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Dimensionality Reduction: SVD & CUR

CS246: Mining Massive Datasets
Jure Leskovec, Stanford University
Mina Ghashami, Amazon
http://cs246.stanford.edu
Reducing Matrix Dimension

- 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 \( r \)

\[
\begin{align*}
A & \approx U_r \Sigma_r V_T^T \\
m \times n & \approx r \times r \times r \\
& \approx U_r \times \Sigma_r \times V_T^T
\end{align*}
\]
## Dimensionality Reduction

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

### Example Matrix

<table>
<thead>
<tr>
<th>customer</th>
<th>day</th>
<th>Week</th>
<th>Thursday</th>
<th>Friday</th>
<th>Saturday</th>
<th>Sunday</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>7/10/96</td>
<td>7/11/96</td>
<td>7/12/96</td>
<td>7/13/96</td>
<td>7/14/96</td>
<td></td>
</tr>
<tr>
<td>ABC Inc.</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>DEF Ltd.</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>GHI Inc.</td>
<td>1</td>
<td>1</td>
<td><strong>1</strong></td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>KLM Co.</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Smith</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td><strong>2</strong></td>
<td><strong>2</strong></td>
<td></td>
</tr>
<tr>
<td>Johnson</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Thompson</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

**New representation**
- ABC Inc.: [1 0]
- DEF Ltd.: [2 0]
- GHI Inc.: [1 0]
- KLM Co.: [5 0]
- Smith: [0 2]
- Johnson: [0 3]
- Thompson: [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, B, C

**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
Reducing Matrix Dimension

- Gives a decomposition of any matrix into a product of three matrices:

\[ A \approx U_r \Sigma_r V_T^T \]

- 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
A ≈ UΣV^T = \sum_i \sigma_i u_i \circ v_i^T

- **A:** Input data matrix
  - m x n matrix (e.g., m documents, n terms)
- **U:** Left singular vectors
  - m x r matrix (m documents, r concepts)
- **Σ:** Singular values
  - r x r diagonal matrix (strength of each ‘concept’)
    (r : rank of the matrix A)
- **V:** Right singular vectors
  - n x r matrix (n terms, r concepts)
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
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.

"Concepts"
AKA Latent dimensions
AKA Latent factors
SVD – Example: Users-to-Movies

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

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

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

Romance-concept: [12.4 0 0 0 9.5 0 0 0 1.3]

\[
\begin{bmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.40 & -0.80 & 0.40 & 0.09 & 0.09 \\
\end{bmatrix}
\]
SVD – Example: Users-to-Movies

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

\[ U \text{ is “user-to-concept” factor matrix} \]

<table>
<thead>
<tr>
<th>Matrix</th>
<th>SciFi-concept</th>
<th>Romance-concept</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alien</td>
<td>1 1 1 0 0</td>
<td>0.13 0.02 -0.01</td>
</tr>
<tr>
<td>Serenity</td>
<td>3 3 3 0 0</td>
<td>0.41 0.07 -0.03</td>
</tr>
<tr>
<td>Casablanca</td>
<td>4 4 4 0 0</td>
<td>0.55 0.09 -0.04</td>
</tr>
<tr>
<td>Amelie</td>
<td>5 5 5 0 0</td>
<td>0.68 0.11 -0.05</td>
</tr>
<tr>
<td>0 2 0 4 4</td>
<td>0.15 -0.59 0.65</td>
<td>0.07 -0.73 -0.67</td>
</tr>
<tr>
<td>0 0 0 5 5</td>
<td>0.07 -0.29 0.32</td>
<td>12.4 0 0</td>
</tr>
<tr>
<td>0 1 0 2 2</td>
<td></td>
<td>0 9.5 0</td>
</tr>
<tr>
<td>0 1 0 2 2</td>
<td></td>
<td>0 0 1.3</td>
</tr>
</tbody>
</table>

\[ \begin{bmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.40 & -0.80 & 0.40 & 0.09 & 0.09
\end{bmatrix} \]
SVD – Example: Users-to-Movies

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

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

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

\[
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3 \\
\end{bmatrix}
\]
SVD – Example: Users-to-Movies

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

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

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

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

\[ \begin{pmatrix}
    0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
    0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
    0.40 & -0.80 & 0.40 & 0.09 & 0.09
\end{pmatrix}
\]
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

\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2 \\
\end{bmatrix}
\times
\begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32 \\
\end{bmatrix}
\times
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3 \\
\end{bmatrix}
\]
SVD – Dimensionality Reduction

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

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

Projection of users on the “Sci-Fi” axis

Movie 1 rating

<table>
<thead>
<tr>
<th></th>
<th>1.61</th>
<th>0.19</th>
<th>-0.01</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5.08</td>
<td>0.66</td>
<td>-0.03</td>
</tr>
<tr>
<td></td>
<td>6.82</td>
<td>0.85</td>
<td>-0.05</td>
</tr>
<tr>
<td></td>
<td>8.43</td>
<td>1.04</td>
<td>-0.06</td>
</tr>
<tr>
<td></td>
<td>1.86</td>
<td>-5.60</td>
<td>0.84</td>
</tr>
<tr>
<td></td>
<td>0.86</td>
<td>-6.93</td>
<td>-0.87</td>
</tr>
<tr>
<td></td>
<td>0.86</td>
<td>-2.75</td>
<td>0.41</td>
</tr>
</tbody>
</table>

Movie 2 rating

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

first right singular vector
More details

Q: How is dim. reduction done?

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

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

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

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

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

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

This is Rank 2 approximation to \( A \).
We could also do Rank 1 approx.
The larger the rank the more accurate the approximation.
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.
More details

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

**A:** Set smallest singular values to zero

\[
\begin{pmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2
\end{pmatrix}
\approx
\begin{pmatrix}
0.92 & 0.95 & 0.92 & 0.01 & 0.01 \\
2.91 & 3.01 & 2.91 & -0.01 & -0.01 \\
3.90 & 4.04 & 3.90 & 0.01 & 0.01 \\
4.82 & 5.00 & 4.82 & 0.03 & 0.03 \\
0.70 & 0.53 & 0.70 & 4.11 & 4.11 \\
-0.69 & 1.34 & -0.69 & 4.78 & 4.78 \\
0.32 & 0.23 & 0.32 & 2.01 & 2.01
\end{pmatrix}
\]

Reconstructed data matrix \( \mathbf{B} \)

Reconstruction Error is quantified by the Frobenius norm:

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

\[
\| \mathbf{A} - \mathbf{B} \|_F = \sqrt{\sum_{ij} (A_{ij} - B_{ij})^2}
\]
is “small”
Fact: SVD gives ‘best’ axis to project on:

‘best’ = minimizing the sum of reconstruction errors

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

- 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” $\mathbf{x}_0$
  - Construct $\mathbf{x}_{k+1} = \frac{M \mathbf{x}_k}{||M \mathbf{x}_k||}$ for $k = 0, 1, ...$
    - $|| ... ||$ denotes the Frobenius norm
  - Stop when consecutive $\mathbf{x}_k$ show little change
Example: Iterative Eigenvector

\[
\mathbf{M} = \begin{pmatrix}
1 & 2 \\
2 & 3 \\
\end{pmatrix} \quad \mathbf{x}_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}
\]

\[
\frac{\mathbf{Mx}_0}{||\mathbf{Mx}_0||} = \frac{\begin{pmatrix} 3 \\ 5 \end{pmatrix}}{\sqrt{34}} = \begin{pmatrix} 0.51 \\ 0.86 \end{pmatrix} = \mathbf{x}_1
\]

\[
\frac{\mathbf{Mx}_1}{||\mathbf{Mx}_1||} = \frac{\begin{pmatrix} 2.23 \\ 3.60 \end{pmatrix}}{\sqrt{17.93}} = \begin{pmatrix} 0.53 \\ 0.85 \end{pmatrix} = \mathbf{x}_2
\]

.....
Once you have the principal eigenvector $x$, you find its eigenvalue $\lambda$ by $\lambda = x^T M x$.

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

**Example**: If we take $x^T = [0.53, 0.85]$, then

$$
\lambda = [0.53 \ 0.85] \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} = 4.25
$$
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:**

$$M^* = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} - 4.25 \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} \begin{bmatrix} 0.53 & 0.85 \end{bmatrix} = \begin{bmatrix} -0.19 & 0.09 \\ 0.09 & 0.07 \end{bmatrix}$$
How to Compute the SVD

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

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

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

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

- Symmetric argument, $A A^T$ 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?

\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2 \\
\end{bmatrix}
\times
\begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32 \\
\end{bmatrix}
\times
\begin{bmatrix}
12.4 \\
0 \\
0 \\
\end{bmatrix}
\]
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?

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

**Project into concept space:**
Inner product with each ‘concept’ vector \( v_i \)
Compactly, we have:

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

E.g.:

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

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

\[ q_{\text{concept}} = \begin{bmatrix} 2.8 & 0.6 \end{bmatrix} \]
**Case study: How to query?**

- How would the user $d$ that rated (‘Alien’, ‘Serenity’) be handled?

$$d_{\text{concept}} = d \ V$$

E.g.:

<table>
<thead>
<tr>
<th>Concept</th>
<th>Matrix</th>
<th>Alien</th>
<th>Serenity</th>
<th>Casablanca</th>
<th>Amelie</th>
</tr>
</thead>
<tbody>
<tr>
<td>SciFi-concept</td>
<td>0.56</td>
<td>0.12</td>
<td>0.59</td>
<td>-0.02</td>
<td>0.09</td>
</tr>
<tr>
<td>SciFi-concept</td>
<td>0.56</td>
<td>0.12</td>
<td>0.09</td>
<td>-0.69</td>
<td>0.09</td>
</tr>
</tbody>
</table>

$$d = \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} \ x \ \begin{bmatrix} 0.56 & 0.12 & 0.56 & 0.12 & 0.09 & -0.69 & 0.09 & -0.69 \end{bmatrix} = \begin{bmatrix} 5.2 & 0.4 \end{bmatrix}$$
## Case study: How to query?

- **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></th>
<th>Matrix</th>
<th>Alien</th>
<th>Serenity</th>
<th>Casablanca</th>
<th>Amelie</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>0</td>
<td>4</td>
<td>5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$q$</td>
<td>5</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

SciFi-concept

![Similarity Matrix](attachment:matrix.png)

Zero ratings in common

Similarity > 0
SVD: Drawbacks

- 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 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 $A$. 

-- Jure Leskovec & Mina Ghashami, Stanford CS246: Mining Massive Datasets
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:

\[
\|X\|_F = \sqrt{\sum_{ij} X_{ij}^2}
\]
CUR Decomposition

- **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 $W = XZYT$
- Then: $W^+ = YZ^+X^T$
  - $Z^+$: reciprocals of non-zero singular values: $Z^+_{ii} = 1/Z_{ii}$

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

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

**Why pseudoinverse works?**

$W = XZYT$ then $W^{-1} = (YT)^{-1}Z^{-1}X^{-1}$

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.
CUR: Row Sampling Algorithm

- 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.
Intuition

- **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)
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
- Big and dense

**CUR:** \[ A = CUR \]
- Huge but sparse
- Big but sparse
- Dense but small
- Sparse and small
SVD vs. CUR: Simple Experiment

- **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:**
  - $\#\text{output matrix entries} / \#\text{input matrix entries}$

- **CPU time**

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