Dimensionality Reduction (Wrap-up)

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Introduction to Machine Learning (CS771A)

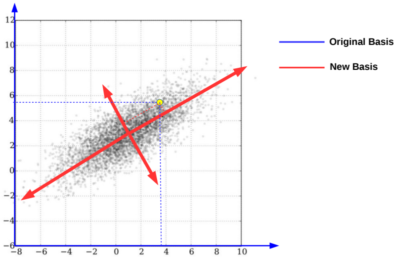
October 11, 2018

Plan for Today

- PCA: The classical view
- Singular Value Decomposition
- A simple technique to compute eigenvectors (Power Iteration)
- Supervised Dimensionality Reduction
- Dimensionality Reduction from Pairwise Distances
- Nonlinear Dimensionality Reduction

Principal Component Analysis: The Key Idea

- We can change the basis in which we represent the data (and get a new co-ordinate system)



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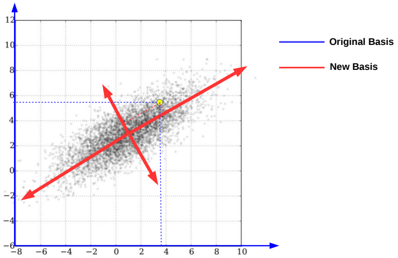

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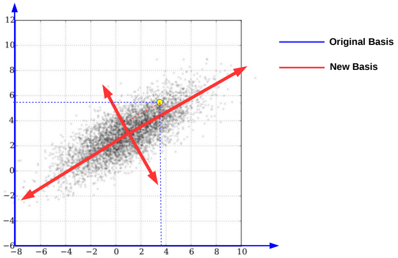

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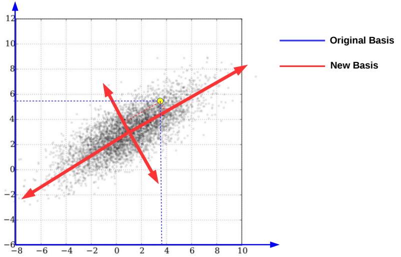

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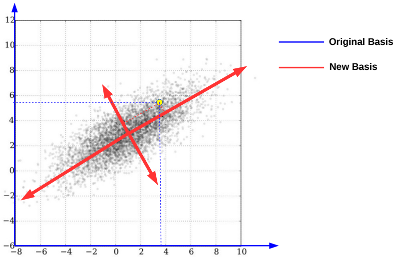

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- PCA finds a new basis such that information loss is minimum if we only keep some dimensions

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- Representing a data point $\boldsymbol{x}_n = [x_{n1}, \ldots, x_{nD}]^\top$ in the standard orthonormal basis $\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_D\}$

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- Note that each new co-ordinate z_{dn} is a projection of $\boldsymbol{x}_n$ along direction $\boldsymbol{u}_d$

$$z_{nd} = \boldsymbol{x}_n^\top \boldsymbol{u}_d = \boldsymbol{u}_d^\top \boldsymbol{x}_n \quad \text{(verify)}$$

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- How to choose K directions $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k$ such that this reconstruction error is minimum?

Directions that Minimize Reconstruction Error..

- Assume $\mathbf{S}$ is the $D \times D$ cov. matrix: $\mathbf{S} = \frac{1}{N}\boldsymbol{x}_n\boldsymbol{x}_n^\top = \frac{1}{N}\mathbf{X}^\top\mathbf{X}$ (assuming already centered data)

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- Thus minimizing recon. error w.r.t. $\boldsymbol{u}_d$ equivalent to maximizing the variance of data along $\boldsymbol{u}_d$

Direction of Maximum Variance

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- Other directions can also be found likewise (with each being orthogonal to all previous ones) using the eigendecomposition of $\mathbf{S}$

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- Thus the variance is maximized when $\boldsymbol{u}_d$ is the (top) eigenvector with largest eigenvalue λ_1
- We denote the top eigenvector as $\boldsymbol{u}_1$ and it called the first Principal Component (PC)
- Other directions can also be found likewise (with each being orthogonal to all previous ones) using the eigendecomposition of $\mathbf{S}$(this is basically the PCA algorithm)

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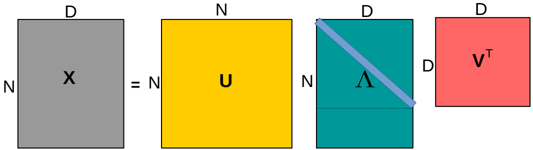
- The K-dimensional projection/embedding of the $N \times D$ data matrix $\mathbf{X}$ is given by

$$\mathbf{Z} = \mathbf{X}\mathbf{U}_K$$

where $\mathbf{U}_K = [\boldsymbol{u}_1 \ \ldots \ \boldsymbol{u}_K]$ is $D \times K$ and embedding matrix $\mathbf{Z}$ is $N \times K$

Singular Value Decomposition (SVD)



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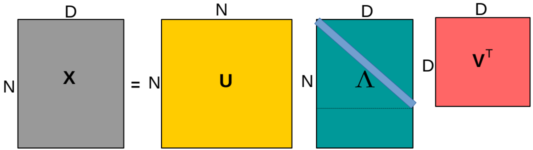

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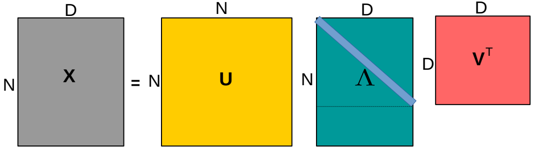

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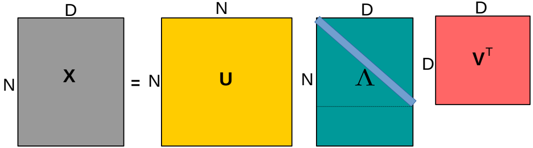

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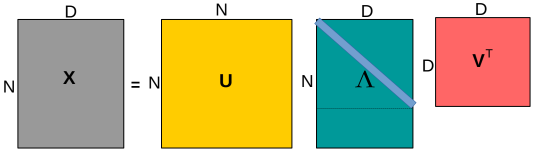

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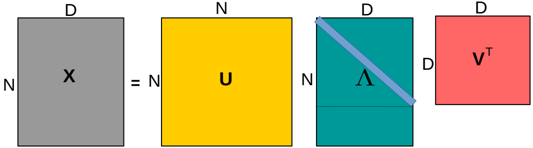

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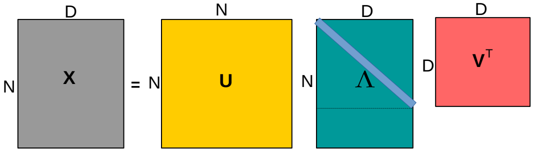

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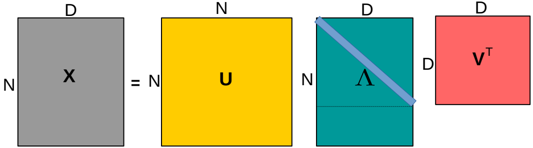

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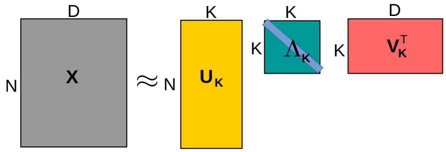
- Note: If $\mathbf{X}$ is symmetric then it is known as eigenvalue decomposition (and $\mathbf{U} = \mathbf{V}$ in that case)

Low-Rank Approximation via SVD



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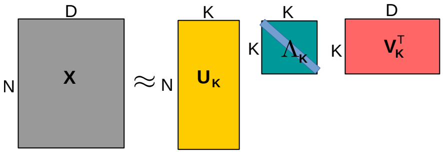

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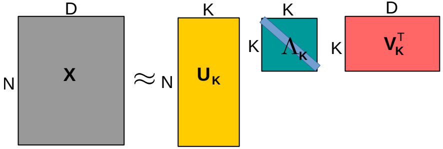

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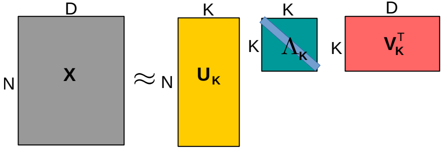

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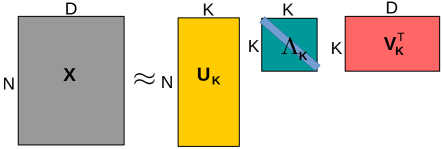

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    - After convergence, $\boldsymbol{x}_M$ is the largest eigenvector and $||\mathbf{S}\boldsymbol{x}_M||$ is the largest eigenvalue
- The main dominant cost is computing $\mathbf{S}\boldsymbol{x}_{m-1}$ which is $O(D^2)$.

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- Each power iteration is $O(D^2)$, overall cost for getting K eigenvectors is $O(KD^2)$

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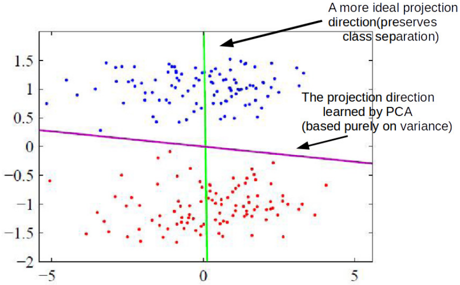

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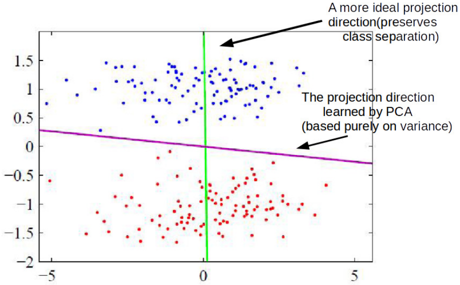

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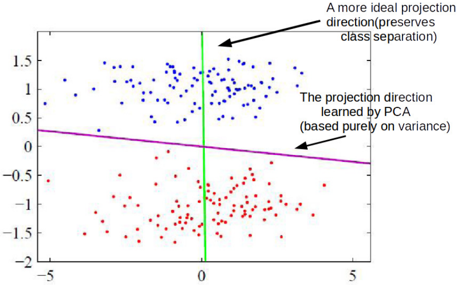
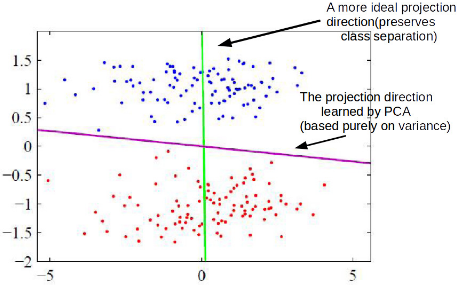


- A better option would be to project such that
  - Points within the same class are close (low intra-class variance)

Supervised Dimensionality Reduction

- Variance based projection directions can sometimes be suboptimal (e.g., if we want to preserve class separation, e.g., when doing classification)



- A better option would be to project such that
  - Points within the same class are close (low intra-class variance)
  - Points from different classes are well separated (the class means are far apart)

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- Solution for $\boldsymbol{u}$ depends on eigendecomposition of within class and between class covariance matrices

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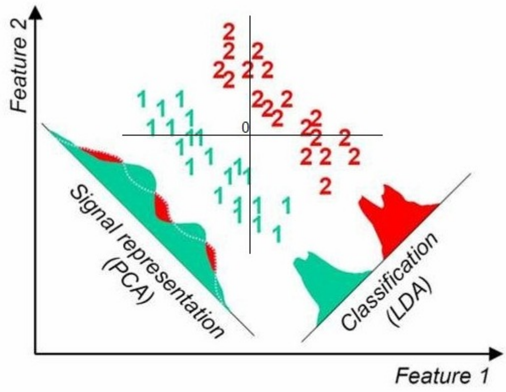

Can be generalized for projections to more than 1 dimensional space

Picture courtesy: Stackoverflow

Dimensionality Reduction given Pairwise Distances between Points

Dimensionality Reduction by Preserving Pairwise Distances

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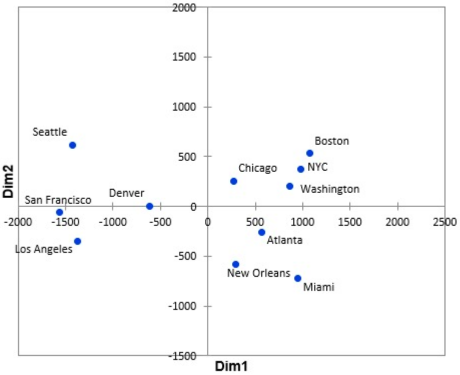
- Can show show that preserving <u>all</u> pairwise <u>Euclidean</u> distances = doing PCA :-)
- Important: Often it is better to only preserve distances between nearest neighbors (helps in learning nonlinear projections), methods like locally linear embedding (LLE) and Isomap do this.

Multi-dimensional Scaling: An Illustration

Result of applying MDS (with $K = 2$) on pairwise distances between some US cities

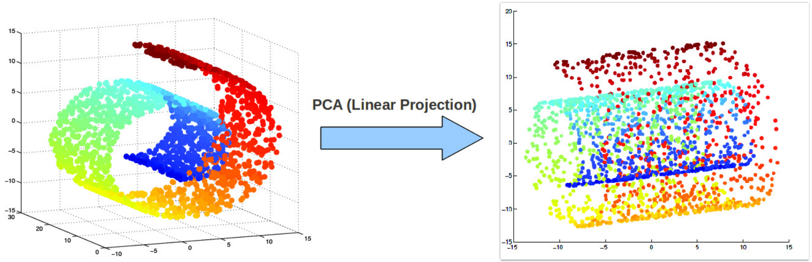


MDS produces a 2D embedding such that geographically close cities are also close in embedding space.

Nonlinear Dimensionality Reduction

Beyond Linear Projections..

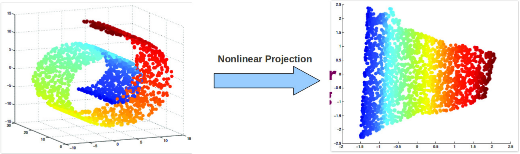
- Consider the swiss-roll dataset (points lying close to a manifold)



- Linear projection methods (e.g., PCA) can't capture intrinsic nonlinearities

Nonlinear Dimensionality Reduction

- We want to a learn nonlinear low-dim projection



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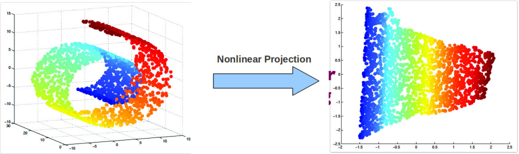

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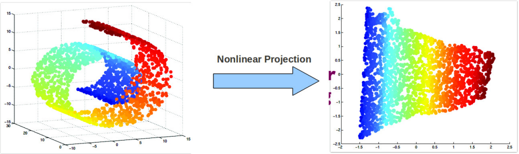

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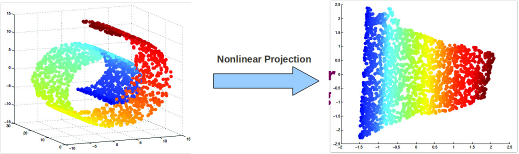

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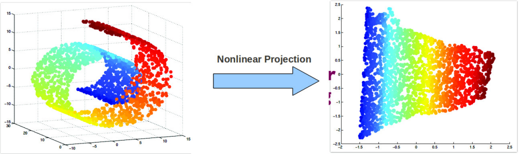

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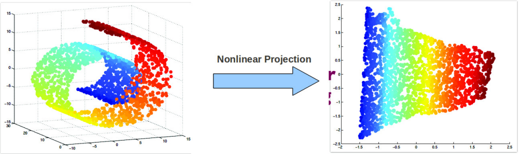

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  - .. or use unsupervised deep learning techniques (later)
- Today, we will briefly look at KPCA, LLE, SNE/tSNE

Kernel PCA

- Recall PCA: Given N observations $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, $\forall \boldsymbol{x}_n \in \mathbb{R}^D$, we define the $D \times D$ covariance matrix (assuming centered data $\sum_n \boldsymbol{x}_n = \mathbf{0}$)

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- This boils down to doing eigendecomposition of the $N \times N$ kernel matrix $\mathbf{K}$ (PRML 12.3)

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- Basically, if point i can be reconstructed from its neighbors in the original space, the same weights W_{ij} should be able to reconstruct it in the new space too.

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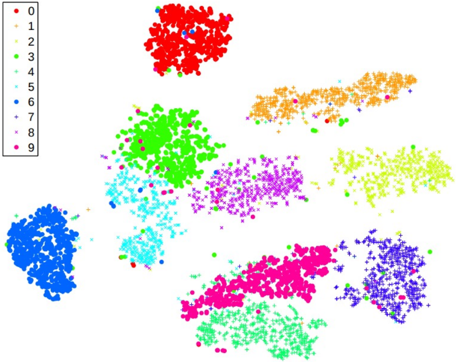
SNE and t-SNE

Especially useful for visualizing data by projecting into 2D or 3D



Result of visualizing MNIST digits data in 2D (Figure from van der Maaten and Hinton, 2008)