PCA / SVD

COMS 4721 Spring 2022

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PCA

Empirical (sample) covariance

Recall: If $\vec{X}$ is a random vector in $\mathbb{R}^d$, its covariance matrix is

$$\mathrm{cov}(\vec{X}) = \mathbb{E}[(\vec{X} - \mathbb{E}(\vec{X}))(\vec{X} - \mathbb{E}(\vec{X}))^{\mathsf{T}}].$$

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If $\vec{x}_1, \ldots \vec{x}_n \in \mathbb{R}^d$ are n data points from $\mathbb{R}^d$, and P_n is the empirical distribution on these points, then their **empirical covariance matrix** (a.k.a. **sample covariance matrix**) is $\mathrm{cov}(\vec{X})$ for $\vec{X} \sim P_n$

More properties of the covariance matrix

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- **Eigenvalue decomposition** (a.k.a. **spectral decomposition**) of $\mathrm{cov}(\vec{X})$:

$$\mathrm{cov}(\vec{X}) = \sum_{i=1}^{d} \lambda_i \vec{v}_i \vec{v}_i^{\mathsf{T}}$$

Example: MNIST data set of handwritten digits

60000 images of handwritten digits, each a 28×28 gray-scale pixel image

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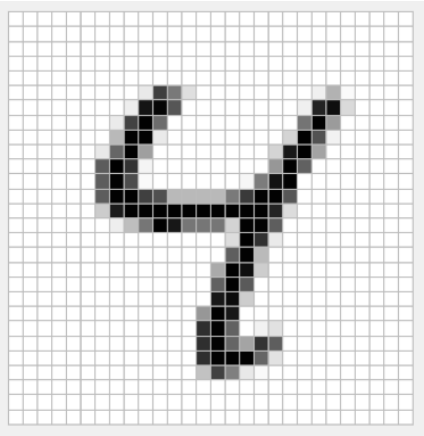
Each image is represented as vector in $[0, 255]^d$ for $d = 28 \times 28 = 784$, one feature per pixel



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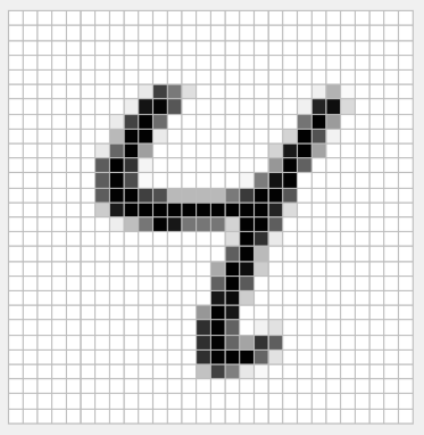

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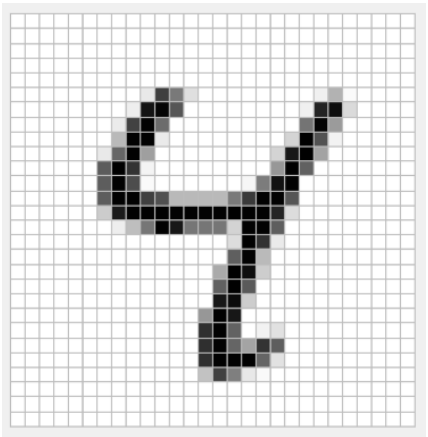

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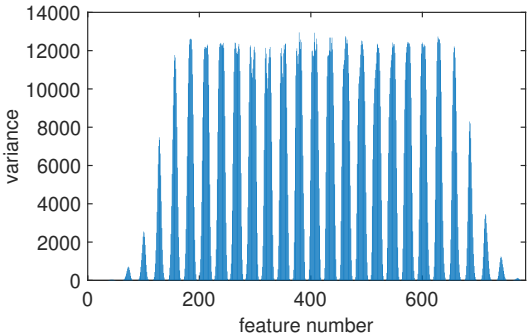

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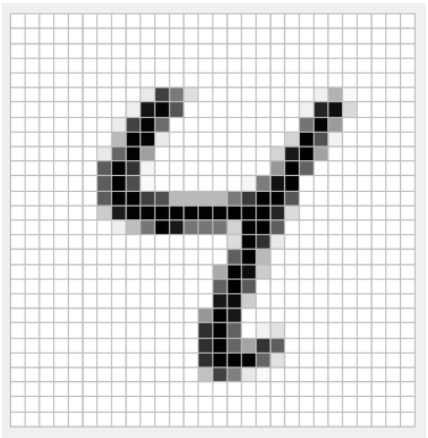

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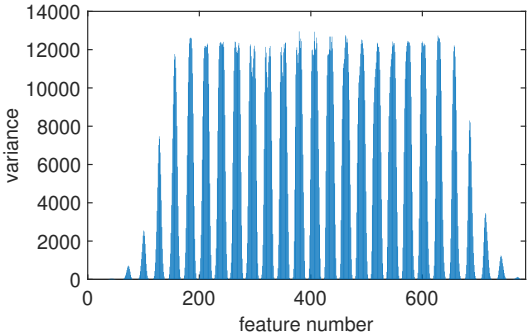

Perhaps not all features are necessary!

Data approximation

Coarse approximation: (our baseline)
Represent each data point by the overall mean $\vec{\mu}$
(where $\vec{\mu} := \mathbb{E}(\vec{X})$)

$$\vec{X} \longmapsto \vec{\mu}$$

Zero features per data point!

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Less coarse approximation:
Represent each data point by overall mean $\vec{\mu}$ plus projection of $\vec{X} - \vec{\mu}$ to subspace $W \subseteq \mathbb{R}^d$

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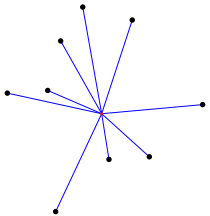

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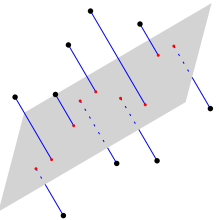

Special case: Coordinate subspaces

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$$10\% \times \underbrace{\mathbb{E}\left[\|\vec{X} - \vec{\mu}\|_2^2\right]}_{\text{our baseline}},$$

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Question: Can we do better by not restricting to coordinate subspaces?

Special case: $k = 1$

Orthogonal projection operator for 1-dimensional subspace W (i.e., a line):

$$\Pi_W \;=\; \vec{\alpha}\vec{\alpha}^{\mathsf{T}}$$

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For $k = 1$, this is same as finding unit vector $\vec{\alpha}$ that maximizes

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Maximum variance linear function of a random vector

Question: What is the maximum variance achievable by a linear function of $\vec{X}$ given as a *unit vector*?

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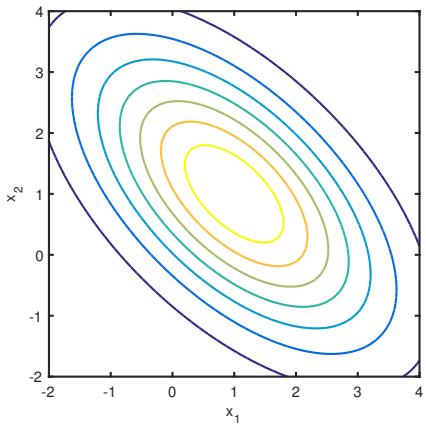
  Achieved by (unit length) eigenvector corresponding to that eigenvalue
  (a.k.a. **top eigenvector**)

Top eigenvector for covariance of a multivariate Gaussian



Top eigenvector direction defines the major axis of each ellipse

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- This is a "weighted" average of the λ_i's; maximized when all "weight" is put on λ_1
- To put all "weight" on λ_1, need $(\vec{\alpha} \cdot \vec{v}_1)^2 = 1$; achieved by $\vec{\alpha} = \pm \vec{v}_1$

Top eigen{value,vector} on MNIST data

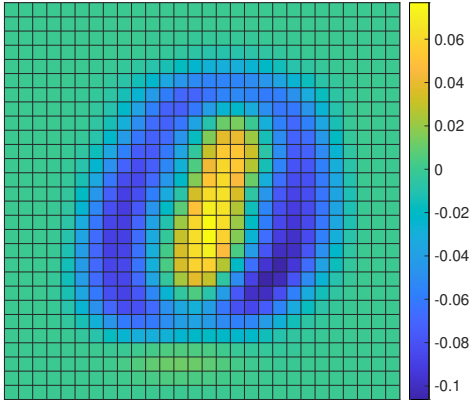
Top eigenvalue:

$$\lambda_1 \approx 0.1 \times \mathbb{E}\|\vec{X} - \vec{\mu}\|_2^2$$

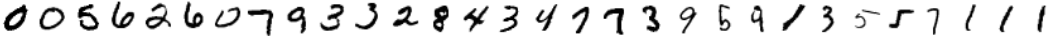
Expected reconstruction error:

$$\approx 0.9 \times \mathbb{E}\|\vec{X} - \vec{\mu}\|_2^2$$

Top eigenvector:



Some MNIST digits sorted by projection to span of top eigenvector:



General case: $k \geq 1$

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This is same as finding orthonormal $\vec{\alpha}_1, \ldots, \vec{\alpha}_k$ that maximizes

$$\mathbb{E}\left[\left\|\sum_{i=1}^{k} \vec{\alpha}_i \vec{\alpha}_i^{\mathsf{T}}(\vec{X} - \vec{\mu})\right\|_2^2\right] = \mathbb{E}\left[\sum_{i=1}^{k} (\vec{\alpha}_i^{\mathsf{T}}(\vec{X} - \vec{\mu}))^2\right] = \sum_{i=1}^{k} \mathrm{var}(\vec{\alpha}_i \cdot \vec{X})$$

Optimality of the top k eigenvectors

Question: What's the maximum variance "accounted for" by k dimensional subspace?

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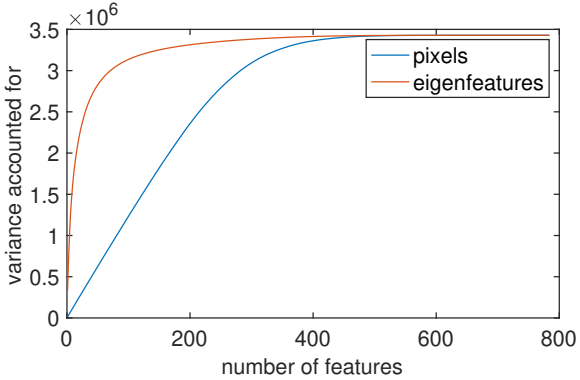
Vectors $\vec{v}_1, \ldots, \vec{v}_k$ are called the **top k principal components** of (the distribution of) $\vec{X}$
Computing these "eigenfeatures" is called **(k-dim.) Principal Components Analysis (PCA)**

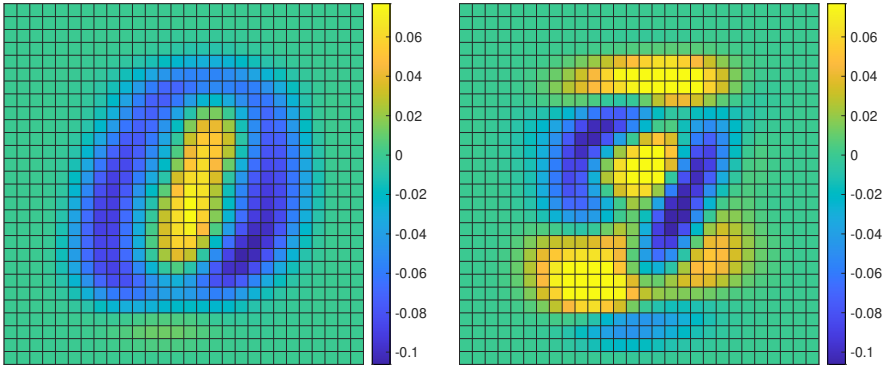
Variance accounted for on MNIST data

MNIST data: Need $k = 87$ "eigenfeatures" to reduce expected reconstruction error to $0.1 \times \mathbb{E}\|\vec{X} - \vec{\mu}\|_2^2$



("Variance accounted for" $= \sum_{i=1}^{k} \mathrm{var}(\vec{\alpha}_i \cdot \vec{X})$)

MNIST eigenvectors



$\vec{v}_1$ $\vec{v}_2$

Orthogonality: $\vec{v}_1 \cdot \vec{v}_2 = 0$

New features from PCA

Properties of eigenfeatures $\vec{v}_i \cdot \vec{X}$ for $i = 1, \ldots, k$:

- $\mathrm{var}(\vec{v}_i \cdot \vec{X}) = \lambda_i$ for all i
- $\mathrm{cov}(\vec{v}_i \cdot \vec{X}, \vec{v}_j \cdot \vec{X}) = 0$ for $i \neq j$

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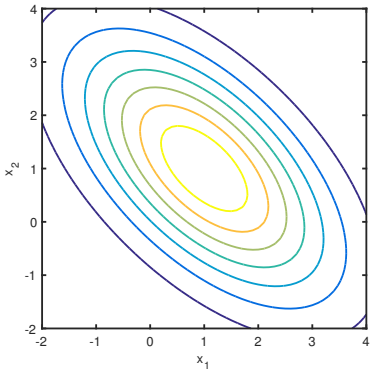
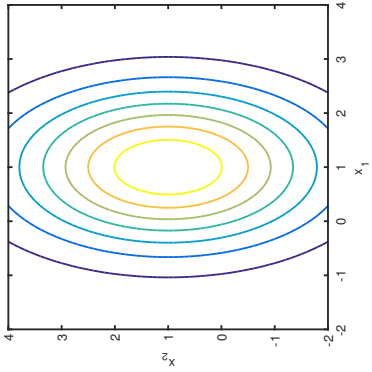


Original features



Eigenfeatures

PCA and beyond

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- Major use of PCA: **Dimension reduction**
  Map data points in $\mathbb{R}^d$ to $\mathbb{R}^k$ for $k < d$
  (When $k = 2$ or $k = 3$, useful for visualization, maybe!)

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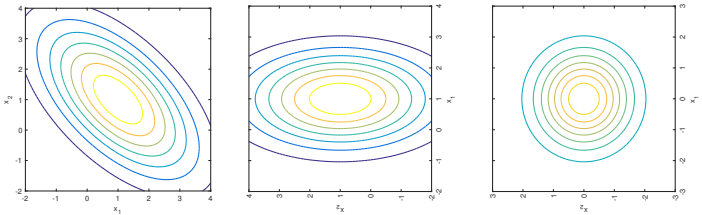
- **Whitening**: Transforming to isotropy

$$\frac{1}{\sqrt{\lambda_i}} \vec{v}_i \cdot \vec{X} \quad \text{for } i = 1, \ldots, k$$



Original features | Eigenfeatures | Whitened features

Postscript: "Un-centered" PCA

Everything about eigen{values,vectors} of $\mathrm{cov}(\vec{X})$ also applies to **second-moment matrix** $\mathbb{E}[\vec{X}\vec{X}^{\mathsf{T}}]$, ... with following changes:

- Replace $\mathrm{var}(\vec{\alpha} \cdot \vec{X})$ with $\mathbb{E}[(\vec{\alpha} \cdot \vec{X})^2]$
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Eigenvector computation

Simple approach to top eigenvector computation

Let eigendecomposition of $A^\mathsf{T}A$ be $\sum_{i=1}^{d} \lambda_i \, \vec{v}_i \, \vec{v}_i^\mathsf{T}$

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If t is large, and $\lambda_1 > \lambda_2$, then

$$(A^\top A)^t \;=\; \lambda_1^t \left(\vec{v}_1 \, \vec{v}_1^\top + \sum_{i=2}^{d} \left(\frac{\lambda_i}{\lambda_1} \right)^t \vec{v}_i \, \vec{v}_i^\top \right) \;\approx\; \lambda_1^t \, \vec{v}_1 \, \vec{v}_1^\top$$

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Main idea:
If t is sufficiently large, multiplying $(A^\mathsf{T}A)^t$ by (almost) any vector yields a vector that is (approximately) in span of $\vec{v}_1$

Power iteration

Slow implementation of main idea: First compute $(A^\top A)^t$, and then multiply by a vector

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Power iteration (a.k.a. power method)

- Initialize $\vec{x}^{(0)} \in \mathbb{R}^d$ randomly (e.g., draw from $\mathrm{N}(\vec{0}, I_d)$)
- For $t = 1, 2, \ldots$ until stopping condition is satisfied:

$$\begin{aligned} \vec{y} &:= A\vec{x}^{(t-1)} \\ \vec{z} &:= A^\top \vec{y} \\ \vec{x}^{(t)} &:= \vec{z}/\|\vec{z}\|_2 \end{aligned}$$

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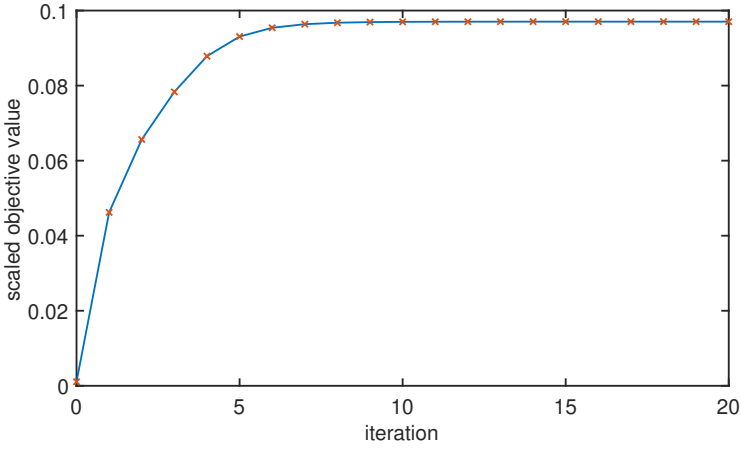
After t iterations, this computes a scaling of $(A^\mathsf{T}A)^t\vec{x}^{(0)}$
(Scaling is due to normalization steps "$\vec{x}^{(t)} := \vec{z}/\|\vec{z}\|_2$")

Example: Power iteration on centered MNIST data

Scaled objective: $J(\vec{x}) = \dfrac{1}{\mathrm{tr}(A^\mathsf{T}A)} \cdot \dfrac{\vec{x}^\mathsf{T}(A^\mathsf{T}A)\vec{x}}{\|\vec{x}\|_2^2}$



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  Can use **deflation**
  If you only care about subspace spanned by $\vec{v}_1, \ldots, \vec{v}_k$: use **subspace iteration**

Low-rank Approximation

Low-rank matrix approximation

Given data matrix $A = [\vec{x}_1 | \cdots | \vec{x}_n]^\mathsf{T} \in \mathbb{R}^{n \times d}$, how can we best approximate it by the product BC for some $B \in \mathbb{R}^{n \times k}$ and $C \in \mathbb{R}^{k \times d}$?

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$$J(B, C) = \|A - BC\|_\mathrm{F}^2$$

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- If B is fixed, then this looks like the SSE objective from OLS!
- Same if C is fixed.
- But apparently more complicated, since both B and C are optimization variables! (E.g., J is not a convex function of (B, C))

Two optimization methods

Gradient descent:

- Start with initial values $B^{(0)} \in \mathbb{R}^{n \times k}$ and $C^{(0)} \in \mathbb{R}^{k \times d}$
- For iteration $t = 1, 2, \ldots$ until stopping condition is satisfied:

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Alternating minimization:

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$$A = \sum_{i=1}^{r} s_i \, \vec{u}_i \, \vec{v}_i^{\mathsf{T}}$$

for some $\{(s_i, \vec{u}_i, \vec{v}_i)\}_{i=1}^{r}$, which satisfy

- $s_1 \geq \cdots \geq s_r > 0$ (**singular values** of A; sorting this way is by convention)
- $\vec{u}_1, \ldots, \vec{u}_r \in \mathbb{R}^n$ are orthonormal (**left singular vectors** of A)
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Can also write as

$$A = USV^{\mathsf{T}}$$

where $U := [\vec{u}_1 | \cdots | \vec{u}_r] \in \mathbb{R}^{n \times r}$, $S := \operatorname{diag}(s_1, \ldots, s_r) \in \mathbb{R}^{r \times r}$, and $V := [\vec{v}_1 | \cdots | \vec{v}_r] \in \mathbb{R}^{d \times r}$

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$$A_k := \sum_{i=1}^{k} s_i \, \vec{u}_i \, \vec{v}_i^{\mathsf{T}},$$

satisfies

$$\|A - A_k\|_{\mathrm{F}}^2 \;=\; \min_{\substack{M \in \mathbb{R}^{n \times d} \\ \text{s.t. } \operatorname{rank}(M) \leq k}} \|A - M\|_{\mathrm{F}}^2 \;=\; \sum_{i=k+1}^{\operatorname{rank}(A)} s_i^2$$

Truncated SVD

Suppose SVD of A is given by

$$A = \sum_{i=1}^{\operatorname{rank}(A)} s_i \, \vec{u}_i \, \vec{v}_i^{\mathsf{T}}$$

Theorem (Schmidt, 1907; Eckart & Young, 1936)**.** The **rank-k SVD** of A (for $k \leq \operatorname{rank}(A)$),

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Can also write $A_k = U_k S_k V_k^{\mathsf{T}}$ where $U_k := [\vec{u}_1 | \cdots | \vec{u}_k] \in \mathbb{R}^{n \times k}$, $S_k := \operatorname{diag}(s_1, \ldots, s_k) \in \mathbb{R}^{k \times k}$, and $V_k := [\vec{v}_1 | \cdots | \vec{v}_k] \in \mathbb{R}^{d \times k}$

Connection to PCA

Observation:

$$A^\mathsf{T}A \;=\; (VSU^\mathsf{T})(USV^\mathsf{T}) \;=\; VS^2V^\mathsf{T} \;=\; \sum_{i=1}^{r} s_i^2\,\vec{v}_i\,\vec{v}_i^\mathsf{T}$$

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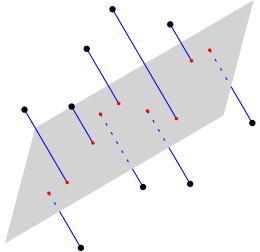
Computing rank-k SVD is same as applying (un-centered) dim. k PCA feature mapping!



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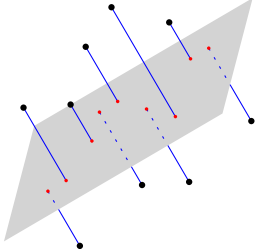
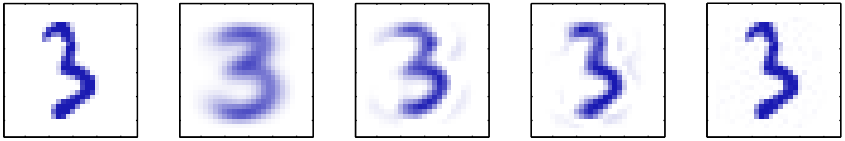


Rows of $U_k S_k$ are the k-dimensional vectors of "eigenfeatures"

MNIST data example

MNIST data example: Compare original image to corresponding row of A_k ($k \in \{1, 10, 50, 200\}$)



Application: Latent Semantic Analysis

Document modeling

Suppose you have corpus of n text documents

- Each document represented using "bag-of-words" count vectors
- $d =$ vocabulary size

$$A := \begin{array}{c|cccc} & \text{aardvark} & \text{abacus} & \text{abalone} & \cdots \\ \hline \text{doc 1} & 3 & 0 & 0 & \cdots \\ \text{doc 2} & 7 & 0 & 4 & \cdots \\ \text{doc 3} & 0 & 4 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{array}$$

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- However, documents about mathematics are likely to contain word that often co-occur with "mathematics" or other math-y words (e.g., "theorem", "proof", "generality")

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(Deerwester, Dumais, Furnas, Landauer, Harshman, 1990)

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- Search queries: Construct "pseudo-document" — i.e., bag-of-words with non-zero counts for query terms — then find documents in corpus of high cosine similarity

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- Hence $A = BC +$ "noise"; hope that A_k avoids the noise

Caveats

- Might hope that splitting apart $A_k = U_k S_k V_k^\mathsf{T}$ as $U_k S_k$ and V_k^T will somehow give something like B and C from the topic model

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  - But these hopes are unlikely to be fulfilled ☹
- Other approaches to finding low-rank approximations with "interpretable" factors:
  - Non-negative Matrix Factorization (Lee & Seung, 1999)
  - Latent Dirichlet Allocation (Pritchard, Stephens, & Donnelly, 2000; Blei, Ng, & Jordan, 2003)
  - etc.

Application: Matrix Completion

Netflix problem

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Common solution (used by Simon Funk in Netflix challenge): Just define objective over entries in Ω

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- Now (attempt to) minimize J_Ω using gradient descent or stochastic gradient descent

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Some close pairs of movie feature vectors $(\vec{c}_i, \vec{c}_j)$:

- Toy Story (1995), Toy Story 2 (1999)
- Sense and Sensibility (1995), Emma (1996)
- Heat (1995), Carlito's Way (1993)
- The Crow (1994), Blade (1998)
- Forrest Gump (1994), Dances with Wolves (1990)
- Mrs. Doubtfire (1993), The Bodyguard (1992)

Summary

- Many applications of low-rank approximations
- Often PCA/SVD is a good approach!
- Sometimes need to go beyond PCA/SVD