- Then it suffices that we compute $-A/2$ to obtain XX^{T}
- Finally, since XX^{T} can be decomposed to recover X

cMDS algorithm

- **Step 1**. Compute matrix CAC

  Given $D = (d_{ij})$, computed CAC

  where

  $A = \left(-\frac{1}{2}d_{ij}^2\right)$

  $C = I - \frac{1}{n}\mathbf{1}^{\mathrm{T}}\mathbf{1}$

  - CAC simultaneously centers the rows and columns of the squared distance matrix A (double centering)
  - It can be shown that $CAC = XX^{\mathrm{T}}$ for centered X (proof in later slides)

    $\Rightarrow$ CAC is positive semi-definite (proof later)

    $\Rightarrow$ CAC decompose to non-negative values

cMDS algorithm

- **Step 2**. Decompose CAC into orthonormal basis

  Method 1: Eigendecompose CAC into $Q\Lambda Q^{\mathrm{T}}$
  - Then, X can be computed as $Q\Lambda^{1/2}$
    - $Q\Lambda Q^{\mathrm{T}} = Q\Lambda^{1/2}\Lambda^{1/2}Q^{\mathrm{T}} = Q\Lambda^{1/2}\left(Q\Lambda^{1/2}\right)^{\mathrm{T}} = XX^{\mathrm{T}}$

  Method 2: Decompose CAC directly into XX^{T} using Cholesky factorization
  - Only works if CAC is positive definite
  - CAC is (positive semi-definite and) positive definite iff all x_i are linearly independent
    - Cholesky in numpy/scipy will not execute unless the input is positive definite
    - Use one that works (e.g. pyre) or write your own with pivoting

cMDS algorithm

- **Step 3**. Choose from the decomposed basis

  Both methods face the problem that the output matrix is not of dimension $n \times m$
  - Eigendecomposition $Q \in \mathbb{R}^{n \times n}$
  - Cholesky factorization $L \in \mathbb{R}^{n \times n}$

- If $n < m$ (fewer datapoints than features)
  - No problem in embedding the points since n points can fit on an $(n-1)$-D plane
  - Naturally suited for dimensionality reduction purpose if use all $n-1$ eigenvectors
    - If need fewer than $(n-1)$-D space, see later slides

cMDS algorithm

- **Step 3**. Choose from the decomposed basis

  Both methods face the problem that the output matrix is not of dimension $n \times m$

  - Eigendecomposition $Q \in \mathbb{R}^{n \times n}$
  - Cholesky factorization $L \in \mathbb{R}^{n \times n}$

- If $n > m$ (more datapoints than features)

  Problem 1

  - CAC is not positive definite since there are insufficient features for linear independence
    - Bad news for Cholesky factorization

cMDS algorithm

- **Step 3**. Choose from the decomposed basis

  Both methods face the problem that the output matrix is not of dimension $n \times m$
  - Eigendecomposition $Q \in \mathbb{R}^{n\times n}$
  - Cholesky factorization $L \in \mathbb{R}^{n\times n}$

- If $n > m$ (more datapoints than features)

  Problem 2
  - Need to deduce m (or fewer) vectors
    - In an ideal eigendecomposition there will be $\mathrm{rank}\left(XX^\mathrm{T}\right)$ $(\leq m)$ positive eigenvalues and $n - \mathrm{rank}(XX^\mathrm{T})$ zero eigenvalues
    - But eigendecomposition usually not ideal with zero eigenvalues, often resulting in complex numbers

cMDS algorithm

- **Step 3**. Choose from the decomposed basis
  - Many implementations will output negative eigenvalues, so extra care is needed
  - For eigendecomposition
    - Remove the eigenpairs with small, negative, or complex eigenvalues, forming Q_1 and Λ_1
    - Choose the set of eigenvalues S from Λ_1 such that $\frac{\sum_{\lambda' \in S} \lambda'}{\sum_{\lambda \in \Lambda_1} \lambda}$ is sufficiently large
    - Finally, compute $Q_1 \Lambda_1^{1/2}$ and retain only those in S
    - Remove extraneous dimensions in $Q_1 \Lambda_1^{1/2}$
  - For Cholesky factorization
    - Choose the vectors with the largest norms

(Proof) $XX^{\mathrm{T}} = CAC$ for centered X

- Will expand XX^{T} and CAC and show equivalence
- Given $X \in \mathbb{R}^{m\times n}$, denote XX^{T} as B, then we can write the Euclidean distance between x_i and x_j as

$$d_{ij}^2 = b_{ii} + b_{jj} - 2b_{ij} \tag{1}$$

- If $\forall k$, $\sum_i x_{ik} = 0$ (X is centered), then

$$\sum_{j=1}^n b_{ij} = \sum_{j=1}^n \sum_{k=1}^m x_{ik}x_{jk} = \sum_{k=1}^m x_{ik}\left(\sum_{j=1}^n x_{jk}\right) = 0$$

Denote $\mathrm{tr}(B) = \sum_{i=1}^n b_{ii}$, $\because \sum_{j=1}^n b_{ij} = 0$, (1) $\Rightarrow$

$$\left.\begin{aligned} \sum_{i=1}^n d_{ij}^2 &= \sum_{i=1}^n b_{ii} + \sum_{i=1}^n b_{jj} = \mathrm{tr}(B) + nb_{jj} \\ \sum_{j=1}^n d_{ij}^2 &= \sum_{j=1}^n b_{ii} + \sum_{j=1}^n b_{jj} = nb_{ii} + \mathrm{tr}(B) \\ \sum_{i,j=1}^n d_{ij}^2 &= \sum_{i,j=1}^n b_{ii} + \sum_{i,j=1}^n b_{jj} = 2n\mathrm{tr}(B) \end{aligned}\right\} (2)$$

(Proof) $XX^{\mathrm{T}} = CAC$ for centered X

Rewrite (1) as $b_{ij} = \frac{1}{2}\left(b_{ii} + b_{jj} - d_{ij}^2\right)$, then (1)+(2)

$$b_{ij} = \frac{1}{2}\left(\frac{1}{n}\left(\sum_{i=1}^{n} d_{ij}^2 - \mathrm{tr}(B) + \sum_{j=1}^{n} d_{ij}^2 - \mathrm{tr}(B)\right) - d_{ij}^2\right)$$

$$= \frac{1}{2}\left(\frac{1}{n}\left(\sum_{i=1}^{n} d_{ij}^2 + \frac{1}{n}\sum_{j=1}^{n} d_{ij}^2 - \frac{1}{n}\sum_{i,j=1}^{n} d_{ij}^2\right) - d_{ij}^2\right)$$

Done, but for notation simplicity let $a_{ij} = -\frac{1}{2}d_{ij}^2$, then

$$b_{ij} = -\frac{1}{n}\sum_{i=1}^{n} a_{ij} - \frac{1}{n}\sum_{j=1}^{n} a_{ij} + \frac{1}{n^2}\sum_{i,j=1}^{n} a_{ij} + a_{ij}$$

Further make things easy to see with

$$a_{i\blacksquare} = \frac{1}{n}\sum_{i=1}^{n} a_{ij},\ a_{\blacksquare j} = \frac{1}{n}\sum_{j=1}^{n} a_{ij},\ a_{\blacksquare\blacksquare} = \frac{1}{n^2}\sum_{i,j=1}^{n} a_{ij}$$

$$\Rightarrow b_{ij} = a_{ij} - a_{i\blacksquare} - a_{\blacksquare j} + a_{\blacksquare\blacksquare}$$

(Proof) $XX^{\mathrm{T}} = CAC$ for centered X

- Now expand CAC into terms consisting of a_{ij}

  Given $A = (a_{ij})$, observe that

$$\left.\begin{aligned} [1\ 1\ \ldots 1]A &= n(a_{i\blacksquare}) \\ A[1\ 1\ \ldots 1] &= n(a_{\blacksquare j}) \\ [1\ 1\ \ldots 1]A[1\ 1 \ldots 1] &= n^2(a_{\blacksquare\blacksquare}) \end{aligned}\right\} \text{(3)}$$

  On the other hand,

$$\begin{aligned} CAC &= \left(I - \frac{1}{n}J\right) A \left(I - \frac{1}{n}J\right) \\ &= A - \frac{1}{n}JA - \frac{1}{n}AJ + \frac{1}{n^2}JAJ \qquad \text{(4)} \end{aligned}$$

  Finally, (3)+(4) gives

$$(CAC)_{ij} = a_{ij} - a_{i\blacksquare} - a_{\blacksquare j} + a_{\blacksquare\blacksquare} = b_{ij}$$

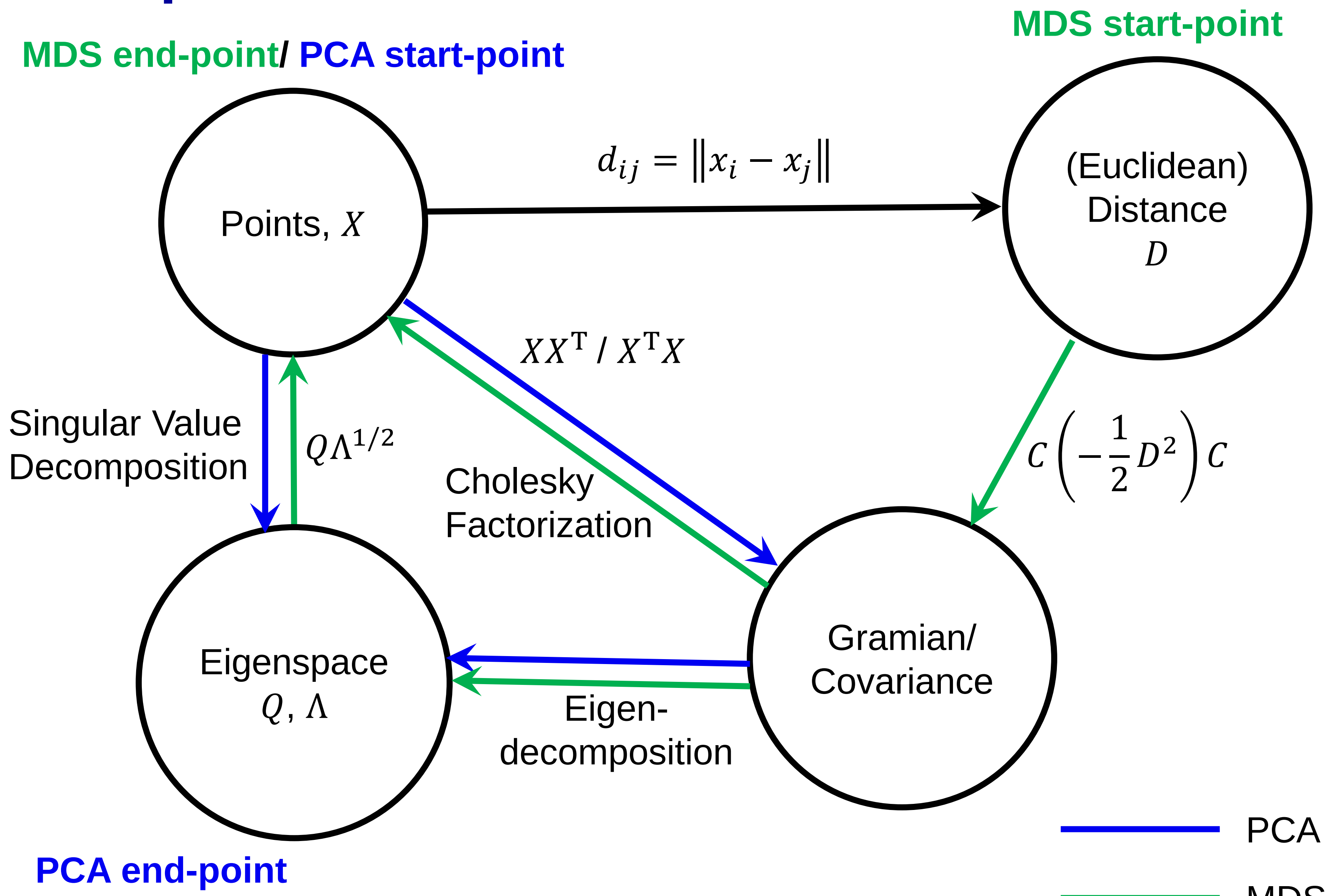
(Proof) CAC is PSD

- Follows immediately from the fact that $CAC = XX^{\mathrm{T}}$, an inner product
  - An inner product $B = XX^{\mathrm{T}}$ of any matrix X (centered or not) is called a Gram matrix, or Gramian
  - Gramians are known to be positive semi-definite (see proof in other slides)

Comparison with PCA

	MDS	**PCA**
Input	$n \times n$ Euclidean distances D	$n \times m$ Dataset X
Matrix considered in theory	$n \times n$ Gramian XX^{T}	$m \times m$ Covariance matrix $X^{\mathrm{T}}X$
Matrix used for decomposition	CAC where $A = -\frac{1}{2}D^2$ and C is the centering matrix	XX^{T} or $X^{\mathrm{T}}X$
Output	Reconstructed X Alternatively, X in lower dimension	Principal components of $X^{\mathrm{T}}X$ (or XX^{T})
Decomposition Method	Cholesky factorization or Eigendecomposition	SVD or Eigendecomposition
$n < m$	Exact reconstruction of X impossible	No problem
$m < n$	For exact reconstruction of X, rank deficiency revealed in eigendecomposition needed to deduce m	No problem

Comparison with PCA



Limitation of cMDS

- For cMDS to work, input distances have to be Euclidean
- More precisely, the Pythagorean principle

$$\left(d_{ij}\right)^2 = \left(x_i - x_j\right)^{\mathrm{T}}\left(x_i - x_j\right)$$

  (or, in terms of the Gramian, $d_{ij}^2 = b_{ii} + b_{jj} - 2b_{ij}$)

  is used in establishing the relation $XX^{\mathrm{T}} = CAC$

  - Such a relationship cannot be assumed for most datasets

- $XX^{\mathrm{T}} = CAC$ does not hold for other metrics

Metric MDS (mMDS)

- Given distance matrix $\left(\delta_{ij}\right)_{n\times n}$ and weights $\left(w_{ij}\right)_{n\times n}$, find $X = [x_1 \quad \cdots \quad x_n]^\mathrm{T}$ where $x_i \in \mathbb{R}^r$, which minimizes

$$\mathrm{stress}(X) = \sum_{i,j,i<j} w_{ij}\left(d\left(x_i, x_j\right) - \delta_{ij}\right)^2$$

where $d\left(x_i, x_j\right)$ denotes the distance between x_i and x_j

  - The weights w_{ij} allow removing entries where δ_{ij} is not available

SMACOF Algorithm for mMDS

- Minimize $\mathrm{stress}(X)$ through majorization
- $\mathrm{stress}(X) = \sum_{i,j,i<j} w_{ij}\left(d(x_i, x_j) - \delta_{ij}\right)^2$

$$= \sum w_{ij} d^2\left(x_i, x_j\right) + \sum w_{ij}\delta_{ij}^2 - 2\sum w_{ij}\delta_{ij} d\left(x_i, x_j\right)$$

Since

- $\sum w_{ij}\delta_{ij}^2$ is constant, C
- $\sum w_{ij} d^2\left(x_i, x_j\right)$ is quadratic, $\mathrm{tr}(X'VX)$
- $\sum w_{ij}\delta_{ij} d\left(x_i, x_j\right) = \mathrm{tr}(X'B(X)X) \geq \mathrm{tr}(X')B(Z)Z$

  where $B(Z) = \left(b_{ij}\right)$ for

$$b_{ij} = \begin{cases} -\frac{w_{ij}\delta_{ij}}{d(x_i, x_j)} & \text{if } d\left(x_i, x_j\right) \neq 0 \text{ and } i \neq j \\ 0 & \text{if } d\left(x_i, x_j\right) = 0 \text{ and } i \neq j \end{cases}$$

$$b_{ii} = -\sum_{j=1, j\neq i}^{n} b_{ij}$$

SMACOF Algorithm for mMDS

- $\text{stress}(X) = C + \text{tr}(X'VX) - 2\text{tr}(X'B(X)X)$ which is bounded above by $C + \text{tr}(X'VX) - 2\text{tr}(X'B(Z)Z) = \tau(X, Z)$
- Majorization iteratively updates X^k at the k^{th} iteration to $\min_X \tau(X, X^{k-1})$
  - $\text{stress}(X)$ will decrease monotonically
  - Stops iteration when $\text{stress}(X^k) - \text{stress}(X^{k-1})$ is below a given threshold
- Proofs for the majorization method requires too much details to provide here

Sammon mapping

- A special case of $\text{stress}(X)$ where weights are inversely proportional to distance δ_{ij}
  - Emphasize accuracy on small δ_{ij} distances
- Given distance matrix $\left(\delta_{ij}\right)_{n\times n}$, find $X = [x_1 \quad \dots \quad x_n]^{\mathrm{T}}$ where $x_i \in \mathbb{R}^r$, which minimizes

$$\text{stress}(X) = \frac{1}{\sum_{i,j,i<j} \delta_{ij}} \sum_{i,j,i<j} \frac{\left(d\left(x_i, x_j\right) - \delta_{ij}\right)^2}{\delta_{ij}}$$

  where $d\left(x_i, x_j\right)$ denotes the distance between x_i and x_j
- The simpler $\text{stress}(X)$ allows a gradient descent optimization

nMDS vs cMDS

- Similarity vs dissimilarity
  - cMDS attempts to recover XX^{T}, a measure of the similarity between x_i and x_j
  - nMDS attempts to recover distances $d\left(x_i, x_j\right)$, a measure of the dissimilarity between x_i and x_j
- Linear vs non-linear
  - cMDS attempts to recover XX^{T}, a linear kernel
  - nMDS, for instance Sammon mapping, can be considered as recovering a non-linear distance measure with an inverse ($1/\delta$) factor
- Closed-form vs iterative method
  - cMDS is solved through a closed-form solution
  - nMDS can only be approximated iteratively using gradient descent or majorization