Linear Dimensionality Reduction: Principal Component Analysis

Piyush Rai

Machine Learning (CS771A)

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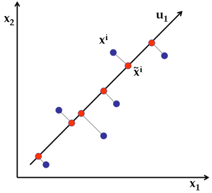

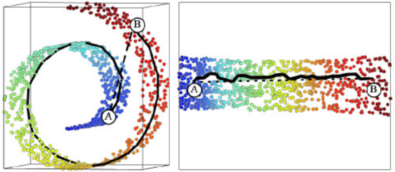

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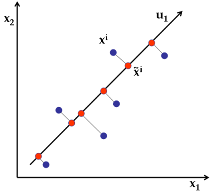

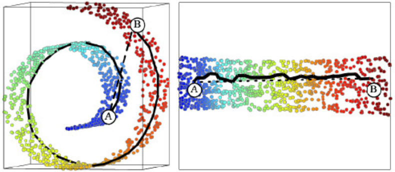

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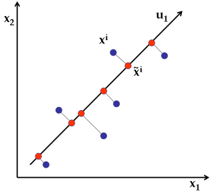

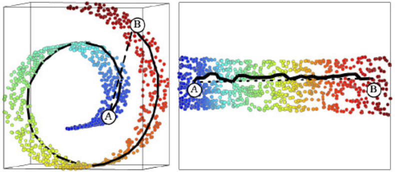

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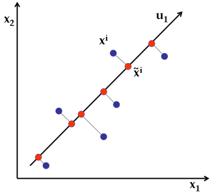

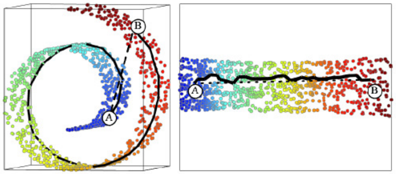

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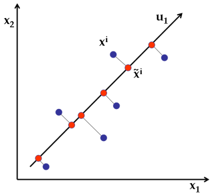

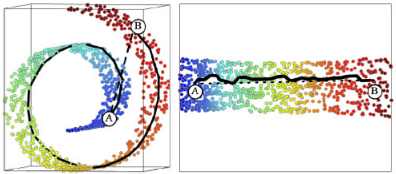

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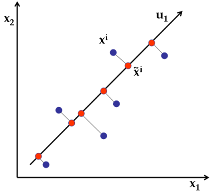

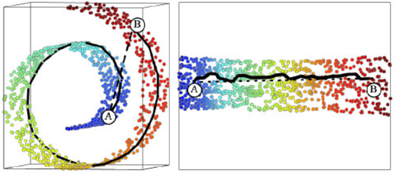

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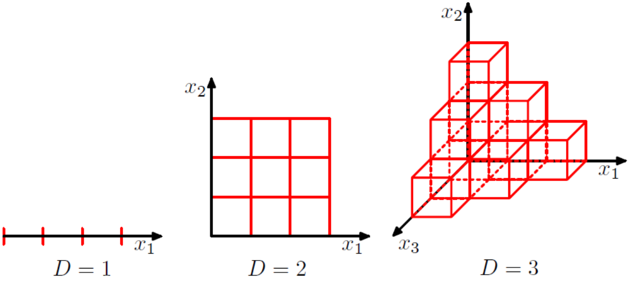
Curse of Dimensionality

- Exponentially large # of examples required to "fill up" high-dim spaces



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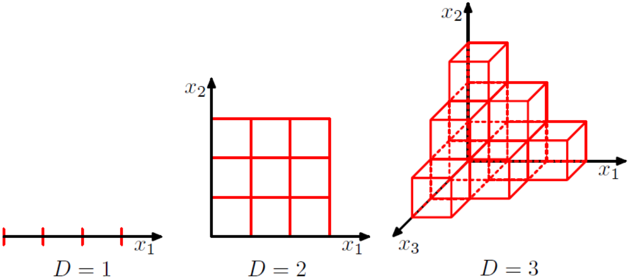

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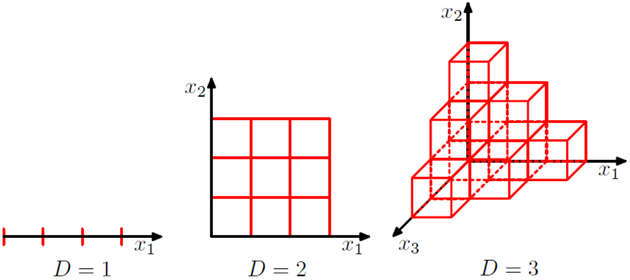

- Fewer dimensions ⇒ Less chances of overfitting ⇒ Better generalization
- Dimensionality reduction is a way to beat the curse of dimensionality

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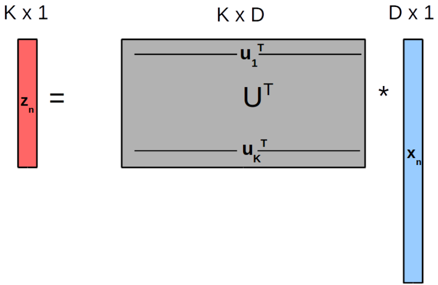

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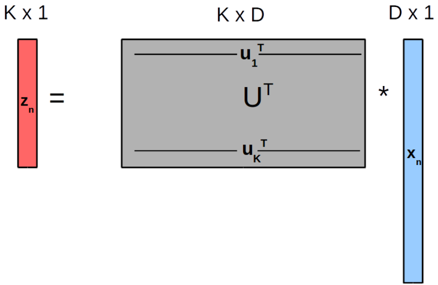

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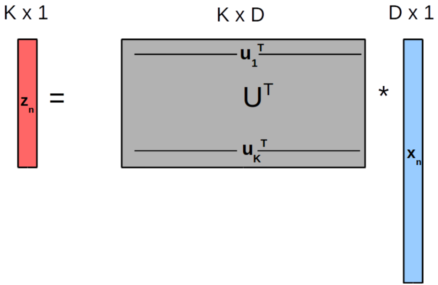

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  - $\boldsymbol{z}_n \in \mathbb{R}^K$ is also called low-dimensional "embedding" of $\boldsymbol{x}_n \in \mathbb{R}^D$

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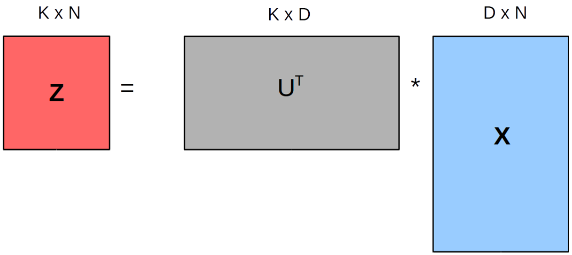

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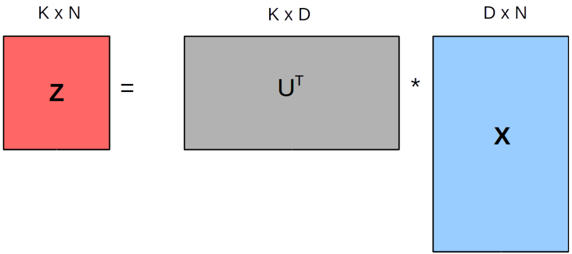

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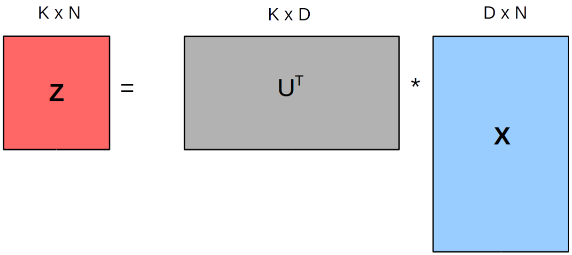

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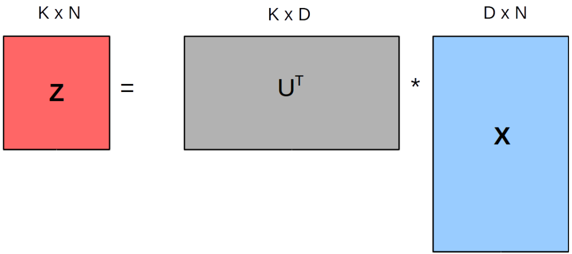

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- Principal Component Analysis (PCA) is an algorithm for doing this

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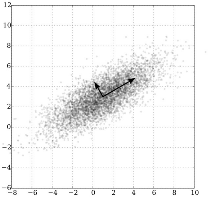

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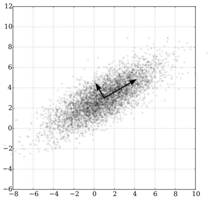

- Also related to other classic methods, e.g., Factor Analysis (Spearman, 1904)

PCA as Maximizing Variance

Variance Captured by Projections

- Consider projecting $\boldsymbol{x}_n \in \mathbb{R}^D$ on a one-dim subspace defined by $\boldsymbol{u}_1 \in \mathbb{R}^D$
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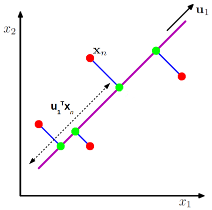

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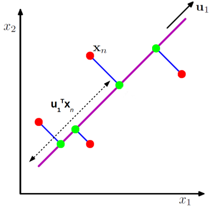

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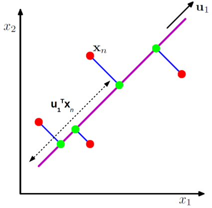

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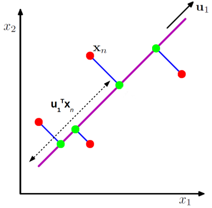

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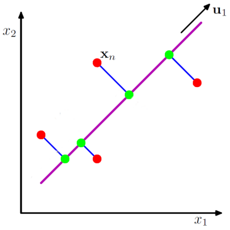
- **S** is the $D \times D$ **data covariance matrix**: $\boldsymbol{S} = \frac{1}{N}\sum_{n=1}^N (\boldsymbol{x}_n - \boldsymbol{\mu})(\boldsymbol{x}_n - \boldsymbol{\mu})^\top$. If data already centered ($\boldsymbol{\mu} = 0$) then $\boldsymbol{S} = \frac{1}{N}\sum_{n=1}^N \boldsymbol{x}_n \boldsymbol{x}_n^\top = \frac{1}{N}\mathbf{X}^\top\mathbf{X}$

Direction of Maximum Variance



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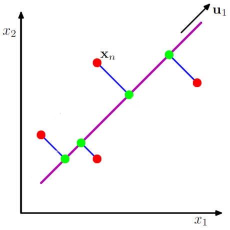

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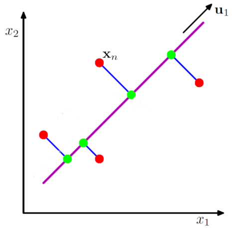

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- We will find $\boldsymbol{u}_1$ by solving the following constrained opt. problem

$$\boxed{\arg\max_{\boldsymbol{u}_1} \; \boldsymbol{u}_1^\top \mathbf{S} \boldsymbol{u}_1 + \lambda_1 (1 - \boldsymbol{u}_1^\top \boldsymbol{u}_1)}$$

where λ_1 is a Lagrange multiplier

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- Var. is maximized when $\boldsymbol{u}_1$ is the (top) eigenvector with largest eigenvalue

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- The objective function: $\arg\max_{\boldsymbol{u}_1} \; \boldsymbol{u}_1^\top \mathbf{S} \boldsymbol{u}_1 + \lambda_1(1 - \boldsymbol{u}_1^\top \boldsymbol{u}_1)$
- Taking the derivative w.r.t. $\boldsymbol{u}_1$ and setting to zero gives

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

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- A word about notation: If $\mathbf{X}$ is $N \times D$, then $\mathbf{S} = \frac{1}{N}\mathbf{X}^\top\mathbf{X}$ (needs to be $D \times D$) and the embedding will be computed as $\mathbf{Z} = \mathbf{X}\mathbf{U}$ where $\mathbf{Z}$ is $N \times K$

PCA as Minimizing the Reconstruction Error

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$$\boxed{\boldsymbol{x}_n = \mathbf{U}\boldsymbol{z}_n \quad \text{and} \quad \boldsymbol{z}_n = \mathbf{U}^\top \boldsymbol{x}_n}$$

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- Also note that each component of vector $\boldsymbol{z}_n$ is $z_{nk} = \boldsymbol{u}_k^\top \boldsymbol{x}_n$

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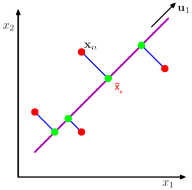
- Total error or "loss" in reconstructing all the data points

$$L(\boldsymbol{u}_1) = \sum_{n=1}^{N} ||\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n||^2 = \sum_{n=1}^{N} ||\boldsymbol{x}_n - \boldsymbol{u}_1 \boldsymbol{u}_1^\top \boldsymbol{x}_n||^2$$



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- It's the same objective that we had when we maximized the variance

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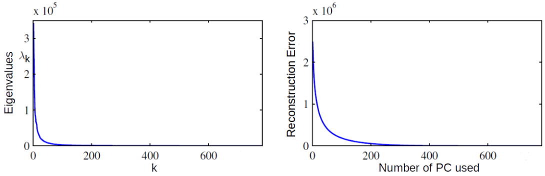

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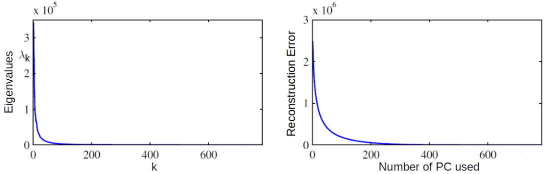

- Can also use other criteria such as AIC/BIC (or more advanced probabilistic approaches to PCA using nonparametric Bayesian methods)

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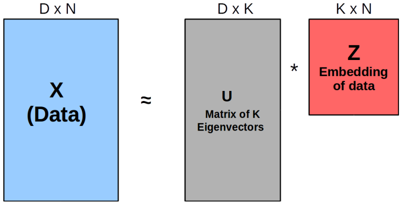

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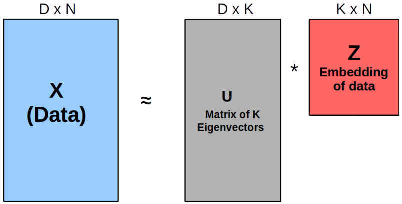

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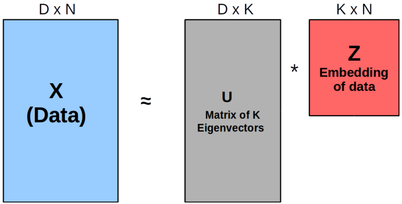

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  - Also closely related to Singular Value Decomposition (SVD); see next slide

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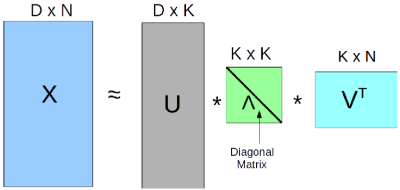
- A rank-K SVD approximates a data matrix $\mathbf{X}$ as follows: $\mathbf{X} \approx \mathbf{U} \Lambda \mathbf{V}^\top$



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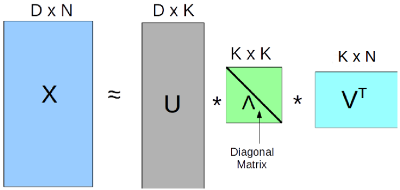

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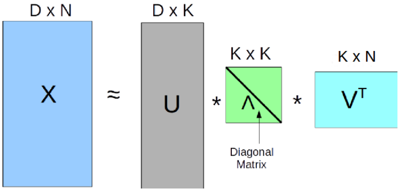

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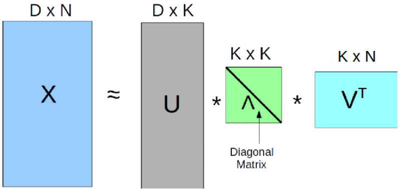

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- Λ is a $K \times K$ diagonal matrix (with top K singular values)
- $\mathbf{V}$ is $N \times K$ matrix with top K right singular vectors of $\mathbf{X}$

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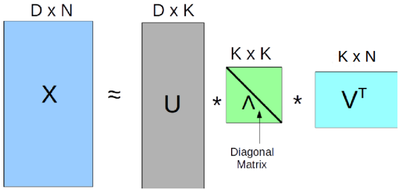

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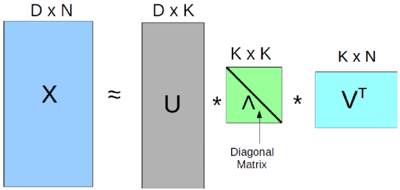

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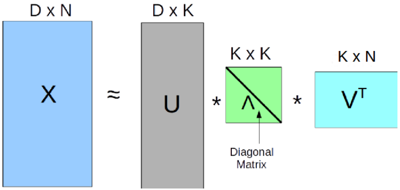

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- PCA is equivalent to the best rank-K SVD after centering the data

PCA: Some Comments

- The idea of approximating each data point as a combination of basis vectors

$$\boldsymbol{x}_n \approx \sum_{k=1}^{K} z_{nk}\boldsymbol{u}_k \quad \text{or} \quad \mathbf{X} \approx \mathbf{UZ}$$

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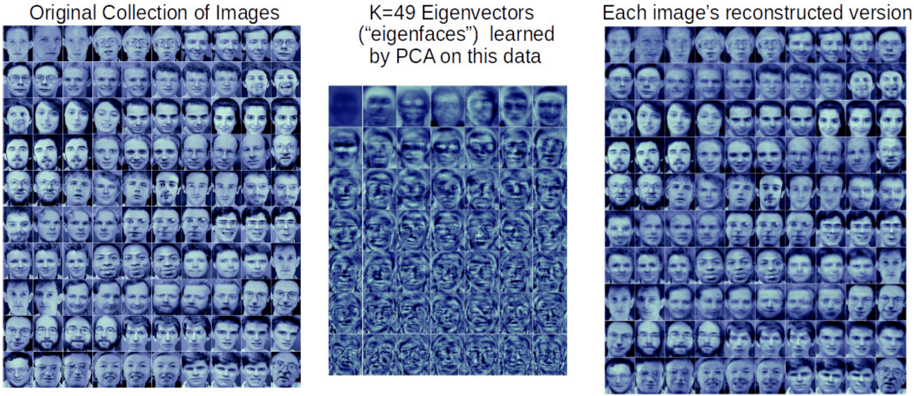
  - Each gene-expression sample as a comb. of a small no of "genetic pathways"
  - The "eigenfaces", "topics", "genetic pathways", etc. are the "basis vectors", which can be learned from data using PCA/SVD or other similar methods

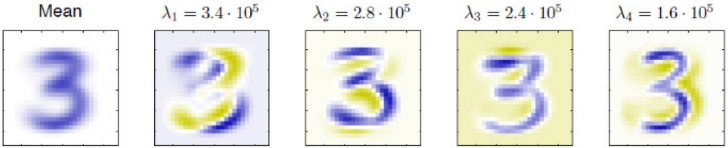
PCA: Example


Original Collection of Images
K=49 Eigenvectors
("eigenfaces") learned
by PCA on this data
Each image's reconstructed version

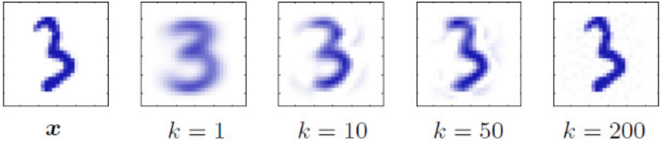
PCA: Example

16×16 pixel images of handwritten 3s (as vectors in $\mathbb{R}^{256}$)

Mean μ and eigenvectors v_1, v_2, v_3, v_4



Reconstructions:



Each input image now represented by just k numbers
(combination weights of each of the k eigenvectors)

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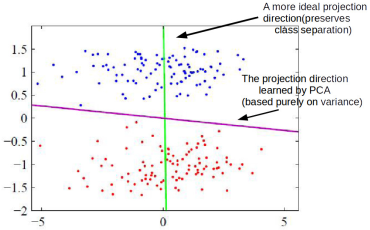

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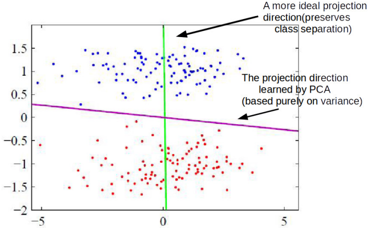

- PCA relies on eigendecomposition of an $D \times D$ covariance matrix
  - Can be slow if done naïvely. Takes $O(D^3)$ time
  - Many faster methods exists (e.g., Power Method)