Mini-Course on Dimensionality Reduction and Manifold Learning
Part 1: Linear Dimensionality Reduction

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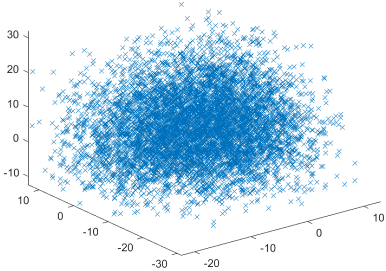
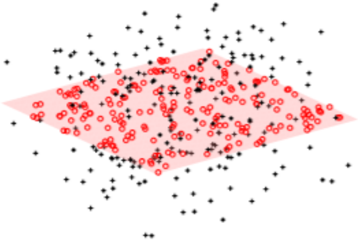
Can be helped by dimensionality reduction, feature selection and compression, quantization

High-dimensional data doesn't typically look like this



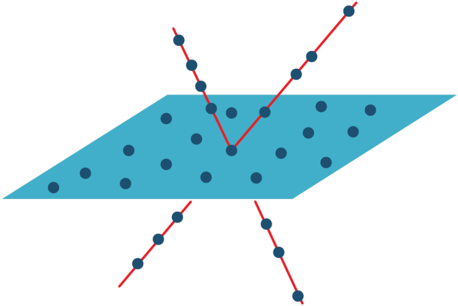
Structure in Data

It could look like this...



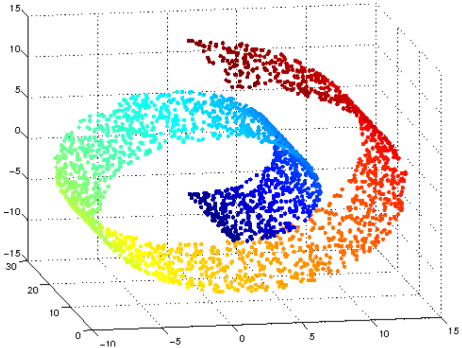
Structure in Data

or this ...



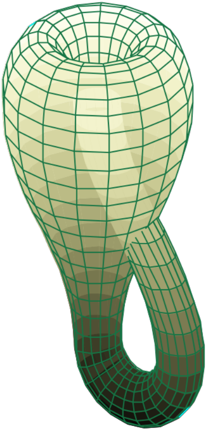
Structure in Data

or maybe this ...



Structure in Data

or what about this?



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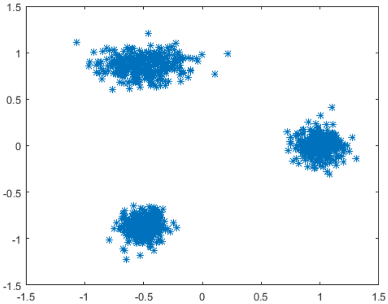
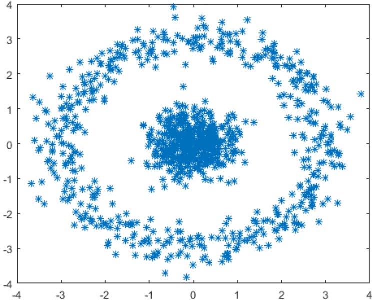


Structure in Data

or even this!



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- Detection (find when a given structure exists)

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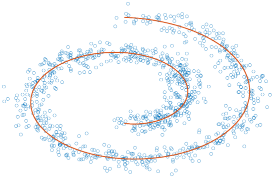
Two Tasks:

- Detection (find when a given structure exists)
- Learning (learn the features necessary to describe the structure – e.g., basis for subspace or charts/tangent spaces for manifold)



Common Structures:

- Subspaces
- Union of subspaces
- Sparsity
- Manifolds
- Union of manifolds
- Clusters (Communities)
- Structure + noise/outliers

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(e.g., weather modeling)

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$$X = \{x_1,\dots x_N\} = C_1 \sqcup \cdots \sqcup C_k$$

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- Classification

$$(x_i, y_i) \Rightarrow \mathcal{C}_\Theta : \mathbb{R}^D \to \{1, \dots, L\}$$

  (e.g., hand-written digits, facial recognition with labelled training

Structure in Data

Techniques:

- Graphs
- (Randomized) Linear Algebra
- Harmonic Analysis
- Statistics
- Optimization
- Neural Networks
- Topological invariants
- . . .

Dimensionality Reduction

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- Find a reduced basis
- Fine low-dimensional parametrization

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- $A(i,:)$ is the i–th column of A and $A(:,j)$ is its j–th row. $A(I,J)$ is a submatrix of entries $(i,j) \in I \times J$

Background: Singular Value Decomposition

Every $A \in \mathbb{R}^{m\times n}$ has a SVD of the form

$$A = U\Sigma V^T = \begin{bmatrix} | & & | \\ u_1 & \dots & u_m \\ | & & | \end{bmatrix} \Sigma \begin{bmatrix} — & v_1 & — \\ & \vdots & \\ — & v_n & — \end{bmatrix}$$

where $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ are *orthogonal* ($U^{-1} = U^T$) and

$$\Sigma = \begin{bmatrix} \mathrm{diag}(\sigma_1, \dots, \sigma_m) & \mathbf{0} \end{bmatrix}, \quad \text{or} \quad \begin{bmatrix} \mathrm{diag}(\sigma_1, \dots, \sigma_n) \\ \mathbf{0} \end{bmatrix}$$

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$\sigma_i^2 = \lambda_i(AA^T) = \lambda_i(A^TA)$, and are ordered $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{\mathrm{rank}(A)} \geq 0$.

SVD Properties

Can be rewritten:

$$A = \sum_{i=1}^{\min\{m,n\}} \sigma_i u_i v_i^T$$

If $\text{rank}(A) = k < m, n$, then we also have

$$A = U_k \Sigma_k V_k^T = \begin{bmatrix} | & & | \\ u_1 & \dots & u_k \\ | & & | \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \end{bmatrix} \begin{bmatrix} — & v_1 & — \\ & \vdots & \\ — & v_k & — \end{bmatrix}$$

$$= \sum_{i=1}^{k} \sigma_i u_i v_i^T$$

SVD Properties

Theorem (Eckart–Young–Mirsky)

Let $k \in \mathbb{N}$ and $A \in \mathbb{R}^{m\times n}$. Then $A_k := U_k \Sigma_k V_k^T$ is a solution of

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Note: $\|A\|_2 = \sigma_1(A)$, and $\|A\|_F = \left(\sum_{i=1}^{\text{rank}(A)} \sigma_i(A)^2\right)^{\frac{1}{2}}$

If 2 is replaced by $p \in [1, \infty]$ these are the family of Schatten p–norms. Unfortunately, $\|\cdot\|_2$ is the Schatten ∞–norm and Frobenius norm is the Schatten 2–norm

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Given: data matrix $A \in \mathbb{R}^{m \times n}$ (columns are data points)

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Note: $S_{ii} = \frac{1}{n-1}\sum_{k=1}^{n}(A_{ik}-\mu_i)^2 = \mathrm{Var}(A_{i:})$

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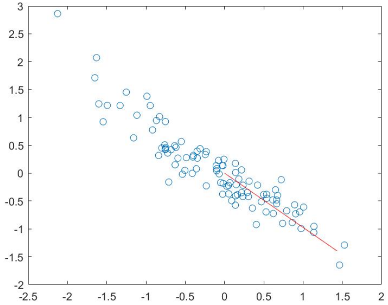
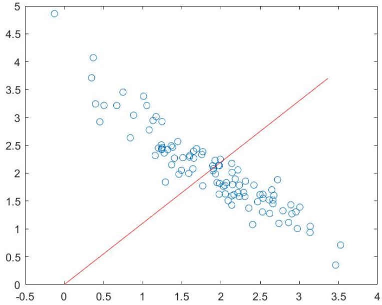
Note: Typically, we ask only for the first few principal components; Eckhart–Young–Mirsky implies that $U_k\Lambda_k U_k^T$ is the best rank k approximation of S

Computational Note: U are the left singular vectors of $\frac{1}{\sqrt{n-1}}\widehat{A}$, so instead of forming the covariance matrix S, we simply take the SVD of $\frac{1}{\sqrt{n-1}}\widehat{A}$

Further Reading: `https://www.cs.princeton.edu/picasso/mats/PCA-Tutorial-Intuition_jp.pdf`

Effect of Centering





PCA on centered data (left) and the same uncentered data (right)

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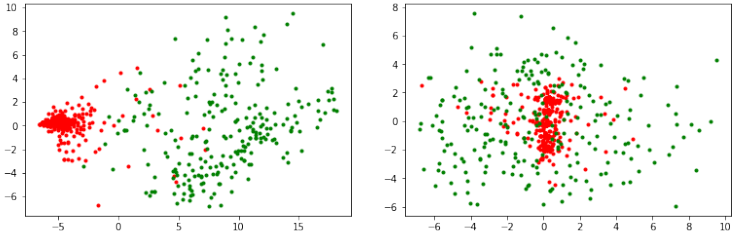
- Identify low-dimensional patterns in data
- Visualization ($k = 2, 3$)

Example



Wisconsin Breast Cancer Dataset `https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic)`
$A \in \mathbb{R}^{32\times 569}$
(Left) Projection onto first two principal components; (Right) Projection onto first and third principal components. Red points are malignant, Green are benign

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a.k.a. What is an *eigengene*? [M. Mahoney and P. Drineas, *CUR Matrix Decompositions for Improved Data Analysis*, Proceedings of the National Academy of Science, 2009]

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Maybe we should look further for a basis for A that is interpretable

Column Subset Selection: Background

Given $A \in \mathbb{R}^{m\times n}$, its Moore–Penrose pseudoinverse is the unique matrix $A^\dagger \in \mathbb{R}^{n\times n}$ such that

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$AA^\dagger : \mathbb{R}^m \to \mathbb{R}^m$ is the orthogonal projection onto the Col(A)

$A^\dagger A : \mathbb{R}^n \to \mathbb{R}^n$ is the orthogonal projection onto Row(A)

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Column Subset Selection Problem (CSSP)

Given $A \in \mathbb{R}^{m\times n}$ and $k < n$, find the column submatrix $C = [a_{i_1} \dots a_{i_k}]$ which minimizes

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Issue: CSSP is NP–hard [Shitov, '17]

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Using actual columns of the data gives an interpretable representation

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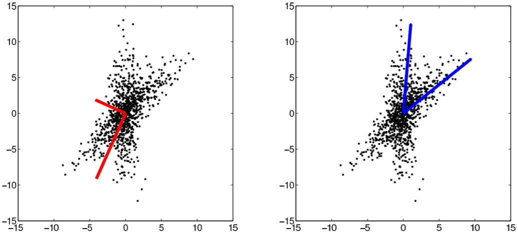
Can capture multiple directions of variability



[Sorensen–Embree, SICOMP '16] Red vectors are Principal Coordinates, Blue vectors are the columns of $CC^\dagger$ for a certain column submatrix

How?

Random Sampling Methods I: Sample w/ or w/out replacement from some distribution over the column indices

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Deterministic Sampling Methods:

- Discrete Empirical Interpolation Method (DEIM) [Gu–Eisenstat, SICOMP '96, Sorensen–Embree, SICOMP '16]
- Greedy Column Selectin [Avron–Boutsidis, SIMAX '13]

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Dimensionality Reduction: $C = U_d \Sigma_d V_d^T \Rightarrow U_d^T A \in \mathbb{R}^{d \times N}$

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Given $X = \{x_1, \ldots, x_N\} \subset \mathbb{R}^D$ find $\Phi : \mathbb{R}^D \to \mathbb{R}^d$ with $d \ll D$ such that

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Relaxation: Given $\varepsilon > 0$, find Φ such that

$$(1-\varepsilon)|x_i - x_j|^2 \leq |\Phi(x_i) - \Phi(x_j)|^2 \leq (1+\varepsilon)|x_i - x_j|^2 \tag{1}$$

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Note: If Q orthogonal and $t \in \mathbb{R}^D$, then

$$|(Qx_i - t) - (Qx_j - t)| = |Q(x_i - x_j)| = |x_i - x_j|.$$

Solution 1: Johnson–Lindenstrauss Embeddings

If Φ is *linear*, then equation reduces to

$$(1-\varepsilon)|y|^2 \leq |\Phi y|^2 \leq (1+\varepsilon)|y|^2, \quad y \in E = \{x_i - x_j\}.$$

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Let $x \in \mathbb{R}^D$ be fixed. Let $\Phi \in \mathbb{R}^{d \times D}$ be a matrix whose entries are i.i.d. Gaussian ($\mathcal{N}(0, \frac{1}{d})$). Then

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Corollary

Gaussian matrices satisfy the Johnson–Lindenstrauss Lemma with high probability.

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General Formulation: Given a similarity measure $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, find $Y \subset \mathbb{R}^d$ which minimizes

$$L(f, D^X, y_1, \dots, y_N) := \left(\frac{\sum_{i,j} (f(y_i, y_j) - D_{ij}^X)^2}{\sum_{i,j} (D_{ij}^X)^2} \right)^{\frac{1}{2}}$$

MDS

The Classical MDS algorithm is a bit simpler: it minimizes

$$\text{Strain}(y_1, \ldots, y_N) := \left(\frac{\sum_{i,j} (B_{ij} - \langle y_i, y_j \rangle)^2}{\sum_{i,j} B_{i,j}^2} \right)^{\frac{1}{2}}$$

where B is an auxiliary matrix defined by

$$B = -\frac{1}{2} J (D^X)^{(2)} J, \qquad J := I - \frac{1}{N} \mathbb{1}\mathbb{1}^T$$

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B is a “double centering" of the distance matrix

MDS

Definition

A matrix $D \in \mathbb{R}^{N \times N}$ is a distance matrix provided

- $D = D^T$,
- $D_{ii} = 0$ for all i
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Note the notion of a distance matrix is much more general. We will characterize when a distance matrix is Euclidean.

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Let D be a distance matrix, and $B = -\frac{1}{2}JD^{(2)}J$. Then D is Euclidean if and only if B is SPSD.

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Theorem (Reverse Direction)

Conversely, if B is SPSD and has rank k, and $B = V\Lambda V^T$ (by the Spectral Theorem), then choosing $X^T = V_k\Lambda_k^{\frac{1}{2}}$ gives $X \subset \mathbb{R}^k$ such that $|x_i - x_j| = D_{ij}$.

Classical MDS Algorithm

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Set: $y_i = (V_d\Lambda_d^{\frac{1}{2}})_{i:}$ – final embedded points

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Recall $V_d \Lambda_d V_d^T$ is a solution to $\min_{X:\text{rank}(X)\leq d} \|B - X\|_F$ by the Eckhart–Young–Mirsky Theorem

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So setting $Y^T = V_d \Lambda_d^{\frac{1}{2}}$ so that $X = Y^T Y$ is a solution to $\min_{Y:\text{rank}(Y) \le d} \|B - Y^T Y\|_F$

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So MDS is E–Y–M in yet another guise!

MDS

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- This version doesn’t necessarily keep our objective of maintaining pairwise distances
- But it is easy because the solution is just the SVD!

Metric MDS

Recall our general loss function:

$$L(f, D^X, y_1, \dots, y_N) := \left(\frac{\sum_{i,j} (f(y_i, y_j) - D_{ij}^X)^2}{\sum_{i,j} (D_{ij}^X)^2} \right)^{\frac{1}{2}}$$

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Metric MDS is when we take $f(y_i, y_j) = |y_i - y_j|$
In this case, the loss function is called stress

$$\text{stress}(D^X, y_1, \ldots, y_N) := \left(\frac{\sum_{i,j} (|y_i - y_j| - D_{ij}^X)^2}{\sum_{i,j} (D_{ij}^X)^2} \right)^{\frac{1}{2}}$$

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Unlike Classical MDS, Metric MDS does not have a closed form solution. The embedded points Y are found via optimization (e.g., stress majorization or (stochastic) gradient descent)

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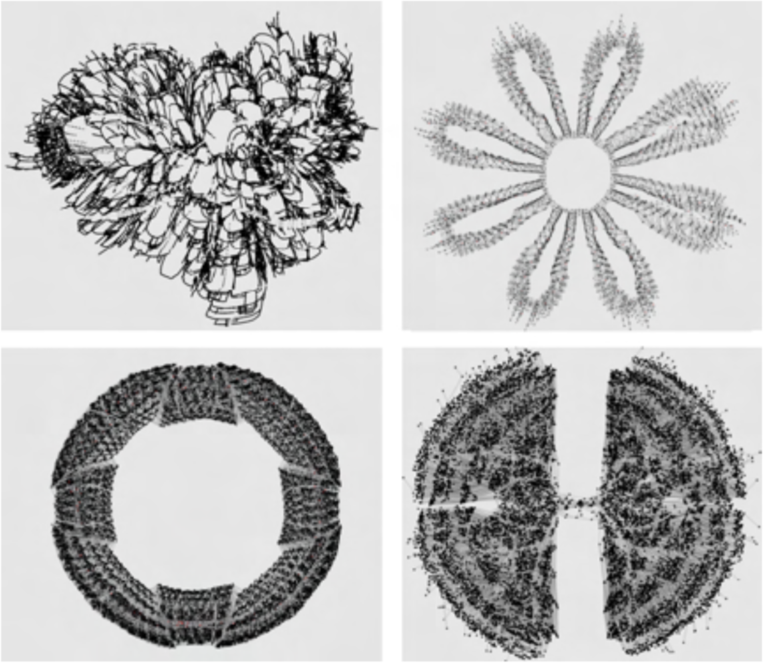
Applications: Graph Drawing

Input: $G = (V, E, w)$, and $D_{ij} = d_G(v_i, v_j)$ (graph-theoretic shortest path distance)

Output: drawing of the graph in $\mathbb{R}^2$ (typically) or $\mathbb{R}^3$

Minimizing stress keeps the points from colliding



Exploratory Data Visualization