PCA (Wrap-up) and Nonlinear Dimensionality Reduction via Kernel PCA

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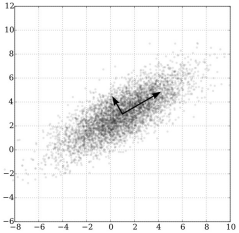
Machine Learning (CS771A)

Sept 7, 2016

Recap/Wrap-up of PCA

Principal Component Analysis (PCA)



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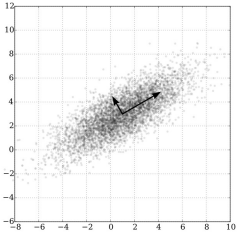

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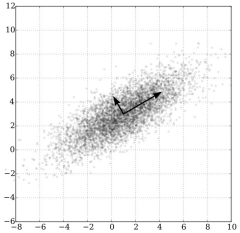

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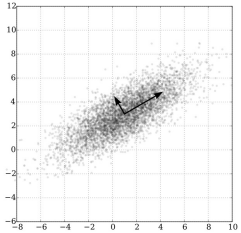

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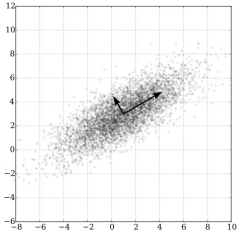

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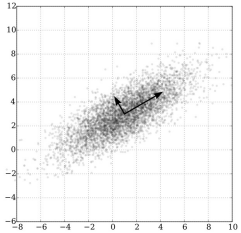

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- PCA uses "amount of data variance captured" to define important directions

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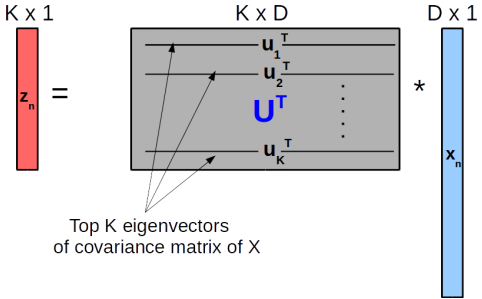
  - Take top K leading eigenvectors $\{\boldsymbol{u}_k\}_{k=1}^K$ with eigenvalues $\{\lambda_k\}_{k=1}^K$
  - $\mathbf{U} = [\boldsymbol{u}_1 \ \ldots \ \boldsymbol{u}_K]$ is $D \times K$ matrix (each column is a projection direction)

PCA as Linear Projection

- Can use $\mathbf{U}$ to linearly project each $\boldsymbol{x}_n \in \mathbb{R}^D$ to a K-dim subspace as

$$\boldsymbol{z}_n = \mathbf{U}^\top \boldsymbol{x}_n = [\boldsymbol{u}_1^\top \boldsymbol{x}_n \ \boldsymbol{u}_2^\top \boldsymbol{x}_n \ \ldots \ \boldsymbol{u}_K^\top \boldsymbol{x}_n]^\top$$



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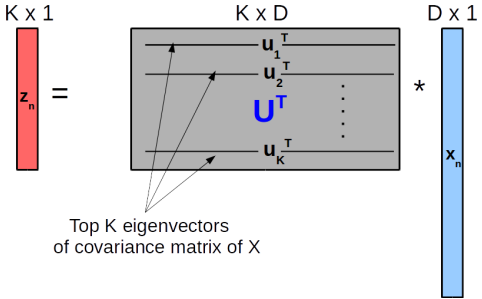
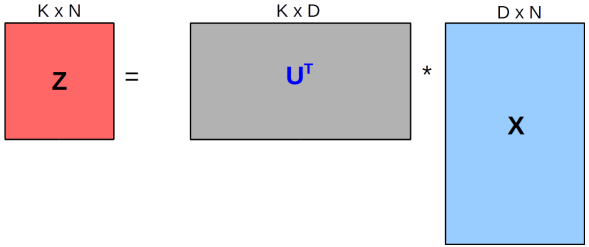


- $\boldsymbol{z}_n \in \mathbb{R}^K$ is also called low-dimensional "embedding" of $\boldsymbol{x}_n \in \mathbb{R}^D$

PCA as Linear Projection

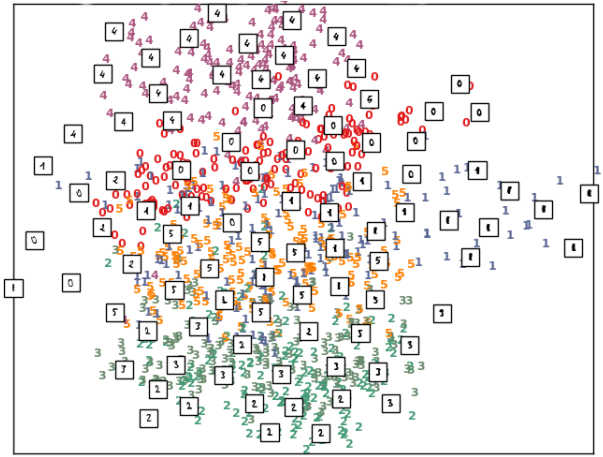
- $\mathbf{Z} = [\boldsymbol{z}_1\ \boldsymbol{z}_2 \ldots\ \boldsymbol{z}_n]$ is the $K \times N$ matrix of embeddings of all the N examples



- $\mathbf{Z}$ can also be thought of as a new, compact feature representation of $\mathbf{X}$

PCA based Embeddings of Handwritten Digits

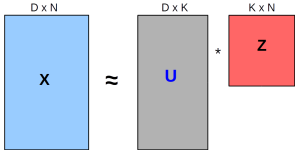
- Shown below are 2-dim embeddings of PCA on a set of handwritten digits (each digit image was originally 8×8, i.e., 64 dimensional)



PCA: Data as Combination of Basis Vectors

- PCA to K-dims is also akin to saying $\boldsymbol{x}_n \approx \sum_{k=1}^{K} z_{nk} \boldsymbol{u}_k$. Thus

$$\mathbf{X} \approx \mathbf{UZ} \qquad \text{(matrix factorization)}$$



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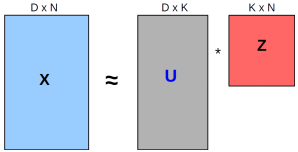

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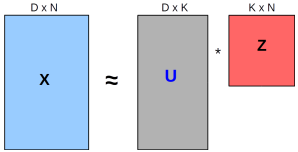

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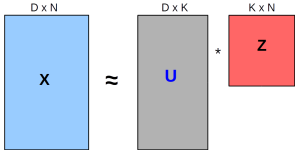

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  - Substantial storage saving if $K \ll D$

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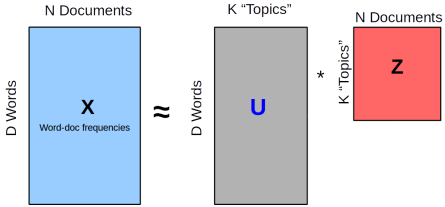

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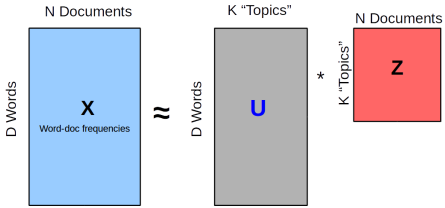

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- This is similar to "Latent Semantic Analysis" (LSA), a well-known document dimensionality reduction technique in information retrieval (basically, LSA does SVD on $\mathbf{X}$, which is equivalent to doing PCA on $\mathbf{X}$)

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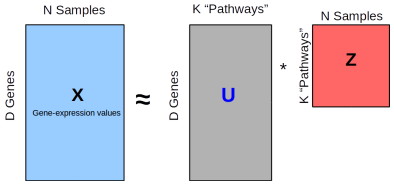
- **X** is (genes $\times$ samples) matrix: Each sample (expression values of a set of D genes) is a weighted combination of K biological "pathways"



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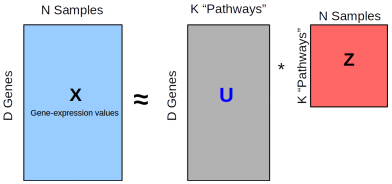
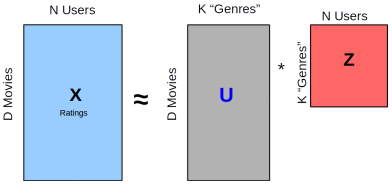
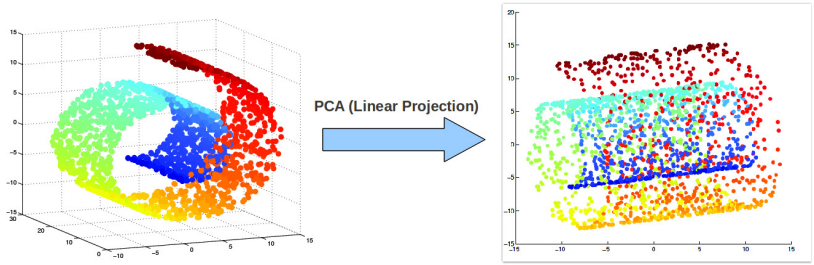


- **X** is (movies $\times$ users) matrix: Each user (represented by the vector of his/her ratings of D movies) is a weighted combination of K genres



Beyond Linear Projections..

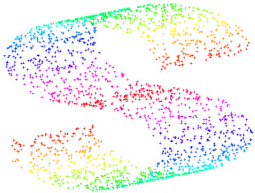
- Consider the swiss-roll dataset (points lying close to a manifold)



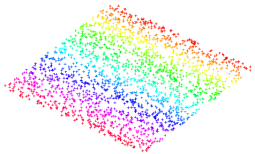
- Linear projection methods (e.g., PCA) can't capture intrinsic nonlinearities

Nonlinear Dimensionality Reduction

- Given: Low-dim. surface embedded **nonlinearly** in high-dim. space
  - Such a structure is called a **Manifold**



- Goal: Recover the low-dimensional surface



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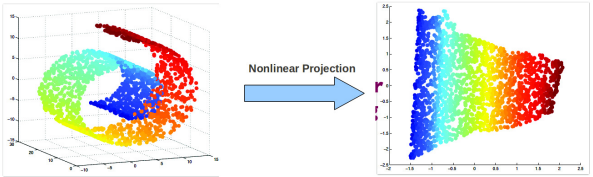

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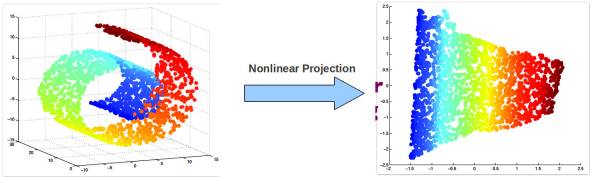

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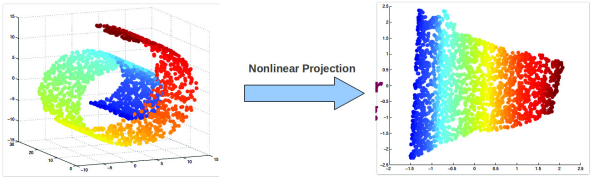

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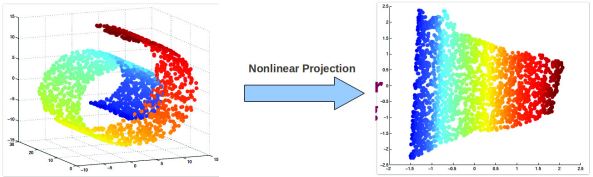

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  - Nonlinearize a linear dimensionality reduction method. E.g.:
    - **Kernel PCA (nonlinear PCA)**
  - Using manifold based methods that intrinsically preserve nonlinear geometry
    - Locally Linear Embedding (LLE)
    - Isomap
    - Maximum Variance Unfolding
    - Laplacian Eigenmaps
    - And others (tSNE, Hessian LLE, etc.)

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 $\sum_n \boldsymbol{x}_n = \boldsymbol{0}$)

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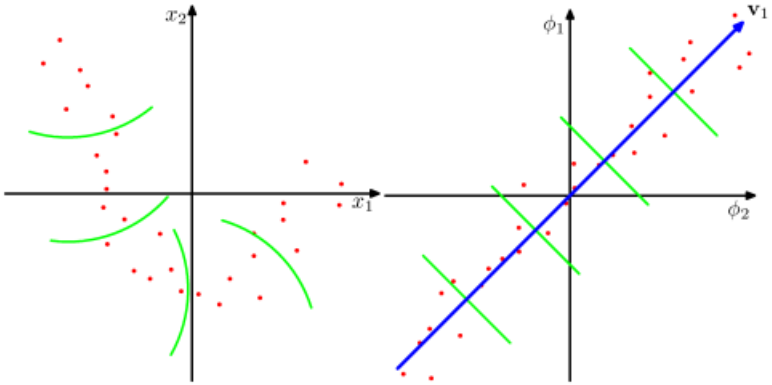
- We would like to do this without having to compute $\mathbf{C}$ or $\phi(\boldsymbol{x}_n)$'s

Kernel PCA



Right figure: After mapping the data via ϕ, data is now close to a linear subspace

Kernel PCA

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- Pre-multiplying both sides by $\phi(\boldsymbol{x}_\ell)^\top$ and re-arranging

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- Note: Since $\boldsymbol{v}_i^\top \boldsymbol{v}_i = 1$ and $\boldsymbol{v}_i = \sum_{n=1}^{N} \alpha_{in}\phi(\boldsymbol{x}_n)$, we have $\boldsymbol{\alpha}_i^\top \mathbf{K}\boldsymbol{\alpha}_i = 1$, which means $\boldsymbol{\alpha}_i^\top \lambda_i N \boldsymbol{\alpha}_i = 1$ and $\boldsymbol{\alpha}_i^\top \boldsymbol{\alpha}_i = 1/(\lambda_i N)$. Thus the original solution with $\boldsymbol{\alpha}_i^\top \boldsymbol{\alpha}_i = 1$ (eigenvec with norm 1) needs to be re-scaled as $\tilde{\alpha}_{in} = \alpha_{in}/\sqrt{\lambda_i N}$

Kernel PCA: Centering the Data

- In PCA, we centered the data before computing the covariance matrix
- For kernel PCA, we need to do the same

$$\tilde{\phi}(\boldsymbol{x}_n) = \phi(\boldsymbol{x}_n) - \frac{1}{N}\sum_{\ell=1}^{N}\phi(\boldsymbol{x}_\ell)$$

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- $\boldsymbol{1}_N$ is the $N \times N$ matrix with every element $= 1/N$
- Eigen-decomposition is then done for the centered kernel matrix $\tilde{\boldsymbol{K}}$

Kernel PCA: Computing the Embeddings

- Suppose $\{\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_L\}$ are the top L eigenvectors of kernel matrix $\tilde{\boldsymbol{K}}$
- The L-dimensional KPCA projection $\boldsymbol{z}_m = [z_{m1}, \ldots, z_{mL}]$ of a point $\boldsymbol{x}_m$:

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- Note: For linear kernel, KPCA reduces to PCA (but more efficient if $N < D$)

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- Re-scale each eigenvector as $\tilde{\boldsymbol{\alpha}}_i = \boldsymbol{\alpha}_i / \sqrt{\lambda_i N}$, $\forall i = 1, \ldots, L$

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- Construct the $N \times N$ kernel matrix $\mathbf{K}$
- Center $\mathbf{K}$ as follows $\tilde{\boldsymbol{K}} = \boldsymbol{K} - \mathbf{1}_N \boldsymbol{K} - \boldsymbol{K}\mathbf{1}_N + \mathbf{1}_N \boldsymbol{K} \mathbf{1}_N$, where $\mathbf{1}_N$ is an $N \times N$ matrix of all $1/N$
- Do eigen-decomposition of $\tilde{\boldsymbol{K}}$ and find top L eigenvecs $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_L$ with eigenvals $\lambda_1, \lambda_2, \ldots, \lambda_L$
- Re-scale each eigenvector as $\tilde{\boldsymbol{\alpha}}_i = \boldsymbol{\alpha}_i / \sqrt{\lambda_i N}$, $\forall i = 1, \ldots, L$
- Finally, compute embedding $\boldsymbol{z}_m \in \mathbb{R}^L$ of any point $\boldsymbol{x}_m$ as

$$z_{m\ell} = \sum_{n=1}^{N} \tilde{\alpha}_{\ell n} k(\boldsymbol{x}_n, \boldsymbol{x}_m)$$

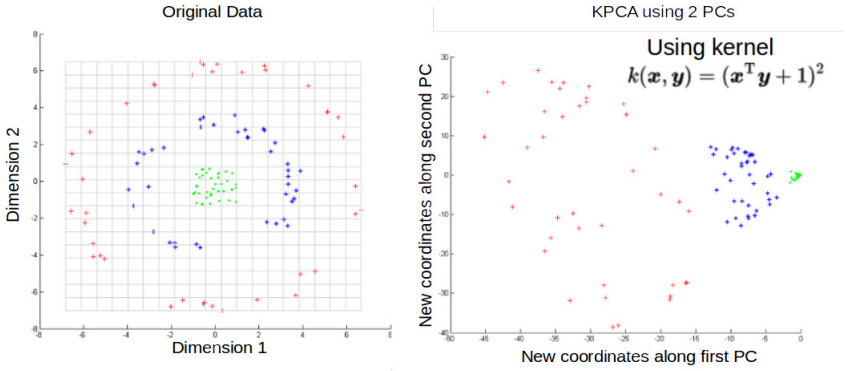
Kernel PCA: Summary of the algorithm

- Construct the $N \times N$ kernel matrix $\mathbf{K}$
- Center $\mathbf{K}$ as follows $\tilde{\mathbf{K}} = \mathbf{K} - \mathbf{1}_N\mathbf{K} - \mathbf{K}\mathbf{1}_N + \mathbf{1}_N\mathbf{K}\mathbf{1}_N$, where $\mathbf{1}_N$ is an $N \times N$ matrix of all $1/N$
- Do eigen-decomposition of $\tilde{\mathbf{K}}$ and find top L eigenvecs $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_L$ with eigenvals $\lambda_1, \lambda_2, \ldots, \lambda_L$
- Re-scale each eigenvector as $\tilde{\boldsymbol{\alpha}}_i = \boldsymbol{\alpha}_i / \sqrt{\lambda_i N}$, $\forall i = 1, \ldots, L$
- Finally, compute embedding $\boldsymbol{z}_m \in \mathbb{R}^L$ of any point $\boldsymbol{x}_m$ as

$$z_{m\ell} = \sum_{n=1}^{N} \tilde{\alpha}_{\ell n} k(\boldsymbol{x}_n, \boldsymbol{x}_m)$$

- Note: For compactness, the $L \times N$ matrix of all L eigenvectors (each is N dimensional) can be written as $\tilde{\boldsymbol{\alpha}} = [\tilde{\boldsymbol{\alpha}}_1 \ \tilde{\boldsymbol{\alpha}}_2 \ \ldots \ \tilde{\boldsymbol{\alpha}}_L]^\top$. Thus we can also write embedding $\boldsymbol{z}_m \in \mathbb{R}^L$ as $\boldsymbol{z}_m = \tilde{\boldsymbol{\alpha}}\boldsymbol{k}_m$ where $\boldsymbol{k}_m$ is $N \times 1$ vector of kernelized similarities of $\boldsymbol{x}_m$ with all the N training data points

Kernel PCA: An Example



Note that even if we throw away the 2nd PC, we get a good 1-D embedding