DD2434 Machine Learning, Advanced Course

Module 7 : high-dimensional data and dimensionality reduction

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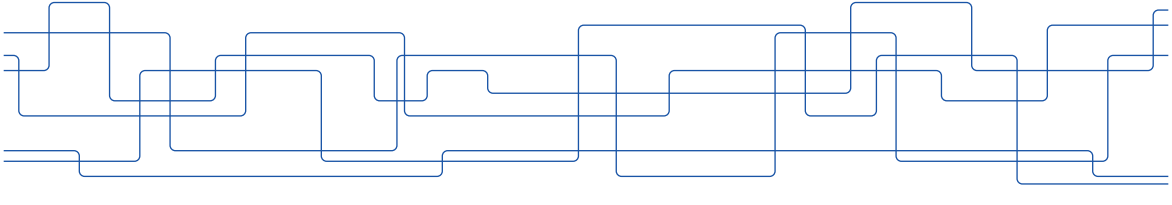


overview of module 7

- high-dimensional data in machine learning
- basic principles of dimensionality reduction
- singular value decomposition (SVD) and eigen-decomposition
- principal component analysis (PCA)
- multidimensional scaling (MDS)
- isomap

reading material

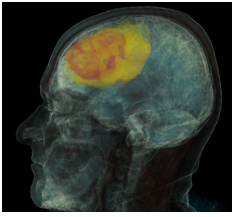
- Lee and Verleysen. Nonlinear dimensionality reduction. Springer, 2007

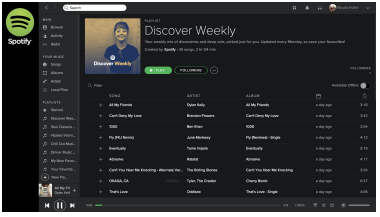
  chapters 1, 2, and 4

  available online in the KTH-library website

machine learning today

- at the heart of an ongoing technological revolution and societal transformation





consider:

- autonomous vehicles
- healthcare (medical imaging, diagnostics, drug design, treatment, etc.)
- recommendation systems (netflix, amazon, etc.)
- searching for information in the web or social media
- intelligent interfaces (personal assistants, face recognition, speech recognition, etc.)
- . . . and many more . . .

data is at the center of machine learning

- data is collected everywhere nowadays
  - in human activities (mobile devices, traffic, sensors, surveillance data, etc.)
  - in science (climate, geological sensing, tracking of animals, biological data, etc.)
  - in industrial processes (monitoring of processes, products, materials)
- data can be used to
  - visualize and gain insights
  - acquire knowledge and make new discoveries
  - validate scientific hypotheses
  - build models, make predictions, optimize processes

data types

- many different types of data
  - relational data
  - text data
  - time series
  - sequential data
  - spatio-temporal data
  - graphs / networks

a very common data representation

- data is a set of observations; each observation consists of values over a set of attributes
  - observations are also called points, or samples
  - attributes are also called dimensions, or variables, or features
- such data is represented by a matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$,

  where n is the number of points and d the number of dimensions

$$\mathbf{Y} = \begin{pmatrix} y_{11} & y_{12} & \cdots & y_{1d} \\ y_{21} & y_{22} & \cdots & y_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ y_{n1} & y_{n2} & \cdots & y_{nd} \end{pmatrix}$$

- sometimes attributes correspond to rows and observations to columns; we make it explicit
- very often data values are not numerical, e.g., categorical
  - it often pays off to transform them to numerical
- in some cases the data values are binary; such data are called transactional

examples of data that can be represented as a matrix

- text data : points = documents, dimensions = words

  $y_{ij} = \{$number of times that document i contains word $j\}$

- movie-ratings data : points = users, dimensions = movies

  $y_{ij} = \{$the rating of user i for movie $j\}$

- purchase data : points = customers, dimensions = products

  $y_{ij} = 1$, if customer i has purchased product j, 0 otherwise (binary)

- stock-market time-series data : points = traded commodities, dimensions = time

  $y_{ij} = \{$the price of commodity i at time $j\}$

  (note that time imposes a natural order on the dimensions)

- social networks : points = individuals, dimensions = individuals

  $y_{ij} = 1$, if individuals i and j are friends, 0 otherwise (binary)

  (note that points and dimensions are the same set of individuals)

data dimensionality can be very large

- *dimensionality* = the number of dimensions of the data
- consider the previous examples
  - tens/hundreds of thousands, or millions, of words, movies, products, individuals, ...
- working with high-dimensional data can be very challenging
- the curse of dimensionality
  - phenomena/challenges that appear when working with high-dimensional data

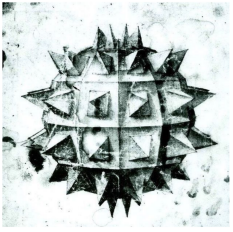
the curse of dimensionality

a term that refers collectively to a number of different phenomena and challenges

- the "host space" of the data increases exponentially with the dimension
  - as a result, high-dimensional data tend to be very sparse
  - also, optimization by exhaustive enumeration is not possible
- certain computational tasks become very challenging
  - e.g., for nearest-neighbor search, it is difficult to do better than exhaustive search
- a large number of dimensions may be irrelevant
  - e.g., may not have any predictive power in a classification task
- visualizing high-dimensional data is difficult
- the geometry of high-dimensional data becomes not intuitive

surprising properties of high-dimensional data

1. "spiky" (but convex) hypercubes



- volume of d-dimensional sphere: $V_s(r) = \pi^{d/2} r^d / \Gamma(1 + d/2)$
- volume of d-dimensional cube: $V_c(r) = (2r)^d$
- it follows

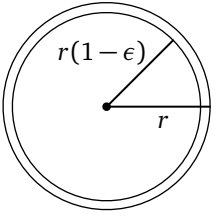
$$\lim_{d \to \infty} \frac{V_s(r)}{V_c(r)} = 0$$

- an exponential number of cube corners "go out" from the sphere
  these corners occupy all the available volume
- e.g., for $r = 1/2$, $V_c(1/2) = 1$, but $\lim_{d \to \infty} V_s(1/2) = 0$
  so, the volume of the sphere vanishes, when dimensionality increases

2. volume of a thin spherical shell

- consider the relative hyper-volume of a thin spherical shell

$$\frac{V_s(r) - V_s((1-\epsilon)r)}{V_s(r)} = \frac{1^d - (1-\epsilon)^d}{1^d} \xrightarrow[d\to\infty]{} 1$$



so, when dimensionality increases, the thin shell contains almost all the volume

3. diagonal of a hypercube

- consider a diagonal of the hypercube $\mathbf{v} = (\pm 1, \ldots, \pm 1)^T$
- and the i-th coordinate axis vector $\mathbf{e}_i = (0, \ldots, 0, 1, 0, \ldots, 0)^T$
- the cosine of their angle is

$$\cos\langle \mathbf{v}, \mathbf{e}_i \rangle = \frac{\mathbf{v}^T \mathbf{e}}{\|\mathbf{v}\| \|\mathbf{e}_i\|} = \frac{\pm 1}{\sqrt{d}} \xrightarrow[d \to \infty]{} 0$$

so, diagonals are nearly orthogonal to all coordinates axes

- we can also show : a random vector is nearly orthogonal to all coordinates axes

4. properties of the unit sphere

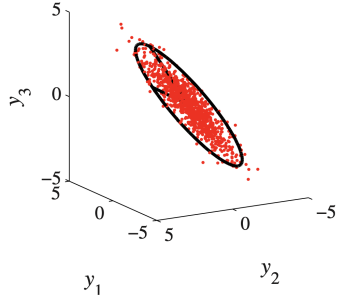
- most vectors lie on the surface of the sphere
- most vectors lie on the "equator"
- most vectors are nearly orthogonal
- most vectors have almost the same distance

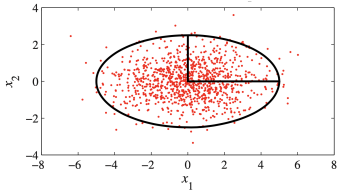
how to cope with high-dimensional data?

- quantify relevance of dimensions (variables), and possibly eliminate irrelevant dimensions
  - a.k.a., feature selection
  - the idea is applied mainly to supervised learning, where we can measure the correlation of variables (or subsets of variables) with the target
- explore correlations between dimensions
  - often pairs (or larger sets) of dimensions are correlated
  - e.g., a subset of dimensions can be explained by a single phenomenon which can be quantified by a latent dimension
  - in such a case we may want to keep only one of the correlated dimensions,
  - or we may want to transform the correlated dimensions into a new (smaller) set of dimensions, which reveal the latent dimensions
  - implementation of these ideas is known as dimensionality reduction

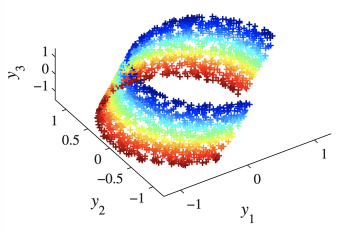
data may reside in lower-dimensional manifolds

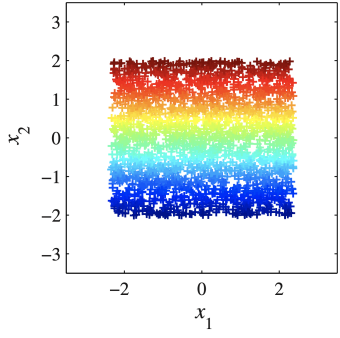
linear manifolds





non-linear manifolds

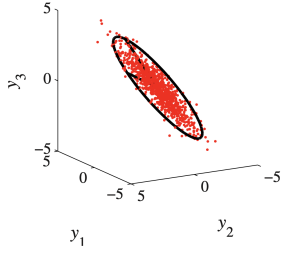


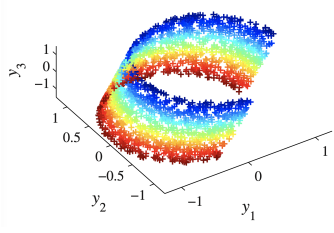


data may reside in lower-dimensional manifolds

- dimensionality reduction can be used to reveal hidden manifolds,
  and represent the data in the latent manifold dimensionality

- motivated by the idea that lower-dimensional manifolds can be either linear or non-linear,
  we have developed methods for linear dimensionality reduction
  or non-linear dimensionality reduction





objectives of dimensionality reduction

- dealing with high-dimensional data is challenging

thus, we need to develop methods to

- embed data in order to reduce their dimensionality
- embed data in order to recover (a potentiall smaller number of) latent variables
- estimate the number of latent variables

a high-level view of dimensionality reduction

- a data point is represented by a vector $\mathbf{y} = (y_1, \ldots, y_d)^T \in \mathbb{R}^d$

  the data is a set of data points $\mathcal{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$

  equivalently, the data is represented by a matrix $\mathbf{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_n) \in \mathbb{R}^{d \times n}$

  (notice that rows represent dimensions and columns represent points)

- the goal of dimensionality reduction is to map the data from $\mathbb{R}^d$ to $\mathbb{R}^k$, with $k \ll d$
  - thus, we want to find a mapping

$$\mathrm{cod} : \mathbb{R}^d \to \mathbb{R}^k, \quad \mathbf{y} \mapsto \mathbf{x} = \mathrm{cod}(\mathbf{y})$$

- the inverse mapping should bring the mapped data close to the original data
  - to reason about this, we use the inverse mapping

$$\mathrm{dec} : \mathbb{R}^k \to \mathbb{R}^d, \quad \mathbf{x} \mapsto \mathbf{y} = \mathrm{dec}(\mathbf{x})$$

linear vs. non-linear dimensionality reduction

- a linear dimensionality reduction method uses linear mappings cod and dec
- a non-linear dimensionality reduction method uses non-linear mappings cod and dec

dimensionality reduction criterion

- to formalize the dimensionality-reduction problem, we need to define an optimization criterion, which captures our intuition about the quality of the dimensionality-reduction mapping
- a commonly-used criterion is mean square error

$$E_{\mathrm{cod},\mathrm{dec}} = \mathbb{E}_{\mathbf{y}}\left[\|\mathbf{y} - \mathrm{dec}(\mathrm{cod}(\mathbf{y}))\|_2^2\right]$$

- other criteria exist, e.g.,
  - maximize the variance of the data on the embedded space
  - make the latent variables independent
  - ...

dimensionality reduction — general scheme

a dimensionality-reduction method has the following components

- a model to specify our data type and the mappings cod and dec
- a criterion to be optimized
- an algorithm to be used to optimize the criterion

the goal is to find optimal mappings cod and dec, within the specified model, which optimize the desired criterion

categorization of dimensionality-reduction methods

- linear vs. non-linear model
- continuous vs. discrete model
- integrated vs. external estimation of the dimensionality
- layered vs. standalone embedding
- batch vs. online algorithm
- exact vs. approximate optimization

matrix decompositions

- we wish to decompose a matrix $\mathbf{A}$ by writing it as a product of two or more matrices:

$$\mathbf{A}_{m\times n} = \mathbf{B}_{m\times k}\,\mathbf{C}_{k\times n} \quad \text{or} \quad \mathbf{A}_{m\times n} = \mathbf{B}_{m\times k}\,\mathbf{C}_{k\times r}\,\mathbf{D}_{r\times n}$$

  ideally k and r are much smaller than m and n

- such a decomposition can yield insights about the nature of matrix $\mathbf{A}$

  or, it can be useful to solve some problem at hand

the singular value decomposition (SVD)

- theorem : any $m \times n$ matrix $\mathbf{A}$, with $m \geq n$, can be factorized into

$$\mathbf{A} = \mathbf{U} \begin{pmatrix} \mathbf{\Sigma} \\ \mathbf{0} \end{pmatrix} \mathbf{V}^T$$

where $\mathbf{U} \in \mathbb{R}^{m \times m}$ and $\mathbf{V} \in \mathbb{R}^{n \times n}$ are orthonormal (i.e., $\mathbf{U}^T\mathbf{U} = \mathbf{I}_{m \times m}$ and $\mathbf{V}^T\mathbf{V} = \mathbf{I}_{n \times n}$) and $\mathbf{\Sigma} \in \mathbb{R}^{n \times n}$ is diagonal

$$\mathbf{\Sigma} = \mathrm{diag}(\sigma_1, \ldots, \sigma_n), \quad \text{where} \quad \sigma_1 \geq \ldots \geq \sigma_n \geq 0$$

- "skinny" version of SVD : $\mathbf{A} = \mathbf{U}_1 \mathbf{\Sigma} \mathbf{V}^T$, where $\mathbf{U}_1 \in \mathbb{R}^{m \times n}$

singular values and singular vectors

- the diagonal elements σ_j of $\mathbf{\Sigma}$ are the singular values of the matrix $\mathbf{A}$
- the columns of $\mathbf{U}$ and $\mathbf{V}$ are the left singular vectors and right singular vectors, resp.
- equivalent form of SVD

$$\mathbf{A}\,\mathbf{v}_j = \sigma_j\,\mathbf{u}_j \quad \text{and} \quad \mathbf{A}^T\mathbf{u}_j = \sigma_j\,\mathbf{v}_j$$

- outer-product form

$$\mathbf{A} = \mathbf{U}_1\mathbf{\Sigma}\mathbf{V}^T = (\mathbf{u}_1 \dots \mathbf{u}_n) \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} (\mathbf{v}_1 \dots \mathbf{v}_n)^T = \sum_{j=1}^{n} \sigma_j\,\mathbf{u}_j\mathbf{v}_j^T$$

which is a sum of rank-one matrices (each term $\sigma_j\,\mathbf{u}_j\mathbf{v}_j^T$ is a rank-one matrix)

matrix approximation using the singular-value decomposition

- theorem : let $\mathbf{A} = \mathbf{U}\,\mathbf{\Sigma}\,\mathbf{V}^T$ be the singular-value decomposition of $\mathbf{A}$
  let $\mathbf{U}_k = (\mathbf{u}_1 \dots \mathbf{u}_k)$, $\mathbf{V}_k = (\mathbf{v}_1 \dots \mathbf{v}_k)$, $\mathbf{\Sigma}_k = \mathrm{diag}(\sigma_1 \dots \sigma_k)$, and define

$$\mathbf{A}_k = \mathbf{U}_k\,\mathbf{\Sigma}_k\,\mathbf{V}_k^T$$

  then,

$$\min_{\mathrm{rank}(\mathbf{B}) \leq k} \|\mathbf{A} - \mathbf{B}\|_2 = \|\mathbf{A} - \mathbf{A}_k\|_2 = \sigma_{k+1}$$

- in other words, $\mathbf{A}_k$ is the best of rank-k approximation for the matrix $\mathbf{A}$
- useful for
  - compression
  - noise reduction
  - and as we will see, dimensionality-reduction

singular-value decomposition and matrix pseudo-inverse

- the Moore–Penrose inverse, or pseudo-inverse, of a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, is a matrix $\mathbf{A}^+ \in \mathbb{R}^{n \times m}$ that generalizes the notion of inverse
- if $\mathbf{A}$ has linearly independent columns (and thus, the matrix $\mathbf{A}^T\mathbf{A}$ is invertible), then $\mathbf{A}^+$ is computed by $\mathbf{A}^+ = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$
  in this case the pseudo-inverse is called left inverse and $\mathbf{A}^+\mathbf{A} = \mathbf{I}$
- if $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ is the singular-value decomposition of $\mathbf{A}$, then

$$\mathbf{A}^+ = \mathbf{V}\mathbf{\Sigma}^+\mathbf{U}^T$$

  where, $\mathbf{\Sigma}^+$ is formed from $\mathbf{\Sigma}$ by taking the reciprocal of all the non-zero elements, leaving all the zeros in place, and making the matrix the right shape

eigen-decomposition

- let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a square matrix
- for a non-zero vector $\mathbf{v}$, the pair $(\lambda, \mathbf{v})$ is an eigenvalue-eigenvector pair, if

$$\mathbf{A}\,\mathbf{v} = \lambda\,\mathbf{v}$$

- an $n \times n$ matrix $\mathbf{A}$ has n eigenvalue-eigenvector pairs
- the eigen-decomposition of matrix $\mathbf{A}$ is

$$\mathbf{A} = \mathbf{Q}\,\mathbf{\Lambda}\,\mathbf{Q}^{-1}$$

where $\mathbf{Q}$ is an $n \times n$ matrix whose i-th column is the eigenvector $\mathbf{v}_i$ of $\mathbf{A}$, and $\mathbf{\Lambda}$ is a diagonal matrix whose diagonal elements are the eigenvalues, $\mathbf{\Lambda}_{ii} = \lambda_i$

- a symmetric matrix has real eigenvalues and orthogonal eigenvectors $(\mathbf{Q}^{-1} = \mathbf{Q}^T)$

in addition, a symmetric positive semidefinite matrix has non-negative eigenvalues

singular value decomposition and eigen-decomposition

- from the singular value decomposition we can write

$$\mathbf{A}^T\mathbf{A} = \mathbf{V}\mathbf{\Sigma}\mathbf{U}^T\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \mathbf{V}\mathbf{\Sigma}^2\mathbf{V}^T$$

$$\mathbf{A}\mathbf{A}^T = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T\mathbf{V}\mathbf{\Sigma}\mathbf{U}^T = \mathbf{U}\mathbf{\Sigma}^2\mathbf{U}^T$$

- it follows :
  - the singular values of $\mathbf{A}$ are the nonnegative square roots of the eigenvalues of $\mathbf{A}^T\mathbf{A}$
  - the columns of $\mathbf{V}$ (right singular vectors of $\mathbf{A}$) are the eigenvectors of $\mathbf{A}^T\mathbf{A}$
  - the columns of $\mathbf{U}$ (left singular vectors of $\mathbf{A}$) are the eigenvectors of $\mathbf{A}\mathbf{A}^T$

principal component analysis (PCA)

- one of the most common dimensionality-reduction techniques
- one of the simplest and most robust
- one of oldest methods, dating back to 1901 [Pearson, 1901]
- has been rediscovered many times
- also known as Karhunen-Loève transformation, or Hotelling transformation

recall our general dimensionality-reduction scheme

we need to specify

- a model to define mappings between $\mathbb{R}^d$ and $\mathbb{R}^k$
- a criterion to be optimized
- an algorithm to be used to optimize the criterion

recall our general dimensionality-reduction scheme

for PCA we use

- a model to define mappings between $\mathbb{R}^d$ and $\mathbb{R}^k$
  - a linear mapping
- a criterion to be optimized
  - mean square error
- an algorithm to be used to optimize the criterion
  - singular-value decomposition

note: employing SVD is not a free choice, it is a consequence of the other two choices

data model of PCA

- a data point is represented by a vector $\mathbf{y} = (y_1, \ldots, y_d)^T \in \mathbb{R}^d$

  the data is a set of data points $\mathcal{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$

  equivalently, the data is represented by a matrix $\mathbf{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_n) \in \mathbb{R}^{d \times n}$

  (notice that rows represent dimensions and columns represent points)

- we assume that each vector $\mathbf{y} = (y_1, \ldots, y_d)^T$ is the result of applying a linear transformation $\mathbf{W} \in \mathbb{R}^{d \times k}$ to a latent vector $\mathbf{x} = (x_1, \ldots, x_k)^T$

$$\mathbf{y} = \mathbf{W}\mathbf{x}$$

- additionally, we assume that the columns of $\mathbf{W}$ are orthonormal, i.e., $\mathbf{W}^T\mathbf{W} = \mathbf{I}_{k \times k}$

  that is, $\mathbf{W}$ is full rank and its columns are a basis of the space that it spans

  (but $\mathbf{W}\mathbf{W}^T$ is not necessarily equal to $\mathbf{I}_{d \times d}$)

data centering

- we assume that the observed points $\mathbf{y}$ and the latent points $\mathbf{x}$ are "centered"

$$\mathbb{E}_{\mathbf{y}}[\mathbf{y}] = \mathbf{0}_d \quad \text{and} \quad \mathbb{E}_{\mathbf{x}}[\mathbf{x}] = \mathbf{0}_k$$

  this can be achieved by removing the expectation $\mathbb{E}_{\mathbf{y}}[\mathbf{y}]$ from each point $\mathbf{y}_i$

$$\mathbf{y}_i \leftarrow \mathbf{y}_i - \mathbb{E}_{\mathbf{y}}[\mathbf{y}]$$

  in practice, the expectation $\mathbb{E}_{\mathbf{y}}[\mathbf{y}]$ is computed by the sample mean

$$\mathbb{E}_{\mathbf{y}}[\mathbf{y}] \approx \frac{1}{n} \sum_{i=1}^{n} \mathbf{y}_i = \frac{1}{n} \mathbf{Y} \mathbf{1}_n$$

- data centering in matrix notation

$$\mathbf{Y} \leftarrow \mathbf{Y} - \frac{1}{n} \mathbf{Y} \mathbf{1}_n \mathbf{1}_n^T$$

PCA linear mapping

- the linear transformation $\mathbf{y} = \mathbf{W}\,\mathbf{x}$ provides the mapping dec from $\mathbb{R}^k$ to $\mathbb{R}^d$

$$\mathrm{dec} : \mathbb{R}^k \to \mathbb{R}^d, \quad \mathbf{x} \mapsto \mathbf{y} = \mathrm{dec}(\mathbf{x}) = \mathbf{W}\,\mathbf{x}$$

- for the mapping from $\mathbb{R}^d$ to $\mathbb{R}^k$ we use the pseudo inverse $\mathbf{W}^+ = (\mathbf{W}^T\mathbf{W})^{-1}\mathbf{W}^T = \mathbf{W}^T$

$$\mathrm{cod} : \mathbb{R}^d \to \mathbb{R}^k, \quad \mathbf{y} \mapsto \mathbf{x} = \mathrm{cod}(\mathbf{y}) = \mathbf{W}^+\mathbf{y} = \mathbf{W}^T\mathbf{y}$$

PCA optimization criterion

- mean square error = reconstruction error

$$E_{\mathbf{W}} = \mathbb{E}_{\mathbf{y}}\left[\|\mathbf{y} - \mathrm{dec}(\mathrm{cod}(\mathbf{y}))\|_2^2\right] = \mathbb{E}_{\mathbf{y}}\left[\|\mathbf{y} - \mathbf{W}\mathbf{W}^T\mathbf{y}\|_2^2\right]$$

recall from previous slide that $\mathrm{cod}(\mathbf{y}) = \mathbf{W}^T\mathbf{y}$ and $\mathrm{dec}(\mathbf{x}) = \mathbf{W}\,\mathbf{x}$

recall that while $\mathbf{W}^T\mathbf{W} = \mathbf{I}_{k\times k}$, matrix $\mathbf{W}\,\mathbf{W}^T$ is not necessarily equal to $\mathbf{I}_{d\times d}$

optimizing the PCA reconstruction-error criterion

$$
\begin{aligned}
E_{\mathbf{W}} &= \mathbb{E}_{\mathbf{y}}\left[\|\mathbf{y} - \mathbf{W}\mathbf{W}^T\mathbf{y}\|_2^2\right] \\
&= \mathbb{E}_{\mathbf{y}}\left[(\mathbf{y} - \mathbf{W}\mathbf{W}^T\mathbf{y})^T(\mathbf{y} - \mathbf{W}\mathbf{W}^T\mathbf{y})\right] \\
&= \mathbb{E}_{\mathbf{y}}\left[\mathbf{y}^T\mathbf{y} - 2\mathbf{y}^T\mathbf{W}\mathbf{W}^T\mathbf{y} + \mathbf{y}^T\mathbf{W}\mathbf{W}^T\mathbf{W}\mathbf{W}^T\mathbf{y}\right] \\
&= \mathbb{E}_{\mathbf{y}}\left[\mathbf{y}^T\mathbf{y} - \mathbf{y}^T\mathbf{W}\mathbf{W}^T\mathbf{y}\right] \\
&= \mathbb{E}_{\mathbf{y}}\left[\mathbf{y}^T\mathbf{y}\right] - \mathbb{E}_{\mathbf{y}}\left[\mathbf{y}^T\mathbf{W}\mathbf{W}^T\mathbf{y}\right]
\end{aligned}
$$

$\mathbb{E}_{\mathbf{y}}\left[\mathbf{y}^T\mathbf{y}\right]$ is constant, so minimizing $E_{\mathbf{W}}$ is equivalent to maximizing $\mathbb{E}_{\mathbf{y}}\left[\mathbf{y}^T\mathbf{W}\mathbf{W}^T\mathbf{y}\right]$

- we use again the sample mean

$$
\begin{aligned}
\mathbb{E}_{\mathbf{y}}\left[\mathbf{y}^T\mathbf{W}\mathbf{W}^T\mathbf{y}\right] &= \frac{1}{n}\sum_{i=1}^{n}\mathbf{y}_i^T\mathbf{W}\mathbf{W}^T\mathbf{y}_i \\
&= \frac{1}{n}\,\mathrm{tr}(\mathbf{Y}^T\mathbf{W}\mathbf{W}^T\mathbf{Y})
\end{aligned}
$$

optimizing the PCA reconstruction-error criterion

- we want to maximize $\mathbb{E}_{\mathbf{y}}\left[\mathbf{y}^T \mathbf{W}\mathbf{W}^T\mathbf{y}\right] = \frac{1}{n}\,\mathrm{tr}(\mathbf{Y}^T\mathbf{W}\mathbf{W}^T\mathbf{Y})$
- consider the singular value decomposition of the data matrix $\mathbf{Y} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$

$$\mathrm{tr}(\mathbf{Y}^T\mathbf{W}\mathbf{W}^T\mathbf{Y}) = \mathrm{tr}(\mathbf{V}\mathbf{\Sigma}\mathbf{U}^T\mathbf{W}\mathbf{W}^T\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T)$$

- we can observe that the above expression reaches its maximum when the k columns of $\mathbf{W}$ are colinear with the columns of $\mathbf{U}$ that are associated with the k largest singular values in $\mathbf{\Sigma}$, i.e.,

$$\mathbf{W} = \mathbf{U}_k$$

- finally, we obtain the projection of point $\mathbf{y}$ to the latent point $\mathbf{x} = \mathbf{W}^T\mathbf{y} = \mathbf{U}_k^T\mathbf{y}$

putting everything together

the PCA method

- input data $\mathbf{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_n) \in \mathbb{R}^{d \times n}$
- data centering $\mathbf{Y} \leftarrow \mathbf{Y} - \frac{1}{n}\mathbf{Y}\mathbf{1}_n\mathbf{1}_n^T$
- singular value decomposition $\mathbf{Y} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$
- take $\mathbf{U}_k$ to be the k columns of $\mathbf{U}$ that correspond to the k largest singular values
- map data to k-dimensional space by $\mathbf{X} = \mathbf{U}_k^T\mathbf{Y}$

explained variance and reconstruction error

- SVD gives a nice connection of explained variance and reconstruction error through singular values
- the variance of the data explained via the first k principal components is

$$V_{\mathbf{W}} = \sum_{i=1}^{k} \sigma_i^2$$

note that the variance of the whole data is $V_{\mathbf{Y}} = \sum_{i=1}^{d} \sigma_i^2$

- on the other hand, the reconstruction error is

$$E_{\mathbf{W}} = \sum_{i=k+1}^{d} \sigma_i^2$$

and thus, the reconstruction error is 0, when $k = d$ and $\mathbf{W} = \mathbf{U}$

selecting the number of latent variables (k)

- selecting the number of latent variables is a mix of science and art
- we can use the concept of explained variance

1. rule of thumb : select k so as to explain at least 85% of the data variance

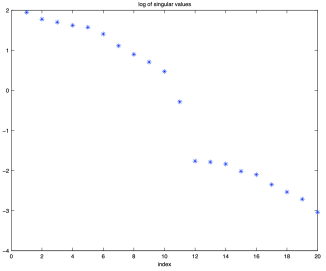
– select the smallest k for which

$$\frac{V_{\mathbf{W}}}{V_{\mathbf{Y}}} = \frac{\sum_{i=1}^{k} \sigma_i^2}{\sum_{i=1}^{d} \sigma_i^2} \geq 0.85$$

(or is it 95%?)

2. plot the singular values and look for a "gap"

– it is often more revealing when ploting the singular values in log scale



example : spatial / linguistic data analysis

- data : 9000 dialect words, 500 counties

  points = words, dimensions = counties

  data matrix $\mathbf{Y}$, so that $y_{ij} = 1$ if word i appears in county j, and $y_{ij} = 0$ otherwise

- apply PCA to this data

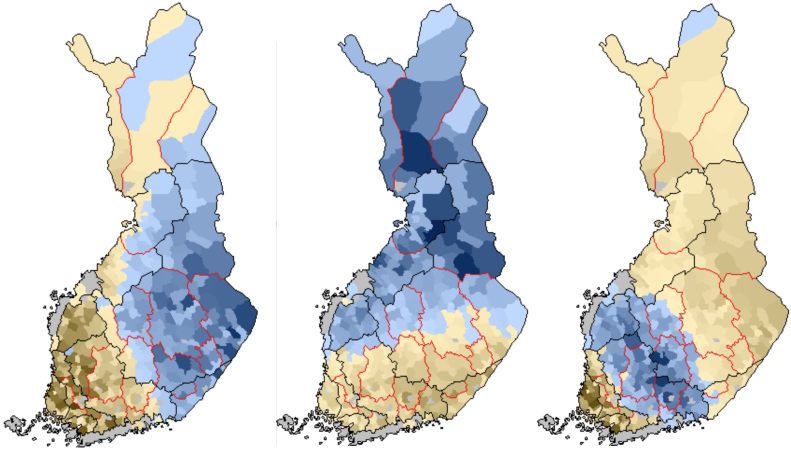
- obtain principal component matrix $\mathbf{W} \in \mathbb{R}^{d \times k}$

  – the i-th column of $\mathbf{W}$ (i-th principal component), $i = 1, \ldots, k$ indicates the counties that explain significant part of the variation left in the data

example credited to Saara Hyvönen

example : spatial / linguistic data analysis

visualizing the first three components



geographical structure of principal components is apparent

note : PCA knows nothing about geography

conclusion and discussion

- PCA is a simple and robust dimensionality-reduction method
  - a few lines of code in `python`, `Matlab`, `R`
  - popular and widely used
- closed-form optimal solution via SVD
- it comes with some rules of thumb to select the number of latent variables
- "layered" method : adds optimal principal components one by one
- main assumption, which can be a limitation in some cases : linear model

distance preservation as a means for dimensionality reduction

- in some cases, data can lie in a non-linear manifold inside a high-dimensional space
  - manifold not known, but we may be able to compute distances on the manifold
- in other cases, data points have no vector representation, but we can compute distances
  - e.g., string edit distance
- in both cases, we can compute distances between pairs of data points
- we want to embed points in a geometric space so that distances are preserved
  - distance between the embedded image of two points $\approx$ original distance
- if distances are preserved in the low-dimensional embedding, intuitively, the embedding has captured the structure of the manifold, and the dimensionality reduction is successful

distance functions

- given a space $\mathcal{Y}$, a distance d is a function $d : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$
- if a distance function d satisfies the following properties

$d(\mathbf{a}, \mathbf{b}) \geq 0$, for all $\mathbf{a}, \mathbf{b} \in \mathcal{Y}$	non-negativity
$d(\mathbf{a}, \mathbf{b}) = 0$ if and only if $\mathbf{a} = \mathbf{b}$	isolation
$d(\mathbf{a}, \mathbf{b}) = d(\mathbf{b}, \mathbf{a})$, for all $\mathbf{a}, \mathbf{b} \in \mathcal{Y}$	symmetry
$d(\mathbf{a}, \mathbf{b}) \leq d(\mathbf{a}, \mathbf{c}) + d(\mathbf{c}, \mathbf{b})$, for all $\mathbf{a}, \mathbf{b}, \mathbf{c} \in \mathcal{Y}$	triangle inequality

we say that the distance d is a metric

we also say that $(\mathcal{Y}, d)$ (the space $\mathcal{Y}$ equipped with distance d) is a metric space

Minkowski distances

- the Minkowski distances is a family of distance functions in the vector space $\mathbb{R}^d$
- for any two points (vectors) $\mathbf{a} = (a_1, \ldots, a_d)$ and $\mathbf{b} = (b_1, \ldots, b_d)$ in $\mathbb{R}^d$ the Minkowski distance L_p between $\mathbf{a}$ and $\mathbf{b}$ is defined as

$$d(\mathbf{a}, \mathbf{b}) = \|\mathbf{a} - \mathbf{b}\|_p = \left(\sum_{i=1}^{d} |a_i - b_i|^p \right)^{\frac{1}{p}}$$

- the following special cases of L_p are most commonly used
  - $p = 1$: city-block or Manhattan distance
  - $p = 2$: Euclidean distance
  - $p = \infty$: maximum distance
- the Minkowski distance is a metric, for all $p \geq 1$

similarity functions

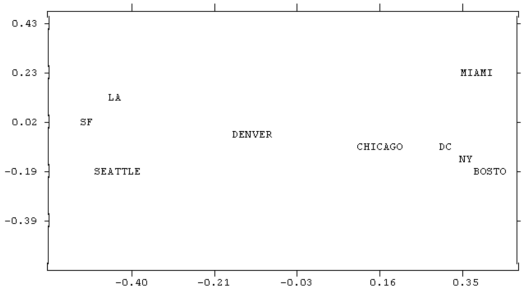
- distances are measures of dissimilarity
- often we work with similarity functions, which are measures of similarity
- similarity functions map pairs of points to reals, i,.e., $\text{sim} : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$
- commonly-used similarity functions are the dot-product, the cosine similarity, the Jaccard coefficient, and more ...
- similarity functions often take values in the range $[0, 1]$, where
  - value 1 indicates that two points are identical, and value 0 indicates that they are totally dissimilar
- on the other hand, for distance functions
  - value 0 indicates that two points are identical, and a large value indicates that they are totally dissimilar
  - sometimes we normalize distances to be in the interval $[0, 1]$

multidimensional scaling (MDS)

- intuitively : given a matrix of pair-wise distances, can be map the data in a low-dimensional space so that distances are preserved?

		1 BOST	2 NY	3 DC	4 MIAM	5 CHIC	6 SEAT	7 SF	8 LA	9 DENV
1	BOSTON	0	206	429	1504	963	2976	3095	2979	1949
2	NY	206	0	233	1308	802	2815	2934	2786	1771
3	DC	429	233	0	1075	671	2684	2799	2631	1616
4	MIAMI	1504	1308	1075	0	1329	3273	3053	2687	2037
5	CHICAGO	963	802	671	1329	0	2013	2142	2054	996
6	SEATTLE	2976	2815	2684	3273	2013	0	808	1131	1307
7	SF	3095	2934	2799	3053	2142	808	0	379	1235
8	LA	2979	2786	2631	2687	2054	1131	379	0	1059
9	DENVER	1949	1771	1616	2037	996	1307	1235	1059	0

distance matrix



mapping to 2D

example credited to Stephen Borgatti, 1997

color perception

[Ekman, 1954]

- study color perception in human vision
- consider 14 colors differing only in their hue
- 31 people rate differences between all pairs of colors, on a five-point scale
- average ratings and convert to distances
  - 0 indicates that two colors are identical, 1 indicates that they are totally different

color perception

pairwise distance matrix

	434	445	465	472	490	504	537	555	584	600	610	628	651
445	0.14												
465	0.58	0.50											
472	0.58	0.56	0.19										
490	0.82	0.78	0.53	0.46									
504	0.94	0.91	0.83	0.75	0.39								
537	0.93	0.93	0.90	0.90	0.69	0.38							
555	0.96	0.93	0.92	0.91	0.74	0.55	0.27						
584	0.98	0.98	0.98	0.98	0.93	0.86	0.78	0.67					
600	0.93	0.96	0.99	0.99	0.98	0.92	0.86	0.81	0.42				
610	0.91	0.93	0.98	1.00	0.98	0.98	0.95	0.96	0.63	0.26			
628	0.88	0.89	0.99	0.99	0.99	0.98	0.98	0.97	0.73	0.50	0.24		
651	0.87	0.87	0.95	0.98	0.98	0.98	0.98	0.98	0.80	0.59	0.38	0.15	
674	0.84	0.86	0.97	0.96	1.00	0.99	1.00	0.98	0.77	0.72	0.45	0.32	0.24

color perception

MDS reproduces the well-known 2-dimensional color circle

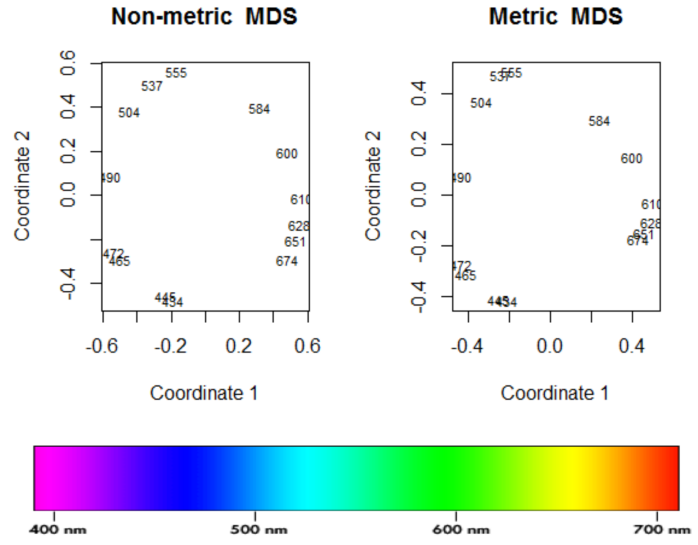


image-retrieval interface with MDS

example from Rubner et al., 1997

2D MDS map of images

example from Rubner et al., 1997

multidimensional scaling (MDS)

a family of related techniques

- scaling refers to constructing a configuration of points in a target metric space from interpoint distance information
- MDS is scaling when the target metric space is the Euclidean space
- classical MDS : the basic MDS formulation
- metric MDS : a generalization of classical MDS, with interpoint distance information, and optimizing a general stress function
- non-metric MDS : a generalization of classical MDS, with rank information

classical MDS with a similarity matrix

- consider dataset $\mathcal{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$, represented as matrix $\mathbf{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_n) \in \mathbb{R}^{d \times n}$
- assume that data is not known, instead pairwise similarities are known
- we know the similarity matrix $\mathbf{S}$, such that $[\mathbf{S}]_{ij} = s_{ij} = \mathbf{y}_i^T \mathbf{y}_j$ (dot-product similarity)
  then, $\mathbf{S} = \mathbf{Y}^T \mathbf{Y}$
- as with PCA, for point i we assume a latent vector $\mathbf{x}_i$, so that $\mathbf{y}_i = \mathbf{W}\mathbf{x}_i$,
  where $\mathbf{W}$ defines a linear transformation
  - we have $\mathbf{Y} = \mathbf{W}\mathbf{X}$
  - we assume again that the columns of $\mathbf{W}$ are orthonormal, i.e., $\mathbf{W}^T\mathbf{W} = \mathbf{I}_{k \times k}$
- we have
$$\mathbf{S} = \mathbf{Y}^T\mathbf{Y} = (\mathbf{W}\mathbf{X})^T(\mathbf{W}\mathbf{X}) = \mathbf{X}^T(\mathbf{W}^T\mathbf{W})\mathbf{X} = \mathbf{X}^T\mathbf{X}$$
  and note again that both $\mathbf{Y}$ and $\mathbf{X}$ are unknown
- the matrix $\mathbf{S}$ is called the Gram matrix

classical MDS with a similarity matrix

- recap : given similarity matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$, we want to find latent matrix $\mathbf{X} \in \mathbb{R}^{k \times n}$, such that $\mathbf{S} = \mathbf{X}^T \mathbf{X}$
- the similarity matrix $\mathbf{S}$ is symmetric positive semi-definite, so its eigen-decomposition is

$$\mathbf{S} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^{-1} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^T = (\mathbf{\Lambda}^{1/2} \mathbf{U}^T)^T (\mathbf{\Lambda}^{1/2} \mathbf{U}^T)$$

  the non-negative eigenvalues of $\mathbf{S}$ are sorted in descending order in the diagonal of $\mathbf{\Lambda}$
- it follows that we can take the $k \times n$ matrix $\mathbf{X}$ to be

$$\mathbf{X} = \mathbf{I}_{k \times n} \mathbf{\Lambda}^{1/2} \mathbf{U}^T$$

- the matrix $\mathbf{X}$ provides a k embedding for each data point
  (point i is taken as the i-th column of $\mathbf{X}$)

classical MDS with a distance matrix

- in many cases, instead of the similarity matrix $\mathbf{S}$, where $[\mathbf{S}]_{ij} = s_{ij} = \mathbf{y}_i^T \mathbf{y}_j$
  we are given as input the pairwise distance matrix $\mathbf{D}$, where $[\mathbf{D}]_{ij} = d_{ij} = \|\mathbf{y}_i - \mathbf{y}_j\|_2$
- we want to perform MDS on the distance matrix $\mathbf{D}$
- we can use the fact
$$d_{ij}^2 = s_{ii} + s_{jj} - 2s_{ij} \quad \Rightarrow \quad s_{ij} = -\frac{1}{2}\left(d_{ij}^2 - s_{ii} - s_{jj}\right)$$
  but note that $s_{ii} = \mathbf{y}_i^T \mathbf{y}_i$ and $s_{jj} = \mathbf{y}_j^T \mathbf{y}_j$ are unknown
- however, we can estimate s_{ij} by a "double centering" trick:
  subtract from each entry of $\mathbf{D}$ the mean of the corresponding row and the mean of the corresponding column, and add back the mean of all entries
- in matrix form
$$\mathbf{S} = -\frac{1}{2}\left(\mathbf{D} - \frac{1}{n}\mathbf{D}\,\mathbf{1}_n\mathbf{1}_n^T - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^T\mathbf{D} + \frac{1}{n^2}\mathbf{1}_n\mathbf{1}_n^T\mathbf{D}\,\mathbf{1}_n\mathbf{1}_n^T\right)$$
- so, we can compute $\mathbf{S}$ from $\mathbf{D}$, and apply MDS with similarities

classical MDS — putting everything together

1. if the similarity matrix $\mathbf{S}$ is available go to step 4
2. if the data matrix $\mathbf{Y}$ is available, compute $\mathbf{S} = \mathbf{Y}^T\mathbf{Y}$, and go to step 4
3. if the distance matrix $\mathbf{D}$ is available, compute $\mathbf{S}$ by the "double centering" trick
4. compute the eigen-decomposition $\mathbf{S} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$
5. a k-dimensional representation of the data is obtained by $\mathbf{X} = \mathbf{I}_{k\times n}\mathbf{\Lambda}^{1/2}\mathbf{U}^T$

metric MDS

- a generalization of classical MDS, where we ask to optimize the stress function (reconstruction error)

$$E_{\mathrm{mMDS}} = \sum_{i<j} w_{ij}(d_{ij} - \hat{d}_{ij})^2$$

  where d_{ij} are the input distances, and $\hat{d}_{ij}$ the distances of the reconstructed points

- when $w_{ij} = 1/d_{ij}$, the method is called Sammon's nonlinear mapping
  - the intuition is to give less importance to errors made on large distances

- for this MDS variant we cannot derive a closed-form optimal solution, instead we search for a solution via a general optimization method, such as gradient descent

non-metric MDS

- in many cases ordinal information is given instead of quantitative distances
  - e.g., in a psychology study people may be able to rank a set of concepts, or indicate relative similarity between groups of objects, without being able to assign quantitative scores
- non-metric MDS asks to optimize a stress function of the form

$$E_{\text{nmMDS}} = \left(\sum_{i<j} w_{ij} \left(f(\delta_{ij}) - \hat{d}_{ij} \right)^2 \right)^{\frac{1}{2}}$$

where δ_{ij} are the ordinal proximities

f is monotone transformation of proximities, such that $f(\delta_{ij}) \approx d_{ij}$

d_{ij} is the Euclidean distance between the unknown data points $\mathbf{y}_i$ and $\mathbf{y}_j$, and

$\hat{d}_{ij}$ the distances of the reconstructed points

- as with metric MDS, we rely on general optimization methods, such as gradient descent

conclusion and discussion

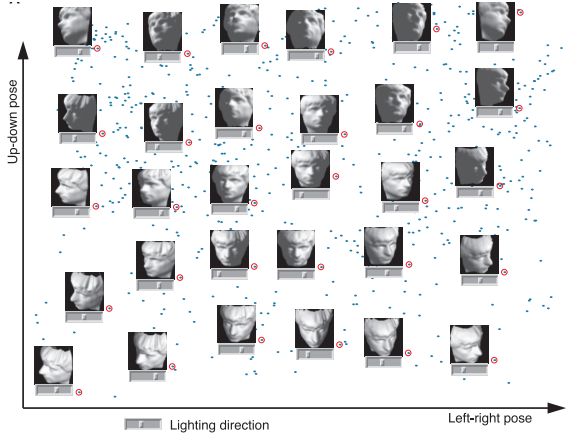
- like PCA, classical MDS is a simple and robust dimensionality-reduction method
- it also assumes a linear model
- optimal solution can be derived and efficiently computed via SVD
- MDS is more flexible than PCA, as it only assumes a similarity or distance matrix, and it is applicable when no vector representation of data is available
- on the other hand, MDS is computationally more intensive when working with matrices of size $n \times n$
- metric and non-metric MDS are more general methods but they come with the cost of having to solve a more difficult optimization problem

nonlinear dimensionality reduction — motivation

many high-dimensional points lie in lower-dimensional manifolds

example

- consider a set of images, of resolution 128×128, depicting an object from different positions, and different lighting
- an image an be considered as a point in a 16384-dimensional space
- arguably, there are 3 degrees of freedom (specifying position and lighting)
- thus, the set of images lies in a 3-dimensional nonlinear manifold within a 16384-dimensional space



example from Tenenbaum et al., 2000

nonlinear dimensionality reduction

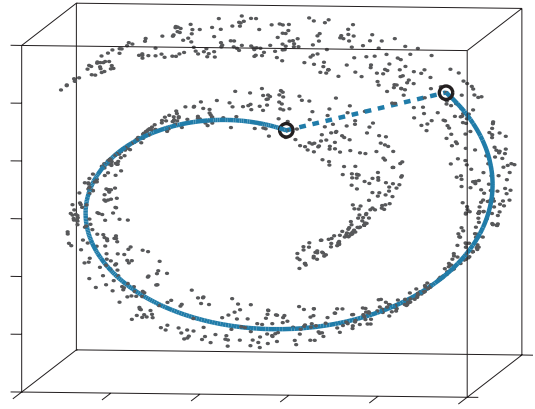
objective

given high-dimensional points $\{\mathbf{y}_i\}$, possibly lying on a non-linear manifold, reconstruct low-dimensional coordinates of the data $\{\mathbf{x}_i\}$, which describe where the points lie on the manifold

isomap

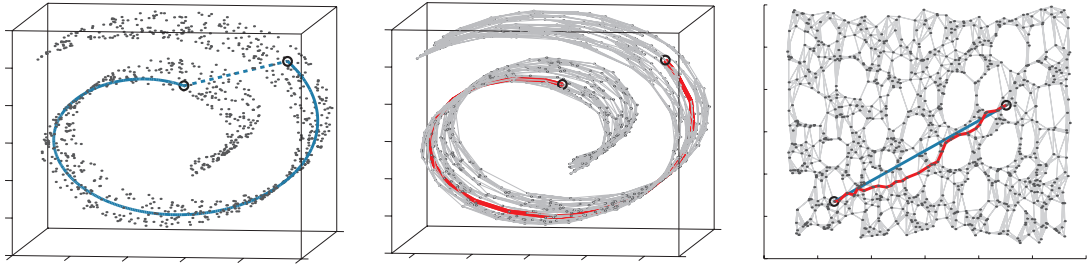
intuition

- Euclidean distance in the original space may be a poor measure of dissimilarity between points
- instead use geodesic distance, distance between points on the manifold
- geodesic distance captures more accurately captures the neighborhood relationships that should be preserved



example from Tenenbaum et al., 2000

calculating geodesic distance



- without knowing the manifold, calculating geodesic distance is impossible
- for nearby points, geodesic distance $\approx$ Euclidean distance
- for faraway points, approximate geodesic distance by a sequence "short hops" between neighboring points

isomap algorithm

given data $\mathcal{Y} = \{\mathbf{y}_i\}$

1. compute distances $\delta_{ij} = \|\mathbf{y}_i - \mathbf{y}_j\|^2$ in the original space
2. construct a graph G, where vertices represent points, and each point is connected to its p nearest points, according to distances δ_{ij}
3. for each pair of points i and j compute the shortest path distance d_{ij} from i to j on the graph G (e.g., using the Floyd-Warshall algorithm)
4. use MDS on the shortest-path distances $\{d_{ij}\}$ to compute the low-dimensional embedding $\{\mathbf{x}_i\}$

conclusion and discussion

- isomap is an algorithm designed to recover low-dimensional non-linear manifolds within high-dimensional spaces
- it works by constructing a graph, which approximates geodesic distances on the manifold, and then uses MDS
- the method can be unstable, for example
  - sensitive to noise
  - sensitive to number of nearest neighbors to construct the graph G
  - if the graph G is disconnected, the algorithm will fail