# Singular Value Decomposition (SVD) 

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## Acknowledgments

- Some examples adapted from Christos Faloutsos' class material (CMU) and also from the following work:
- Quantifiable Data Mining Using Ratio Rules.
F. Korn, A. Labrinidis, Y. Kotidis, C. Faloutsos. The VLDB Journal, Volume 8(3+4), February 2000.
(available at http://pages.aueb.gr/users/kotidis/Publications/index.html)


## Applications

- Find similar "concepts" in large datasets
- Basket analysis
- Explore customer-product relationships
- Find similar customers, products
- Document indexing \& retrieval
- Dimensionality reduction/feature selection
- Reduce data size by projecting items into a lowerdimensionality concept-space
- Remove noise, detect outliers, visualization
- Web-link analysis
- Compute "importance" of web-pages


## Basket Data Analysis



## Singular Value Decomposition (SVD)

- Factorization of matrix A into three matrices

$$
\mathrm{A}=\mathrm{U} \wedge \mathrm{~V}^{\top}
$$

- Such that:
- A: n x m matrix (e.g. n customers, m products)
- U: $\mathrm{n} \times \mathrm{r}$ matrix (customers to concepts)
$-\Lambda: r \times r$ diagonal matrix
-V : $\mathrm{m} \times \mathrm{r}$ matrix (products to concepts)
- $\mathrm{U}($ resp. V ) is a column-orthonormal matrix
- Its columns are mutually orthogonal unit vectors


## 乞та $\mathrm{E} \lambda \lambda \eta \nu \iota \kappa \alpha \alpha^{. . .}$



- Concepts:'Evvotءs

- Eigen value: Iסıotıนń


## SVD Example



## Different Column Ratios

1:2:3 $\Longleftrightarrow 0.27: 0.53: 0.80$


## Mixed preferences (rounding near-zero values)

## What are the concepts now?

## Geometric Interpretation

- Recall V: products to concepts matrix

$$
\mathbf{V}^{\top}=\left(\begin{array}{lllll}
0.58 & 0.58 & 0.58 & 0 & 0 \\
0 & 0 & 0 & 0.71 & 0.71
\end{array}\right) \text { concepts }
$$

products
( $\mathrm{U} \wedge=\mathrm{AV}$ ) gives the coordinates of the projection

Second-best direction to project customers (meat-eaters concept)
"best" direction to project customers (vegetarians concept)

Each point is a customer depicted in the products space
\#dims = \#products !

## SVD using R

```
a=matrix
c(1,1,1,0,0,
        2,2,2,0,0,
        1,1,1,0,0,
        5,5,5,0,0,
        0,0,0,2,2,
        0,0,0,3,3,
        0,0,0,1,1),
    nrow=7,ncol=5, byrow = TRUE)
    svd(a)
$d
[1] 9.643651e+00 5.291503e+00 7.529899e-16 0.000000e+00 0.000000e+00
$u
\begin{tabular}{l|rr|}
{\([1]\),} & -0.1796053 & 0.0000000 \\
{\([2]\),} & -0.3592106 & 0.0000000 \\
{\([3]\),} & -0.1796053 & 0.0000000 \\
{\([4]\),} & -0.8980265 & 0.0000000 \\
{\([5]\),} & 0.0000000 & -0.5345225 \\
{\([6]\),} & 0.0000000 & -0.8017837 \\
{\([7]\),} & 0.0000000 & -0.2672612
\end{tabular}
\$v
```

| $[1]$, | -0.5773503 | 0.0000000 |
| ---: | ---: | ---: |
| $[2]$, | -0.5773503 | 0.0000000 |
| $[3]$, | -0.5773503 | 0.0000000 |
| $[4]$, | 0.0000000 | -0.7071068 |
| $[5]$, | 0.0000000 | -0.7071068 |

「,1] [,2]
$[1$,
$[2$,
$[3$,
$[4] \quad 0.0000000-$,
$[5] \quad 0.0000000-$,
$[, 3]$
0.97298719 0.05552004 0.02776002 0.22235746 0.00000000 $0.00000000-0.42857143$ $0.00000000-0.14285714$
[, 3]
0.8164966
0.4082483
0.4082483
0.0000000
0.0000000
[,4]
0.0000000
0.0000000
0.0000000
-0.7071068
0.7071068
[,5]
0.0000000
-0.7071068
0.7071068
0.0000000
0.0000000

## SVD in Python



## Applications of SVD

- John : "I like tomatoes"
- Think of John as a customer (row) vector
- $\overrightarrow{\mathrm{C}}_{\text {John }}=\left[\begin{array}{llll}0 & 0 & 3 & 0\end{array} 0\right.$ O
- Mary : "I like lettuce and asparagus"
- $\overrightarrow{\mathrm{c}}_{\text {Mary }}=\left[\begin{array}{lllll}2 & 2 & 0 & 0 & 0\end{array}\right]$
- Vectors don't look similar (inner-product = zero)
$-\operatorname{sim}\left(\vec{c}_{\text {John }}, \vec{c}_{\text {Mary }}\right)=0 * 2+0 * 2+3 * 0+0 * 0+0 * 0=0$ (equivalently their cosine similarity $=0$ )


## Map to the concepts space

Also... this is an example of dim-reduction (from 5-dims $\rightarrow$ 2-dims)
$\left(\begin{array}{lllll}0 & 0 & 0 & 0\end{array}\right) \times\left(\begin{array}{ll}0.58 & 0 \\ 0.58 & 0 \\ 0.58 & 0 \\ 0 & 0.71 \\ 0 & 0.71\end{array}\right)=\left(\begin{array}{ll}1.74 & 0\end{array}\right)$

Products that John/Mary buy (or prefer)

products-to-concepts $V$

Now John \& Marry look similar (cos=1) even though their baskets don't contain common products

## Building Recommendations

- John : "I like tomatoes"
- Think of John as a customer (row) vector
- $\overrightarrow{\mathrm{c}}_{\text {John }}=\left[\begin{array}{llll}0 & 0 & 3 & 0\end{array}\right]$
- Which additional products could John find appealing?


## Map to the concepts space (a), and back (b)




## Map to the concepts' space



## Rank of Matrix



## Dimensionality Reduction



## Truncated SVD

- Concentrate on the most important parts using a rank-k approximation of the matrix
- How to select the value of k ?


## Example (Image Compression)



## Another example*



[^0]
## How do we achieve compression?

- Original image: $\mathrm{n} \times \mathrm{m}$ values
- By selecting the first $k$ singular values we store
- $k$ singular values
- First $k$ columns of matrix $U\left(n^{*} k\right.$ values)
- First $k$ rows of matrix $V^{\top}\left(m^{*} k\right.$ values)
- Thus, we need a total of $k^{*}(1+n+m)$ values
- Compare with $\mathrm{n} \times \mathrm{m}$


## Scree plot

- Plot the value of successive singular values (or their squared values) against the rank order
- Decision is subjective



## Use truncated SVD for removing noise



[^1]
## More on denoising

| (11100) |  | 11100 |
| :---: | :---: | :---: |
| 22200 |  | 22200 |
| 11100 |  | 11100 |
| 55500 | K=2 | 55500 |
| 00022 |  | 00022 |
| 00033 |  | 0002.93 .1 |
| 00001 |  | 0000.50 .5 |

$$
\mathrm{V}^{\top}=\left(\begin{array}{lllll}
0.58 & 0.58 & 0.58 & 0 & 0 \\
0 & 0 & 0 & 0.69 & 0.72 \\
0 & 0 & 0 & -0.72 & 0.69
\end{array}\right) \quad \Lambda=\left(\begin{array}{lll}
9.64 & 0 & 0 \\
0 & 5.15 & 0 \\
0 & 0 & 0.70
\end{array}\right)
$$

## Frobenious norm (a.k.a. Euclidean Norm) <br> $\|\boldsymbol{A}\|_{F} \equiv \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n}\left|a_{i j}\right|^{2}}$

original matrix


$\sigma_{1}{ }^{2}+\sigma_{2}{ }^{2}=121$
$\|A\|_{F}^{2}=3 * 1^{2}+3 * 2^{2}+3 * 1^{2}+3 * 5^{2}+2 * 2^{2}+2 * 3^{2}+2 * 1^{2}=121$

## $\|A\|_{F}$ v.s. singular values

original matrix

products

$$
3 * 1^{2}+3 * 2^{2}+3 * 1^{2}+3 * 5^{2}+2 * 2^{2}+2 * 3^{2}+2 * 1^{2}=121
$$

$$
\sigma_{1}^{2}+\sigma_{2}^{2}=121
$$

1-rank approximation

$3 * 1^{2}+3 * 2^{2}+3 * 1^{2}+3 * 5^{2}=93$

$$
\sigma_{1}^{2}=93
$$

## Select k based on $\|A\|_{F}^{2}$

- Recall $\|A\|_{F}^{2}=\Sigma\left(\sigma_{\mathrm{i}}{ }^{2}\right)$
- List singular values in decreasing order:

$$
\sigma_{1}, \sigma_{2}, \sigma_{3} \ldots
$$

- Select $k$ singular values such that the sum of their squares is (for example) $\geq 80 \%$ of the total sum of the squared singular values
- Ensures that 80\% of the squared Frobenious norm is preserved

$$
\Lambda=\left(\begin{array}{cc}
9.64 & 0 \\
0 & 5.29
\end{array}\right] \begin{aligned}
& \sigma_{1}{ }^{2}+\sigma_{2}{ }^{2}=121 \\
& \sigma_{1}{ }^{2}=93
\end{aligned} \longleftrightarrow \begin{aligned}
& 1^{\text {st }}=\text {-rank approximation preserves } \\
& 93 / 121=77 \% \text { of the energy }
\end{aligned}
$$

## Consideration

- Results depend on magnitude of data values
- E.g.: first column is customer age (18..65)
second column is income (5000..100000)
- Then, income seems more important than age
- For some datasets this may be true, but not for all


## Suggestion

- First do mean normalization (center to zero) by subtracting the mean value per column
- Optionally do feature scaling
- e.g. divide by standard deviation (normalize magnitude) per column
- other approach is to reduce features with large magnitude (e.g. take square roots/logarithms)


## Mean Normalization




## Feature Scaling

(e.g. standardization in this example)


## Another interpretation: Ratio Rules

$$
\begin{gathered}
V^{\top}=\left[\begin{array}{lllll}
0.58 & 0.58 & 0.58 & 0 & 0 \\
0 & 0 & 0 & 0.71 & 0.71
\end{array}\right] \text { concepts } \\
\text { products }
\end{gathered}
$$

- RR1: "A (vegetarian)customer spends
0.58:0.58:0.58 € on asparagus:lettuce:tomatoes"
- Ratio Rules Construction
- Obtain matrix A
- Compute $\mathrm{A}_{\mathrm{c}}$ (zero mean) from A by subtracting column averages
- Compute $\mathrm{C}=\mathrm{A}_{c}{ }^{\top} \mathrm{A}$ product-to-product similarity matrix
- Ratio Rules in $V$ are the eigenvectors of $C$


## What-if-Analysis

- Simple case: exactlyspecified
- Example
- RR1: bread:butter
- A customer spends 5\$ on bread
- How much is she
 expected to spend on butter?


## Harder cases*


*See: "Quantifiable Data Mining Using Ratio Rules"

## Other use: detect outlier values

- Inspect Customer x:
$-(5,2,3,0,51) \longrightarrow$ Looks suspicious
- Remove suspected value(s), replace with unknown (5,2,3,0,?)
- Run previous algorithm, reconstruct missing value from RRs
- (5,2,3,0,48)
- Compare against guessed value


## Sample of V matrix for NBA 1991-2 season stats

| field | $R R_{1}$ | $R R_{2}$ | $R R_{3}$ |
| :---: | :---: | :---: | :---: |
| minutes played <br> field goals <br> goal attempts <br> free throws <br> throws attempted <br> blocked shots <br> fouls | .808 | -.4 |  |
| points <br> offensive rebounds <br> total rebounds <br> assists <br> steals | .406 | .199 |  |

RR1: level of activity (stars vs bench players)
RR2: field position (offensive/defensive players)
defensive players are good rebounders but score less points per minutes played than offensive players RR3: height of a players (tall guys get more rebounds but have less steals/assists

## Visualization



## Latent Semantic Indexing (Information Retrieval)

- Assume $A$ is a (terms) $x$ (documents) matrix
- Values denote the term frequencies (or e.g. tf*idf scores)

|  | d1 | d2 | d3 | $\ldots$ |
| :---: | :---: | :---: | :---: | :---: |
| Term1 | 4 | 0 | 2 | $\ldots$ |
| Term2 | 0 | 2 | 0 | $\ldots$ |
| Term3 | 3 | 2 | 0 | $\ldots$ |
| Term4 | 2 | 0 | 1 | $\ldots$ |
| Term5 | 11 | 7 | 0 | $\ldots$ |
| $\ldots$ | 0 | 0 | 0 | $\ldots$ |
| $\ldots$ | 0 | 0 | 1 | $\ldots$ |

## How to define similarity between docs?

|  |  | $\bigcirc$ | $\bigcirc$ |  |
| :---: | :---: | :---: | :---: | :---: |
|  | d1 | d2 | d3 | ... |
| Term1 | 4 | 0 | 2 | ... |
| Term2 | 0 | 2 | 0 | ... |
| Term3 | 3 | 2 | 0 | ... |
| Term4 | 2 | 0 | 1 | ... |
| Term5 | 11 | 7 | 0 | ... |
| ... | 0 | 0 | 0 | ... |
| ... | 0 | 0 | 1 | ... |

## Issue 1: Synonymy

- Different words with the same meaning


|  | d1 | d2 | d3 | $\ldots$ |
| :---: | :---: | :---: | :---: | :---: |
| Car | 4 | 0 | 2 | $\ldots$ |
| Term2 | 0 | 2 | 0 | $\ldots$ |
| Automobile | 3 | 2 | 0 | $\ldots$ |
| Term4 | 2 | 0 | 1 | $\ldots$ |
| Term5 | 11 | 7 | 0 | $\ldots$ |
| $\ldots$ | 0 | 0 | 0 | $\ldots$ |
| $\ldots$ | 0 | 0 | 1 | $\ldots$ |

## Issue 2: Polysemy

- The same word having other meanings

|  | d 1 | d 2 | d 3 | $\ldots$ |
| :---: | :---: | :---: | :---: | :---: |
| Term1 | 4 | 0 | 2 | $\ldots$ |
| Term2 | 0 | 2 | 0 | $\ldots$ |
| Term3 | 3 | 2 | 0 | $\ldots$ |
| Term4 | 2 | 0 | 1 | $\ldots$ |
| Apple | 11 | 7 | 0 | $\ldots$ |
| $\ldots$ | 0 | 0 | 0 | $\ldots$ |
| $\ldots$ | 0 | 0 | 1 | $\ldots$ |
|  |  |  |  |  |

mentioned as a fruit
mentioned as a technology company

## Latent Semantic Indexing

- SVD (LSI) discovers the "topics" (=concepts) discussed
- Handle synonymy: e.g. car, automobile, autoкivnto, $\alpha \mu \alpha ́ \xi ı ~ a l l ~ r e f e r ~ t o ~ t h e ~ s a m e ~ t o p i c ~$
- Handle polysemy: if apple is mentioned along with other fruits in a document it will be mapped to the apple-the-fruit concept (crude analogy)


## SVD vs PCA

- SVD: $A=U \wedge V^{\top}$
- PCA : $A=X L X^{\top}$
- A is symmetric
$-\mathrm{U}, \mathrm{V}, \mathrm{X}$ are orthonormal $\rightarrow \mathrm{X}^{\top} \mathrm{X}=\mathrm{I}, \mathrm{V}^{\top} \mathrm{V}=\mathrm{I}, \mathrm{U}^{\top} \mathrm{U}=\mathrm{I}$
- Given a non-symmetric matrix $A$
$-A^{\top} \mathrm{A}$ is symmetric (thus PCA applies)
$-A^{\top} A=V \Lambda^{\top} U^{\top}\left(U \wedge V^{\top}\right)=V \Lambda^{2} V^{\top}=X L X^{\top}$
- for $\mathrm{X}=\mathrm{V}, \mathrm{L}=\Lambda^{2}$
- also, $I_{i}=\lambda_{1}^{2}$
eigen-values
singular-values


## Quick Note: table multiplication

- Let $\mathrm{M}_{\mathrm{nxm}}=X_{\mathrm{nx\mid}} * \mathrm{Y}_{\mathrm{Ixm}}$
- Then:

$$
\begin{aligned}
& \mathrm{M}_{\mathrm{ij}}=\sum_{k=1}^{l}\left(\mathrm{X}_{\mathrm{ik}} * \mathrm{Y}_{\mathrm{kj}}\right) \\
= & \overrightarrow{\mathrm{x}}_{\mathrm{i}} \cdot \overrightarrow{\mathrm{y}}_{\mathrm{j}}
\end{aligned}
$$



## Dot products

- $\vec{x} \cdot \vec{y}=\Sigma\left(x_{k}^{*} y_{k}\right)$
- Example:

$$
\begin{aligned}
& \vec{x}=(1,3,0,5) \\
& \vec{y}=(1,0,1,6)
\end{aligned}
$$

- Then:

$$
\begin{aligned}
\vec{x} \cdot \vec{y} & =1^{*} 1+3^{*} 0+0^{*} 1+5^{*} 6=31 \\
& =|\vec{x}|^{*}|\vec{y}|^{*} \cos (\theta(\vec{x}, \vec{y}))
\end{aligned}
$$

## More interesting properties of SVD

- Recall $A_{n \times m}$ :
customers to products matrix
- SVD: $A=U \wedge V^{\top}$
- Then $\mathrm{A}^{\top} \mathrm{A}=\mathrm{V} \wedge^{2} \mathrm{~V}^{\top}$ (product-to-product similarity matrix)
- Similarity based on their customers



## Exploring User's similarities

- Let $\mathrm{v}^{\prime}$ be a mx 1 vector denoting the preferences of customer "John"
- What is $A v^{\prime}$ ?

$A v^{\prime}$ denotes similarities of customers to John


## Exploring User's similarities

- $A v^{\prime}$ denotes similarities of customers to John
- What is $\mathrm{A}^{\top}\left(A v^{\prime}\right)$ ?
- Products that customers similar to John buy
- a high value indicates that the customers for this product are similar to the customers that are similar to John


In "facebook terms" what friends of John like (assuming "friend of John" means similar to John)

## Take it further

- $\left(A^{\top} A\right) v^{\prime}=$ what the friends of John like
- Via similar arguments:
- $\left(A^{\top} A\right)^{2} v^{\prime}=$ what the friends of the friends of John like
- $\left(A^{\top} A\right)^{k} v^{\prime}=$ what $k$-hops away friends like


## Visually



WHAT IS THIS?

## Interesting property

- Computation converges to a vector parallel to $\mathrm{v}_{1}$
$-\left(A^{\top} A\right)^{k}=V \wedge^{2 k} V^{\top}=^{\sim} v_{1} \lambda_{1}{ }^{2 k} v_{1}^{\top}$ for $k \gg 1$
- Recall that $v_{1}$ is also the $1^{\text {st }}$ eigenvector of $A^{\top} A$
- By definition $\left(A^{\top} A\right) v_{1}=\lambda_{1}{ }^{2} v_{1}$
- Therefore: $\left(A^{\top} A\right)^{k} v^{\prime}=\sim$ constant $* v_{1}$
- After k steps it doesn't matter where we started from. Will converge to the first (strongest) eigenvector
- property used for computing pageRank ( A is derived from the adjacency matrix of the web)


## Example

Dataset A (Customer x Products)

| 1 | 1 | 1 | 0 | 0 | 0 | 3 | Customer 1 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2 | 2 | 2 | 0 | 0 | 0 | 6 | Customer 2 |
| 1 | 1 | 1 | 0 | 0 | 3 | 3 | Customer 3 |
| 5 | 5 | 5 | 0 | 0 | 0 | 15 | Customer 4 |
| 0 | 0 | 0 | 2 | 2 | 0 | 0 | Customer 5 |
| 0 | 0 | 0 | 3 | 3 |  | 0 | Customer 6 |
| 0 | 0 | 0 | 1 | 1 |  | 0 | Customer 7 |

Customers-to-John similarity vector

## Conclusion: first four customers are similar to John

Dataset A (Customer x Products)

| $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{1}$ | $\mathbf{0}$ | $\mathbf{0}$ |
| :--- | :--- | :--- | :--- | :--- |
| $\mathbf{2}$ | $\mathbf{2}$ | $\mathbf{2}$ | $\mathbf{0}$ | $\mathbf{0}$ |
| $\mathbf{1}$ | $\mathbf{1}$ | 1 | $\mathbf{0}$ | $\mathbf{0}$ |
| $\mathbf{5}$ | $\mathbf{5}$ | $\mathbf{5}$ | $\mathbf{0}$ | $\mathbf{0}$ |
| 0 | 0 | 0 | 2 | 2 |
| 0 | 0 | 0 | 3 | 3 |
| 0 | 0 | 0 | 1 | 1 |



Customers-to-John similarity vector

## Moreover, customers that are like John buy vegetables



## Complication

$A^{\top}$ A (Product x Product)

|  | a | 1 | t | b | p |
| :---: | :---: | :---: | :---: | :---: | :---: |
| a | 31 | 31 | 31 | 0 | 0 |
| I | 31 | 31 | 31 | 0 | - |
| t | 31 | 31 | 31 | 0,' | 0 |
| b | 0 | 0 | 0 | 14 | 14 |
| $p$ | 0 | 0 | 6 | 14 | 14 |



## PageRank* (informal)

Page $x$ is important if many important pages link to it


Page $y$ has more incoming links but lower PageRank than page $x$

## PageRank

## (less informal but not complete)

- Let matrix W denote the web graph

From:

To: |  |  | $1 / 3$ | 1 |
| :--- | :--- | :--- | :--- |
|  | $1 / 2$ |  |  |
| $1 / 2$ |  | $1 / 3$ |  |
|  | 1 | $1 / 3$ |  |

$$
\mathrm{p}_{1}=1 / 3 \mathrm{p}_{3}+\mathrm{p}_{4}
$$

- Look for vector $p$ such that W.p = 1.p

|  |  | $1 / 3$ | 1 |
| :--- | :--- | :--- | :--- |
| $1 / 2$ |  |  |  |
| $1 / 2$ |  | $1 / 3$ |  |
|  | 1 | $1 / 3$ |  |$\cdot$| $p_{1}$ |
| :--- |
| $p_{2}$ |
| $p_{3}$ |
| $p_{4}$ |$=$| $p_{1}$ |
| :--- |
| $p_{2}$ |
| $p_{3}$ |
| $p_{4}$ |

## Complications

- Some (even important) pages may have no outgoing links
- PageRank leaks out from these nodes instead of being re-distributed back to the net
- Existence of cycles

- spider traps/closed communities
- PageRank get’s "trapped"



## Summary

- SVD: algebraic tool that has many potential uses
- Dimensionality reduction
- Indexing (LSI)
- Visualization/clustering of high-dimensional objects
- Similarity computations/outlier detection
- Rule mining, treatment of missing/wrong values


[^0]:    * credit: https://towardsdatascience.com/understanding-singular-value-decomposition-and-its-application-in-data-science-388a54be95d

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