COMS 4771
Dimensionality Reduction

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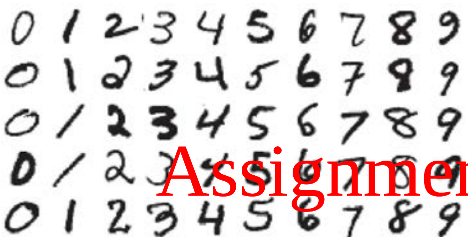
Example: Handwritten digits

Handwritten digit data, but with no labels



What can we do?

- Suppose know that there are 10 groupings, can we find the groups?
- What if we don't know there are 10 groups?
- How can we discover/explore other structure in such data?

A 2D visualization of digits dataset

Dimensionality Reduction

Data: $\vec{x}_1, \vec{x}_2, \ldots \vec{x}_n \in \mathbf{R}^d$

Goal: find a 'useful' transformation $\phi : \mathbf{R}^d \to \mathbf{R}^k$ that helps in the downstream prediction task.

Some previously seen useful transformations:

- z-scoring $(x_1, \ldots, x_d) \mapsto \left(\frac{x_1 - \mu_1}{\sigma_1}, \ldots, \frac{x_d - \mu_d}{\sigma_d}\right)$ *Keeps same dimensionality but with better scaling*

- Kernel transformations. *Higher dimensionality, making data linearly separable*

What are other desirable feature transformations?

How about lower dimensionality while keeping the relevant information?

Principal Components Analysis (PCA)

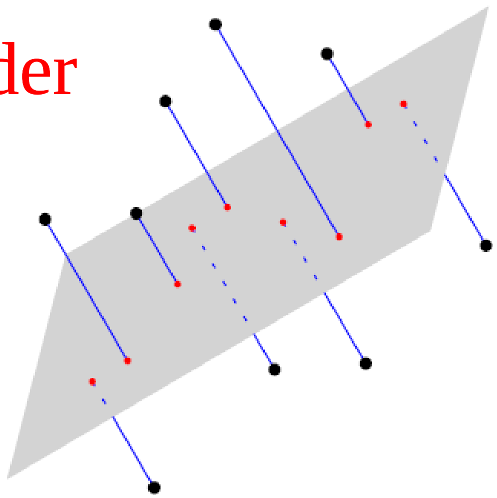
Data: $\vec{x}_1, \vec{x}_2, \ldots \vec{x}_n \in \mathbf{R}^d$

Goal: find the best **linear** transformation $\phi : \mathbf{R}^d \to \mathbf{R}^k$ that best maintains reconstruction accuracy.

Equivalently, minimize aggregate residual error

Define: $\Pi^k : \mathbf{R}^d \to \mathbf{R}^d$ *k-dimensional orthogonal linear projector*

$$\underset{\Pi^k}{\textit{minimize}} \quad \frac{1}{n}\sum_{i=1}^{n} \left\| \vec{x}_i - \Pi^k(\vec{x}_i) \right\|^2$$

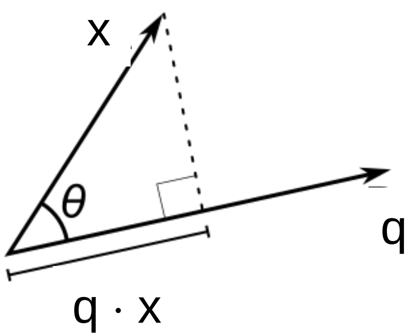


How do we optimize this?

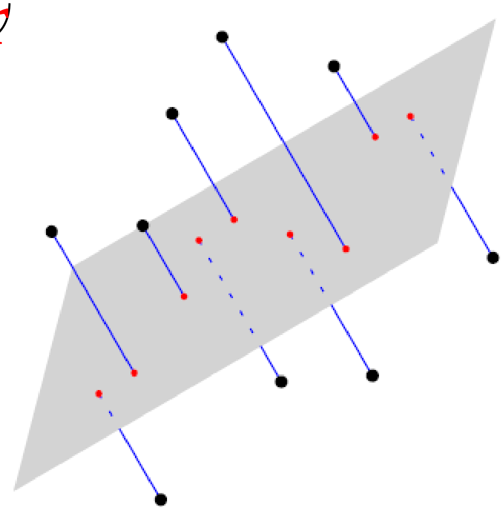
Dimensionality Reduction via Projections

A *k* dimensional subspace can be represented by $\vec{q}_1, \ldots, \vec{q}_k \in \mathbf{R}^d$ orthonormal vectors.

The projection of any $\vec{x} \in \mathbf{R}^d$ in the $\mathrm{span}(\vec{q}_1, \ldots, \vec{q}_k)$ is given by



$$\sum_{i=1}^{k} (\vec{q}_i \cdot \vec{x})\, \vec{q}_i = \underbrace{\left(\sum_{i=1}^{k} \vec{q}_i \vec{q}_i^{\mathsf{T}} \right)}_{\Pi^k} \vec{x}$$



To represent it in $\mathbf{R}^k$ (using basis $\vec{q}_1, \ldots, \vec{q}_k$) the coefficients simply are: $(\vec{q}_1 \cdot \vec{x}), \ldots, (\vec{q}_k \cdot \vec{x})$

PCA: k = 1 case

If projection dimension k = 1, then looking for a q such that

$$\textit{minimize}_{\|q\|=1} \quad \frac{1}{n}\sum_{i=1}^{n} \left\| \vec{x}_i - (\vec{q}\,\vec{q}^{\top})\vec{x}_i \right\|^2$$

$$\frac{1}{n}\sum_{i=1}^{n} \left\| \vec{x}_i - (\vec{q}\,\vec{q}^{\top})\vec{x}_i \right\|^2 = \left(\frac{1}{n}\sum_{i=1}^{n} \vec{x}_i^{\top}\vec{x}_i\right) - \vec{q}^{\top}\left(\frac{1}{n}\sum_{i=1}^{n} \vec{x}_i\vec{x}_i^{\top}\right)\vec{q}$$

$$\propto -\,\vec{q}^{\top}\left(\frac{1}{n}XX^{\top}\right)\vec{q}$$

Equivalent formulation:

$$\textit{maximize}_{\|q\|=1} \quad \vec{q}^{\top}\left(\frac{1}{n}XX^{\top}\right)\vec{q}$$

How to solve?

Eigenvectors and Eigenvalues

Recall for any matrix *M*, the (λ,v) pairs of the fixed point equation

$$Mv = \lambda v$$

are the eigenvalue and the eigenvectors of *M*. ($v \neq 0$)

$$v^{\mathsf{T}} M v = \lambda v^{\mathsf{T}} v$$

$$\lambda = \frac{v^{\mathsf{T}} M v}{v^{\mathsf{T}} v} = \bar{v}^{\mathsf{T}} M \bar{v} \qquad \text{where } \bar{v} = \frac{v}{\|v\|}$$ *(ie, unit length)*

So,

maximize$_{\|q\|=1}$ $\vec{q}^{\mathsf{T}} \left(\frac{1}{n} X X^{\mathsf{T}} \right) \vec{q}$

Basically is the top eigenvector of matrix (1/n) XX^{T}!

PCA: k = 1 case

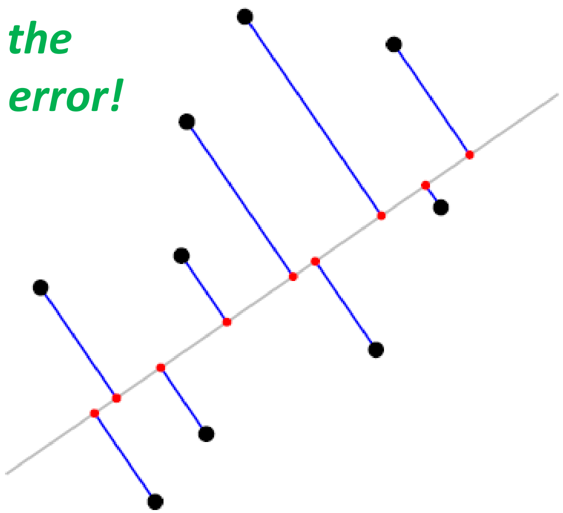
maximize$_{||q||=1}$ $\vec{q}^\top \left(\frac{1}{n} X X^\top\right) \vec{q}$

Covariance of data (if mean = 0)

For any q the quadratic form $\vec{q}^\top \left(\frac{1}{n} X X^\top\right) \vec{q}$ is the empirical

variance of data in the direction q, ie, of data $\vec{q}^\top \vec{x}_1, \ldots, \vec{q}^\top \vec{x}_n$ *why?*

Therefore, the top eigenvector solution implies that the direction of maximum variance minimizes the residual error!



What about general k?

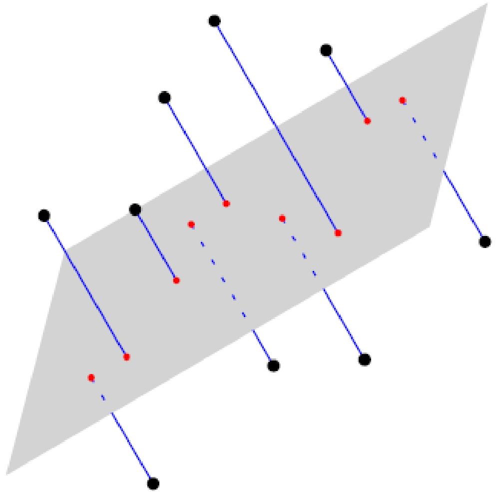
PCA: general k case

$$\arg\min_{\substack{Q \in \mathbf{R}^{d\times k} \\ Q^\top Q = I}} \frac{1}{n}\sum_{i=1}^{n} \left\| \vec{x}_i - QQ^\top \vec{x}_i \right\|^2 = \arg\max_{\substack{Q \in \mathbf{R}^{d\times k} \\ Q^\top Q = I}} \operatorname{tr}\left(Q^\top \left(\frac{1}{n} X X^\top\right) Q\right)$$

Solution: Basically is the top k eigenvectors of the matrix $XX^\top$!

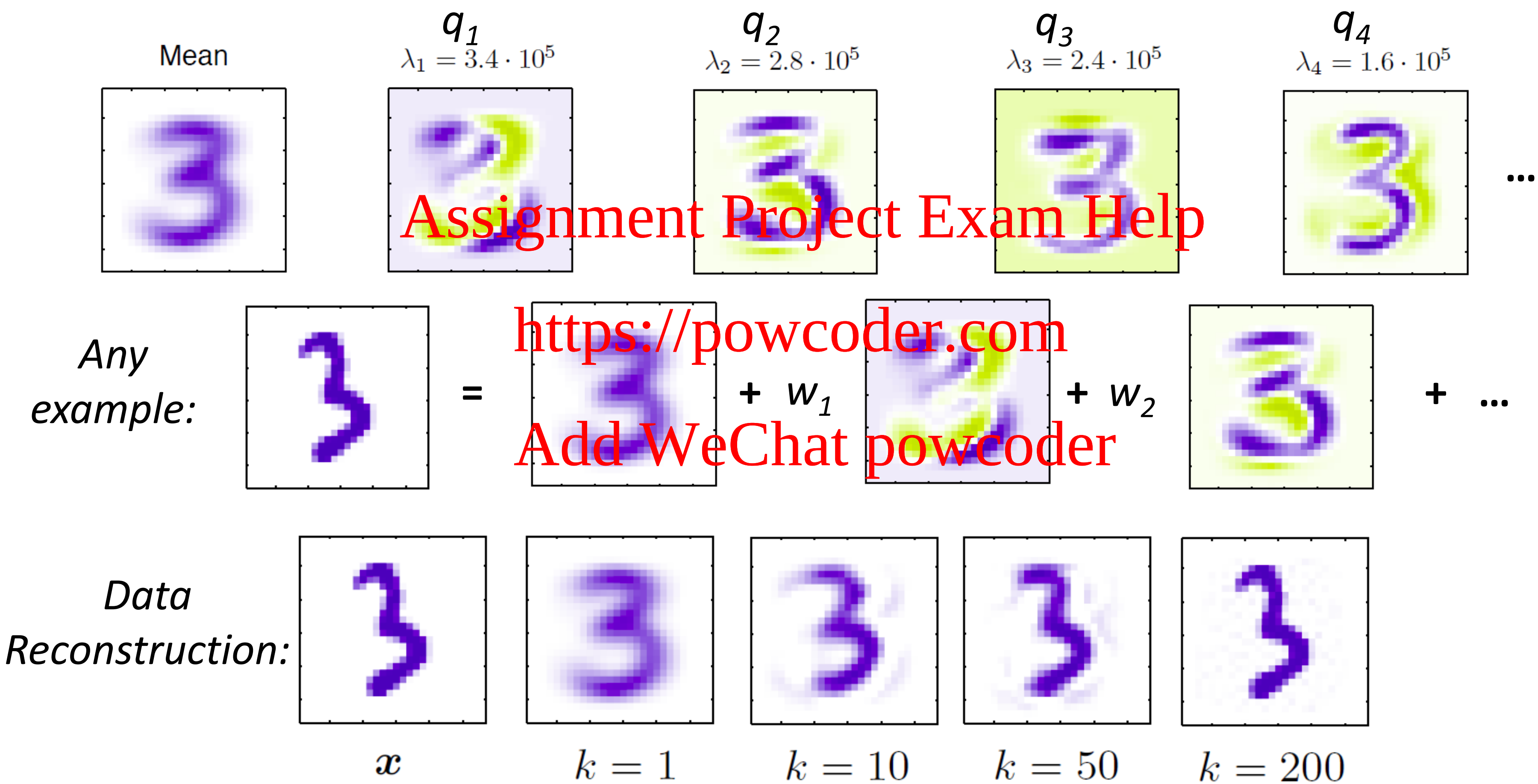
$$\operatorname{tr}\left(Q^\top \left(\frac{1}{n} X X^\top\right) Q\right) = \sum_{i=1}^{k} \text{empirical variance of } \vec{q}_i^{\,\top} x$$

k-dimensional subspace preserving maximum amount of variance



PCA: Example Handwritten Digits

Images of handwritten 3s in $\mathbf{R}^{784}$



We can compress the each datapoint to just k numbers!

Other Popular Dimension Reduction Methods

Multi-dimensional Scaling

Independent Component Analysis (ICA) (for blind source separation)

Non-negative matrix factorization (to create additive models)

Dictionary Learning

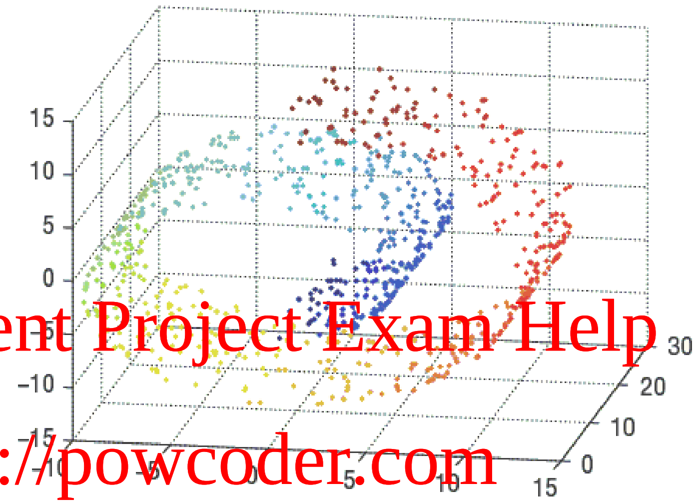
Random Projections

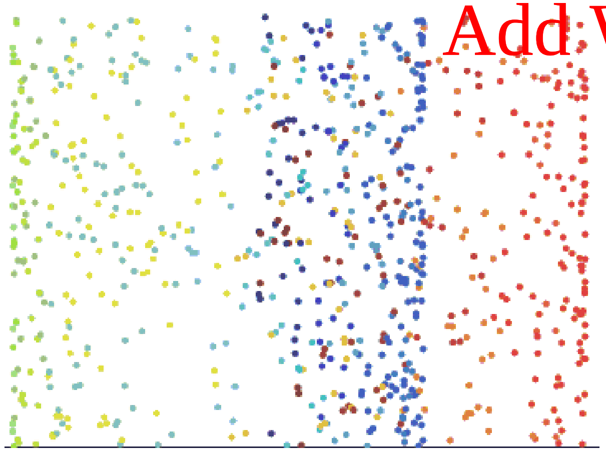
...

*All of them are **linear** methods*

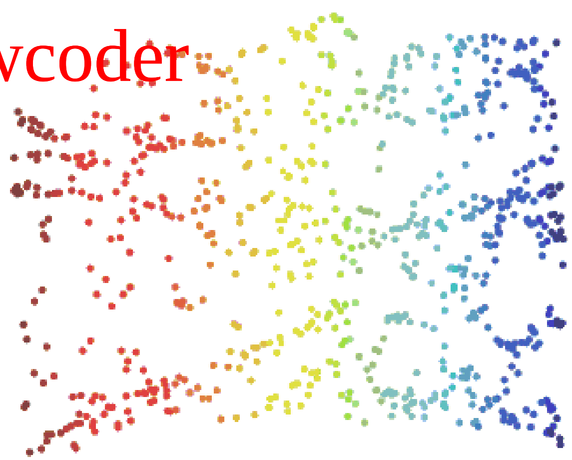
Non-Linear Dimensionality Reduction

Consider non-linear data





Linear embedding



non-linear embedding

Non-Linear Dimensionality Reduction

Basic optimization criterion:

Find an embedding that:

- Keeps neighboring points close
- Keeps far-off points far

Example variation 1:

Distort neighboring distances by at most ($1 \pm \varepsilon$) factor, while maximizing non-neighbor distances.

Example variation 2:

Compute ***geodesic*** *(local hop) distances, and find an embedding that best preserves geodesics.*

Non-linear embedding: Example

Popular Non-Linear Methods

Locally Linear Embedding (LLE)

Isometric Mapping (IsoMap)

Laplacian Eigenmaps (LE)

Local Tangent Space Alignment (LTSA)

Maximum Variance Unfolding (MVU)

...

What We Learned…

- Dimensionality Reduction

    Linear vs non-linear Dimensionality Reduction

- Principal Component Analysis

Questions?