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Dimensionality Reduction: SVD & CUR

CS246: Mining Massive Datasets
Jure Leskovec, Stanford University
Charilaos Kanatsoulis, Stanford University
http://cs246.stanford.edu
Often, our data can be represented by an $m$-by-$n$ matrix

And this matrix can be closely approximated by the product of three matrices that share a small common dimension $r$
## Dimensionality Reduction

- **Compress / reduce dimensionality:**
  - $10^6$ rows; $10^3$ columns; no updates
  - Random access to any cell(s); **small error: OK**

<table>
<thead>
<tr>
<th>customer</th>
<th>day</th>
<th>7/10/96</th>
<th>7/11/96</th>
<th>7/12/96</th>
<th>7/13/96</th>
<th>7/14/96</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABC Inc.</td>
<td>We</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DEF Ltd.</td>
<td>Th</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>GHI Inc.</td>
<td>Fr</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>KLM Co.</td>
<td>Sa</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Smith</td>
<td>Su</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Johnson</td>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Thompson</td>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

**New representation**
- $[1 \ 0]$
- $[2 \ 0]$
- $[1 \ 0]$
- $[5 \ 0]$
- $[0 \ 2]$
- $[0 \ 3]$
- $[0 \ 1]$

**Note:** The above matrix is really “2-dimensional.” All rows can be reconstructed by scaling $[1 \ 1 \ 1 \ 0 \ 0]$ or $[0 \ 0 \ 0 \ 1 \ 1]$
There are hidden, or **latent factors, latent dimensions** that – to a close approximation – explain why the values are as they appear in the data matrix.
The axes of these dimensions can be chosen by:

- The first dimension is the direction in which the points exhibit the greatest variance.
- The second dimension is the direction, orthogonal to the first, in which points show the 2nd greatest variance.
- And so on..., until you have enough dimensions that variance is really low.
Q: What is rank of a matrix A?  
A: Number of linearly independent rows of A  

Cloud of points in 3D space:  
- Think of point coordinates as a matrix:  
  \[
  \begin{bmatrix}
  1 & 2 & 1 \\
  -2 & -3 & 1 \\
  3 & 5 & 0
  \end{bmatrix}
  \]
  
  1 row per point:  
  A: \[1 0\], B: \[0 1\], C: \[1 -1\]  

We can rewrite coordinates more efficiently!  
- Old basis vectors: \([1 0 0]\) \([0 1 0]\) \([0 0 1]\)  
- New basis vectors: \([1 2 1]\) \([-2 -3 1]\)  
- Then A has new coordinates: \([1 0]\), B: \([0 1]\), C: \([1 -1]\)  
  - Notice: We reduced the number of dimensions/coordinates!
Goal of dimensionality reduction is to discover the axes of data!

Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

By doing this we incur a bit of error as the points do not exactly lie on the line.
SVD: Singular Value Decomposition
Reduction Matrix Dimension

- Gives a decomposition of any matrix into a product of three matrices:
  - \( A \approx U \Sigma V^T \)

- There are strong constraints on the form of each of these matrices
  - Results in a unique decomposition
  - From this decomposition, you can choose any number \( r \) of intermediate concepts (latent factors) in a way that minimizes the reconstruction error
**SVD – Definition**

\[ A \approx U \Sigma V^T = \sum_i \sigma_i u_i \circ v_i^T \]

- **A: Input data matrix**
  - \( m \times n \) matrix (e.g., \( m \) documents, \( n \) terms)
- **U: Left singular vectors**
  - \( m \times r \) matrix (\( m \) documents, \( r \) concepts)
- **Σ: Singular values**
  - \( r \times r \) diagonal matrix (strength of each ‘concept’)
    - \( r : \) rank of the matrix \( A \)
- **V: Right singular vectors**
  - \( n \times r \) matrix (\( n \) terms, \( r \) concepts)
A ≈ UΣV^T = \sum_i \sigma_i u_i \circ v_i^T

If we set \( \sigma_2 = 0 \), then the green columns may as well not exist.
It is **always** possible to decompose a real matrix $A$ into $A = U \Sigma V^T$, where

- $U, \Sigma, V$: unique
- $U, V$: column orthonormal
  - $U^T U = I; \ V^T V = I$ (I: identity matrix)
  - (Columns are orthogonal unit vectors)
- $\Sigma$: diagonal
  - Entries (**singular values**) are non-negative, and sorted in decreasing order ($\sigma_1 \geq \sigma_2 \geq ... \geq 0$)

Nice proof of uniqueness: [https://www.cs.cornell.edu/courses/cs322/2008sp/stuff/TrefethenBau_Lec4_SVD.pdf](https://www.cs.cornell.edu/courses/cs322/2008sp/stuff/TrefethenBau_Lec4_SVD.pdf)
Consider a matrix. What does SVD do?

Ratings matrix where each column corresponds to a movie and each row to a user. First 4 users prefer SciFi, while others prefer Romance.
**SVD – Example: Users-to-Movies**

- \( A = U \Sigma V^T \) - example: Users to Movies

<table>
<thead>
<tr>
<th>User</th>
<th>SciFi</th>
<th>Romance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>Alien</td>
<td>Serenity</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

\[
\begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32
\end{bmatrix}
\times
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3
\end{bmatrix}
\times
\begin{bmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.40 & -0.80 & 0.40 & 0.09 & 0.09
\end{bmatrix}
\]
SVD – Example: Users-to-Movies

\[ A = U \Sigma V^T \] - example: Users to Movies

<table>
<thead>
<tr>
<th>SciFi-concept</th>
<th>Romance-concept</th>
</tr>
</thead>
<tbody>
<tr>
<td>SciFi</td>
<td></td>
</tr>
<tr>
<td>Romance</td>
<td></td>
</tr>
</tbody>
</table>

Matrix

\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2 \\
\end{bmatrix}
\]

SciFi-concept

\[
\begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32 \\
\end{bmatrix}
\]

Romance-concept

\[
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.40 & -0.80 & 0.40 & 0.09 & 0.09 \\
\end{bmatrix}
\]
A = U Σ V^T - example:

U is “user-to-concept” factor matrix

Matrix | Alien | Serenity | Casablanca | Amelie
--- | --- | --- | --- | ---
1 | 1 | 0 | 0 | 0
3 | 3 | 0 | 0 | 0
4 | 4 | 0 | 0 | 0
5 | 5 | 0 | 0 | 0
0 | 2 | 4 | 4 | 0
0 | 0 | 5 | 5 | 0
0 | 1 | 2 | 2 | 0

SciFi-concept

Romance-concept

SciFi

Romance

= 

\[
\begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.40 & -0.80 & 0.40 & 0.09 & 0.09 \\
\end{bmatrix}
\]
A = U \Sigma V^T - example:

\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2
\end{bmatrix}
\begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32
\end{bmatrix}
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3
\end{bmatrix}
\]
A = U Σ Vᵀ - example:

SciFi

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Alien</th>
<th>Serenity</th>
<th>Casablanca</th>
<th>Amelie</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>3</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>4</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>0</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

SciFi-concept

| 0.13 | 0.02 | -0.01 |
| 0.41 | 0.07 | -0.03 |
| 0.55 | 0.09 | -0.04 |
| 0.68 | 0.11 | -0.05 |
| 0.15 | -0.59 | 0.65 |
| 0.07 | -0.73 | -0.67 |
| 0.07 | -0.29 | 0.32 |

V is “movie-to-concept” factor matrix

\[
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3
\end{bmatrix}
\]
Movies, users and concepts:

- $U$: user-to-concept matrix
- $V$: movie-to-concept matrix
- $\Sigma$: its diagonal elements: ‘strength’ of each concept
Dimensionality Reduction with SVD
Instead of using two coordinates \((x, y)\) to describe point positions, let’s use only one coordinate.

Point’s position is its location along vector \(v_1\).
**SVD – Dimensionality Reduction**

- **A = U \Sigma V^T - example:**
  - **U:** “user-to-concept” matrix
  - **V:** “movie-to-concept” matrix

\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2
\end{bmatrix}
= \begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32
\end{bmatrix}
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3
\end{bmatrix}
\begin{bmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.40 & -0.80 & 0.40 & 0.09 & 0.09
\end{bmatrix}
\]
\[ A = U \Sigma V^T - \text{example:} \]

\[
\begin{pmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2
\end{pmatrix}
\begin{pmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32
\end{pmatrix}
\begin{pmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3
\end{pmatrix}
\begin{pmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.40 & -0.80 & 0.40 & 0.09 & 0.09
\end{pmatrix}

variance (‘spread’) on the \( v_1 \) axis
A = U \Sigma V^T - example:

- **U \Sigma**: Gives the coordinates of the points in the projection axis

\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2 \\
\end{bmatrix}
\]

Project the users on the “Sci-Fi” axis using **U \Sigma**:

\[
\begin{bmatrix}
1.61 & 0.19 & -0.01 \\
5.08 & 0.66 & -0.03 \\
6.82 & 0.85 & -0.05 \\
8.43 & 1.04 & -0.06 \\
1.86 & -5.60 & 0.84 \\
0.86 & -6.93 & -0.87 \\
0.86 & -2.75 & 0.41 \\
\end{bmatrix}
\]
More details

**Q:** How is dim. reduction done?

$$\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2 \\
\end{bmatrix} = \begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32 \\
\end{bmatrix} \times \begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3 \\
\end{bmatrix} \times \begin{bmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.40 & -0.80 & 0.40 & 0.09 & 0.09 \\
\end{bmatrix}$$
More details

Q: How exactly is dim. reduction done?
A: Set smallest singular values to zero

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \times \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 & 0.65 \\ 0.07 & -0.73 & -0.67 \\ 0.07 & -0.29 & 0.32 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 3 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.40 & -0.80 & 0.40 & 0.09 & 0.09 \end{bmatrix}$$
More details

Q: How exactly is dim. reduction done?
A: Set smallest singular values to zero
More details

Q: How exactly is dim. reduction done?

A: Set smallest singular values to zero

This is Rank 2 approximation to A. We could also do Rank 1 approx. The larger the rank the more accurate the approximation.
SVD – Interpretation #2

More details
- **Q:** How exactly is dim. reduction done?
- **A:** Set smallest singular values to zero

This is Rank 2 approximation to $A$. We could also do Rank 1 approx. The larger the rank the more accurate the approximation.

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx \begin{bmatrix} 0.13 & 0.02 \\ 0.41 & 0.07 \\ 0.55 & 0.09 \\ 0.68 & 0.11 \\ 0.15 & -0.59 \\ 0.07 & -0.73 \\ 0.07 & -0.29 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \end{bmatrix}$$
Q: How exactly is dim. reduction done?
A: Set smallest singular values to zero

More details

Reconstructed data matrix B

Reconstruction Error is quantified by the Frobenius norm:

\[ \| M \|_F = \sqrt{\sum_{ij} M_{ij}^2} \]

\[ \| A - B \|_F = \sqrt{\sum_{ij} (A_{ij} - B_{ij})^2} \]

is “small”
Fact: SVD gives ‘best’ axis to project on:

- ‘best’ = minimizing the sum of reconstruction errors

\[ \|A - B\|_F = \sqrt{\sum_{ij} (A_{ij} - B_{ij})^2} \]

\[ A = U \Sigma V^T \]

\[ B \] is best approximation of \( A \):

\[ B = U \Sigma V^T \]
Theorem:
Let $A = U \Sigma V^T$ and $B = U S V^T$ where $S = \text{diagonal } r \times r \text{ matrix}$ with $s_i=\sigma_i$ ($i=1\ldots k$) else $s_i=0$
then $B$ is a best $\text{rank}(B)=k$ approx. to $A$

What do we mean by “best”:

- $B$ is a solution to $\min_B \|A-B\|_F$ where $\text{rank}(B)=k$

Refer to the MMDS book for a proof.

$$\|A - B\|_F = \sqrt{\sum_{ij} (A_{ij} - B_{ij})^2}$$
SVD – Conclusions so far

- **SVD**: $A = U \Sigma V^T$: **unique**
  - $U$: user-to-concept factors
  - $V$: movie-to-concept factors
  - $\Sigma$: strength of each concept

- **Q**: So what’s a good value for $r$ (# of latent factors)?
  - Let the **energy** of a set of singular values be the sum of their squares.
  - Pick $r$ so the retained singular values have at least 90% of the total energy.

- **Back to our example:**
  - With singular values 12.4, 9.5, and 1.3, total energy = 245.7
  - If we drop 1.3, whose square is only 1.7, we are left with energy 244, or over 99% of the total
How to Compute SVD
How do we actually compute SVD?

First we need a method for finding the principal eigenvalue (the largest one) and the corresponding eigenvector of a symmetric matrix.

- $M$ is symmetric if $m_{ij} = m_{ji}$ for all $i$ and $j$

Method:

- Start with any “guess eigenvector” $x_0$
- Construct $x_{k+1} = \frac{Mx_k}{\|Mx_k\|}$ for $k = 0, 1, \ldots$
  - $\| \ldots \|$ denotes the Frobenius norm
- Stop when consecutive $x_k$ show little change
Example: Iterative Eigenvector

\[
M = \begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix} \quad x_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}
\]

\[
\frac{Mx_0}{\|Mx_0\|} = \begin{pmatrix} 3 \\ 5 \end{pmatrix} / \sqrt{34} = \begin{pmatrix} 0.51 \\ 0.86 \end{pmatrix} = x_1
\]

\[
\frac{Mx_1}{\|Mx_1\|} = \begin{pmatrix} 2.23 \\ 3.60 \end{pmatrix} / \sqrt{17.93} = \begin{pmatrix} 0.53 \\ 0.85 \end{pmatrix} = x_2
\]

.....
Once you have the principal eigenvector \( \mathbf{x} \), you find its eigenvalue \( \lambda \) by \( \lambda = \mathbf{x}^T \mathbf{M} \mathbf{x} \).

- **In proof:** We know \( \mathbf{x} \lambda = \mathbf{M} \mathbf{x} \) if \( \lambda \) is the eigenvalue; multiply both sides by \( \mathbf{x}^T \) on the left.
- Since \( \mathbf{x}^T \mathbf{x} = 1 \) we have \( \lambda = \mathbf{x}^T \mathbf{M} \mathbf{x} \)

**Example:** If we take \( \mathbf{x}^T = [0.53, 0.85] \), then

\[
\begin{bmatrix}
0.53 & 0.85
\end{bmatrix}
\begin{bmatrix}
1 & 2 \\
2 & 3
\end{bmatrix}
\begin{bmatrix}
0.53 \\
0.85
\end{bmatrix}
= 4.25
\]
Finding More Eigenpairs

- Eliminate the portion of the matrix $M$ that can be generated by the first eigenpair, $\lambda$ and $x$:
  \[
  M^* := M - \lambda \, x \, x^T
  \]

- Recursively find the principal eigenpair for $M^*$, eliminate the effect of that pair, and so on

**Example:**

\[
M^* = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} - 4.25 \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} \begin{bmatrix} 0.53 & 0.85 \end{bmatrix} = \begin{bmatrix} -0.19 & 0.09 \\ 0.09 & 0.07 \end{bmatrix}
\]
Start by supposing $A = U \Sigma V^T$

$A^T = (U \Sigma V^T)^T = (V^T)^T \Sigma^T U^T = V \Sigma U^T$

- **Why?** (1) Rule for transpose of a product; (2) the transpose of the transpose and the transpose of a diagonal matrix are both the identity functions

$A^T A = V \Sigma U^T U \Sigma V^T = V \Sigma^2 V^T$

- **Why?** $U$ is orthonormal, so $U^T U$ is an identity matrix
- Also note that $\Sigma^2$ is a diagonal matrix whose $i$-th element is the square of the $i$-th element of $\Sigma$

$A^T A V = V \Sigma^2 V^T V = V \Sigma^2$

- **Why?** $V$ is also orthonormal
Since $A^TA = V\Sigma^2V^T \rightarrow AVA^T = V\Sigma^2$

- **Note** that therefore the $i$-th column of $V$ is an eigenvector of $A^TA$, and its eigenvalue is the $i$-th element of $\Sigma^2$

- Thus, we can find $V$ and $\Sigma$ by finding the eigenpairs for $A^TA$

  - Once we have the eigenvalues in $\Sigma^2$, we can find the singular values by taking the square root of these eigenvalues

- Symmetric argument, $AA^T$ gives us $U$
To compute the full SVD using specialized methods:
- $O(nm^2)$ or $O(n^2m)$ (whichever is less)

But:
- Less work, if we just want singular values
- or if we want the first $k$ singular vectors
- or if the matrix is sparse

Implemented in linear algebra packages like
- LINPACK, Matlab, SPlus, Mathematica ...
Example of SVD
**Case study: How to query?**

- **Q:** Find users that like ‘Matrix’
- **A:** Map query into a ‘concept space’ – how?

\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2 \\
\end{bmatrix}
\begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32 \\
\end{bmatrix}
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3 \\
\end{bmatrix}
\begin{bmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.40 & -0.80 & 0.40 & 0.09 & 0.09 \\
\end{bmatrix}
\]
Case study: How to query?

- **Q:** Find users that like ‘Matrix’
- **A:** Map query into a ‘concept space’ – how?

Project into concept space:
Inner product with each ‘concept’ vector $v_i$
Case study: How to query?

- Q: Find users that like ‘Matrix’
- A: Map query into a ‘concept space’ – how?

Project into concept space:
Inner product with each ‘concept’ vector $v_i$
Case study: How to query?

Compactly, we have:

\[ q_{\text{concept}} = q \, V \]

E.g.:

\[
\begin{bmatrix}
5 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
0.56 & 0.12 & 0.59 & -0.02 & 0.09 & 0.12 & 0.09 & -0.69 & 0.09 & -0.69
\end{bmatrix}
= \begin{bmatrix}
2.8 & 0.6
\end{bmatrix}
\]

SciFi-concept
Case study: How to query?

- How would the user \( d \) that rated ('Alien', 'Serenity') be handled?

\[
d_{\text{concept}} = d \, V
\]

E.g.:

\[
d = \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix}
\]

\[
V = \begin{bmatrix} 0.56 & 0.12 & 0.59 & -0.02 & 0.56 & 0.12 & 0.09 & -0.69 & 0.09 & -0.69 \end{bmatrix}
\]

\[
x = \begin{bmatrix} 0.56 & 0.12 \end{bmatrix}
\]

\[
SciFi-concept = \begin{bmatrix} 5.2 & 0.4 \end{bmatrix}
\]
**Observation:** User $d$ that rated (‘Alien’, ‘Serenity’) will be similar to user $q$ that rated (‘Matrix’), although $d$ and $q$ have zero ratings in common!

<table>
<thead>
<tr>
<th>SciFi-concept</th>
<th>5.2</th>
<th>0.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zero ratings in common</td>
<td>2.8</td>
<td>0.6</td>
</tr>
<tr>
<td>Similarity &gt; 0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Optimal low-rank approximation in terms of Frobenius norm

- **Interpretability problem:**
  - A singular vector specifies a linear combination of all input columns or rows

- **Lack of sparsity:**
  - Singular vectors are \textit{dense}!
CUR Decomposition
It is common for the matrix $A$ that we wish to decompose to be very sparse.

But $U$ and $V$ from a SVD decomposition will not be sparse.

**CUR** decomposition solves this problem by using only (randomly chosen) rows and columns of $A$. 
Goal: Express $A$ as a product of matrices $C, U, R$

Make $\|A - C \cdot U \cdot R\|_F$ small

“Constraints” on $C$ and $R$:

\[
\begin{pmatrix}
A
\end{pmatrix}
\approx
\begin{pmatrix}
C
\end{pmatrix}
\cdot
\begin{pmatrix}
U
\end{pmatrix}
\cdot
\begin{pmatrix}
R
\end{pmatrix}
\]

Frobenius norm:

\[
\|X\|_F = \sqrt{\sum_{ij} X_{ij}^2}
\]
Goal: Express $A$ as a product of matrices $C, U, R$

Make $\|A - C \cdot U \cdot R\|_F$ small

“Constraints” on $C$ and $R$:

$$\begin{pmatrix} A \\ \end{pmatrix} \approx \begin{pmatrix} C \\ \end{pmatrix} \cdot \begin{pmatrix} U \\ \end{pmatrix} \cdot \begin{pmatrix} R \\ \end{pmatrix}$$

Pseudo-inverse of the intersection of $C$ and $R$

Frobenius norm: $\|X\|_F = \sqrt{\sum_{ij} X_{ij}^2}$
Let \( W \) be the “intersection” of sampled columns \( C \) and rows \( R \).

**Def:** \( W^+ \) is the pseudoinverse

- Let SVD of \( W = X Z Y^T \)
- Then: \( W^+ = Y Z^+ X^T \)
  - \( Z^+ \): reciprocals of non-zero singular values: \( Z^+_{ii} = 1/Z_{ii} \)

Let: \( U = Y (Z^+)^2 X^T \)

**Why the intersection?** These are high magnitude numbers

**Why pseudoinverse works?**

\( W = X Z Y^T \) then \( W^{-1} = (Y^T)^{-1} Z^{-1} X^{-1} \)

Due to orthonormality: \( X^{-1} = X^T, \ Y^{-1} = Y^T \)

Since \( Z \) is diagonal \( Z^{-1} = 1/Z_{ii} \)

Thus, if \( W \) is nonsingular, pseudoinverse is the true inverse
To decrease the expected error between $A$ and its decomposition, we must pick rows and columns in a nonuniform manner.

The *importance* of a row or column of $A$ is the square of its Frobenius norm.

- That is, the sum of the squares of its elements.

When picking rows and columns, the probabilities must be proportional to importance.

**Example:** $[3,4,5]$ has importance 50, and $[3,0,1]$ has importance 10, so pick the first 5 times as often as the second.
Sampling columns (similarly for rows):

Input: matrix $A \in \mathbb{R}^{m \times n}$, sample size $c$

Output: $C_d \in \mathbb{R}^{m \times c}$

1. for $x = 1 : n$ [column distribution]
2. $P(x) = \sum_i A(i, x)^2 / \sum_{i,j} A(i, j)^2$
3. for $i = 1 : c$ [sample columns]
4. Pick $j \in 1 : n$ based on distribution $P(x)$
5. Compute $C_d(:, i) = A(:, j) / \sqrt{cP(j)}$

Note this is a randomized algorithm, same column can be sampled more than once
Rough and imprecise intuition behind CUR

- CUR is more likely to pick points away from the origin
  - Assuming smooth data with no outliers these are the directions of maximum variation

Example: Assume we have 2 clouds at an angle

- SVD dimensions are orthogonal and thus will be in the middle of the two clouds
- CUR will find the two clouds (but will be redundant)
CUR: Provably good approx. to SVD

For example:

- Select $c = O\left(\frac{k \log k}{\varepsilon^2}\right)$ columns of $A$ using ColumnSelect algorithm (slide 56)

- Select $r = O\left(\frac{k \log k}{\varepsilon^2}\right)$ rows of $A$ using RowSelect algorithm (slide 56)

- Set $U = Y (Z^+)^2 X^T$

Then: $\left\| A - CUR \right\|_F \leq (2 + \varepsilon) \left\| A - A_K \right\|_F$

with probability 98%

In practice: Pick $4k$ cols/rows for a “rank-k” approximation
**CUR: Pros & Cons**

+ **Easy interpretation**
  - Since the basis vectors are actual columns and rows

+ **Sparse basis**
  - Since the basis vectors are actual columns and rows

- **Duplicate columns and rows**
  - Columns of large norms will be sampled many times
SVD vs. CUR

**SVD:** \[ A = U \Sigma V^T \]
- Huge but sparse
- Sparse and small
- Big and dense

**CUR:** \[ A = CUR \]
- Huge but sparse
- Big but sparse
- Dense but small
DBLP bibliographic data
- Author-to-conference big sparse matrix
- $A_{ij}$: Number of papers published by author $i$ at conference $j$
- 428K authors (rows), 3659 conferences (columns)
  - Very sparse

Want to reduce dimensionality
- How much time does it take?
- What is the reconstruction error?
- How much space do we need?
**Results: DBLP - big sparse matrix**

- **Accuracy:**
  - $1 - \text{relative sum squared errors}$
- **Space ratio:**
  - $\frac{\text{#output matrix entries}}{\text{#input matrix entries}}$
- **CPU time**

Sun, Faloutsos: *Less is More: Compact Matrix Decomposition for Large Sparse Graphs*, SDM ’07.