# **Dimensionality Reduction**

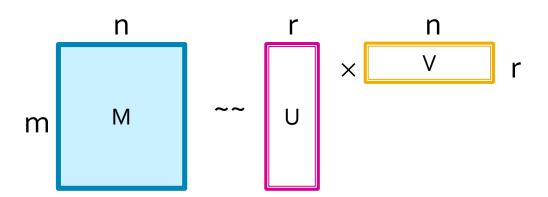
UV Decomposition
Singular-Value Decomposition
CUR Decomposition

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# 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 two matrices that share a small common dimension r.

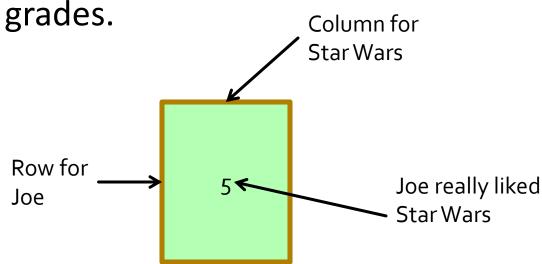


### Why Is That Even Possible?

- There are hidden, or latent factors that to a close approximation – explain why the values are as they appear in the matrix.
- Two kinds of data may exhibit this behavior:
  - 1. Matrices representing a many-many-relationship.
  - Matrices that are really a relation (as in a relational database).

#### Matrices as Relationships

- Our data can be a many-many relationship in the form of a matrix.
  - Example: people vs. movies; matrix entries are the ratings given to the movies by the people.
  - Example: students vs. courses; entries are the grades.
    Column for



### Matrices as Relationships — (2)

- Often, the relationship can be explained closely by latent factors.
  - Example: genre of movies or books.
    - I.e., Joe liked Star Wars because Joe likes science-fiction, and Star Wars is a science-fiction movie.
  - Example: good at math?

#### Matrices as Relational Data

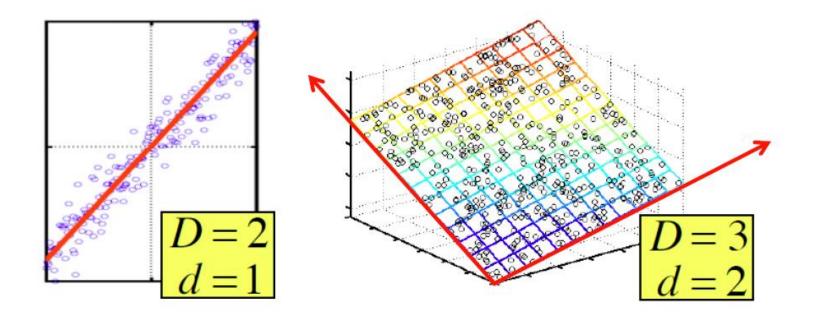
- Another closely related form of data is a collection of rows (tuples), each representing one entity.
- Columns represent attributes of these entities.
- Example: Stars can be represented by their mass, brightness in various color bands, diameter, and several other properties.
- But it turns out that there are only two independent variables (latent factors): mass and age.

# **Example: Stars**

Star	Mass	Luminosity	Color	Age
Sun	1.0	1.0	Yellow	4.6B
Alpha Centauri	1.1	1.5	Yellow	5.8B
Sirius A	2.0	25	White	0.25B

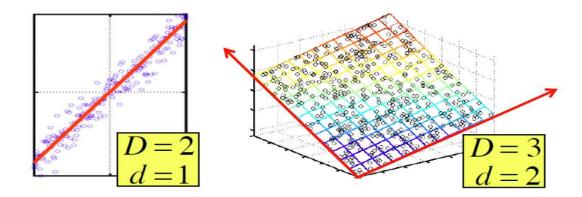
The matrix

# D-Dimensional Data Lying Close to a d-Dimensional Subspace



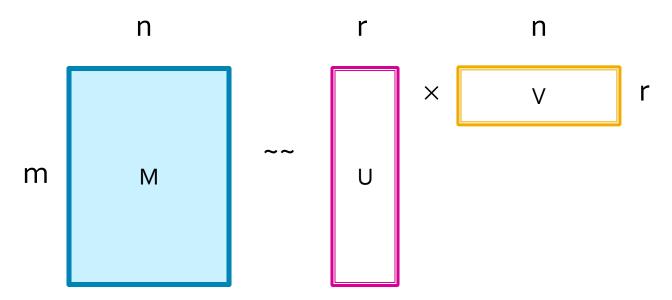
#### Intuition

- The axes of the subspace 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 greatest variance.
  - And so on..., until you have "enough" dimensions.



#### **UV** Decomposition

The simplest form of matrix decomposition is to find a pair of matrixes, the first (U) with few columns and the second (V) with few rows, whose product is close to the given matrix M.



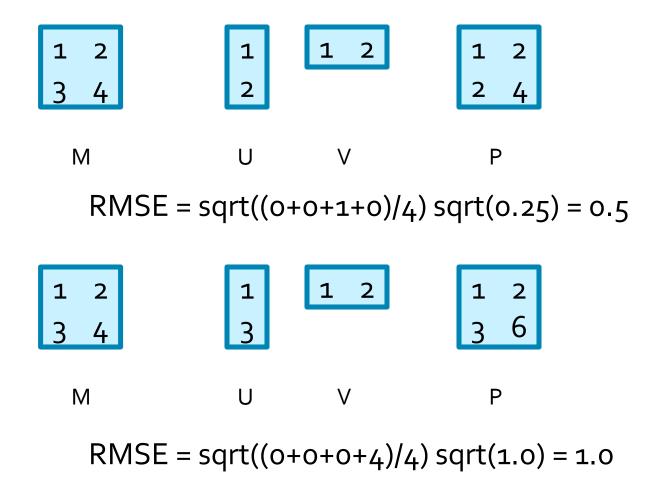
#### Latent Factors

- This decomposition works well if r is the number of "hidden factors" that explain the matrix M.
- Example: m<sub>ij</sub> is the rating person i gives to movie j; u<sub>ik</sub> measures how much person i likes genre k; v<sub>kj</sub> measures the extent to which movie j belongs to genre k.

## Measuring the Error

- Common way to evaluate how well P = UV approximates M is by RMSE (root-mean-square error).
- Average  $(m_{ij} p_{ij})^2$  over all i and j.
- Take the square root.
  - Square-rooting changes the scale of error, but doesn't really effect which choice of U and V is best.

#### Example: RMSE

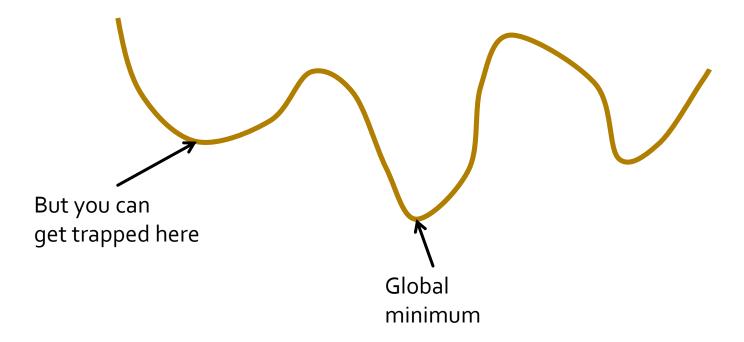


## Optimizing U and V

- Pick r, the number of latent factors.
- Think of U and V as composed of variables,  $u_{ik}$  and  $v_{ki}$ .
- Express the RMSE as (the square root of)  $E = \sum_{ij} (m_{ij} - \sum_{k} u_{ik} v_{kj})^{2}.$
- Gradient descent: repeatedly find the derivative of E with respect to each variable and move each a small amount in the direction that lowers the value of E.
  - Many options more later in the course.

#### Local Versus Global Minima

- Expressions like this usually have many minima.
- Seeking the nearest minimum from a starting point can trap you in a local minimum, from which no small improvement is possible.



#### **Avoiding Local Minima**

- Use many different starting points, chosen at random, in the hope that one will be close enough to the global minimum.
- Simulated annealing: occasionally try a leap to someplace further away in the hope of getting out of the local trap.
  - Intuition: the global minimum might have many nearby local minima.
    - As Mt. Everest has most of the world's tallest mountains in its vicinity.

#### **Application: Recommendations**

- UV decomposition can be used even when the entire matrix M is not known.
- Example: recommendation systems, where M represents known ratings of movies (e.g.) by people.
- Jure will cover recommendation systems next week.

# Singular-Value Decomposition

Rank of a Matrix
Orthonormal Bases
Eigenvalues/Eigenvectors
Computing the Decomposition
Eliminating Dimensions

# Why SVD?

- Gives a decomposition of any matrix into a product of three matrices.
- There are strong constraints on the form of each of these matrices.
  - Results in a decomposition that is essentially unique.
- From this decomposition, you can choose any number r of intermediate concepts (latent factors) in a way that minimizes the RMSE error given that value of r.

#### Rank of a Matrix

- The rank of a matrix is the maximum number of rows (or equivalently columns) that are linearly independent.
  - I.e., no nontrivial sum is the all-zero vector.
- Example: No two rows dependent.
  - One would have to be a multiple of the other.
- But any 3 rows are dependent.
  - Example: First + third twice the second = [0,0,0].
- Similarly, the 3 columns are dependent.
- Therefore, rank = 2.

#### Important Fact About Rank

- If a matrix has rank r, then it can be decomposed exactly into matrices whose shared dimension is r.
- Example, in Sect. 11.3 of MMDS, of a 7-by-5 matrix with rank 2 and an exact decomposition into a 7-by-2 and a 2-by-5 matrix.

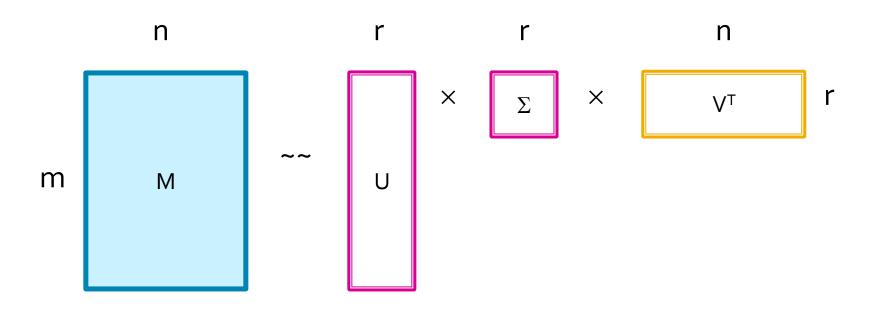
#### Orthonormal Bases

- Vectors are orthogonal if their dot product is 0.
- Example: [1,2,3].[1,-2,1] = 0, so these two vectors are orthogonal.
- A unit vector is one whose length is 1.
  - Length = square root of sum of squares of components.
    - No need to take square root if we are looking for length = 1.
- Example: [0.8, -0.1, 0.5, -0.3, 0.1] is a unit vector, since 0.64 + 0.01 + 0.25 + 0.09 + 0.01 = 1.
- An orthonormal basis is a set of unit vectors any two of which are orthogonal.

#### **Example: Columns Are Orthonormal**

3/√116	1/2	$7/\sqrt{116}$	1/2
3/√116	-1/2	7/√ <del>11</del> 6	-1/2
7/√ <del>116</del>	1/2	-3/√ <del>11</del> 6	-1/2
7/√ <del>116</del>	-1/2	-3/\(\sqrt{116}\)	1/2

#### Form of SVD



Special conditions:

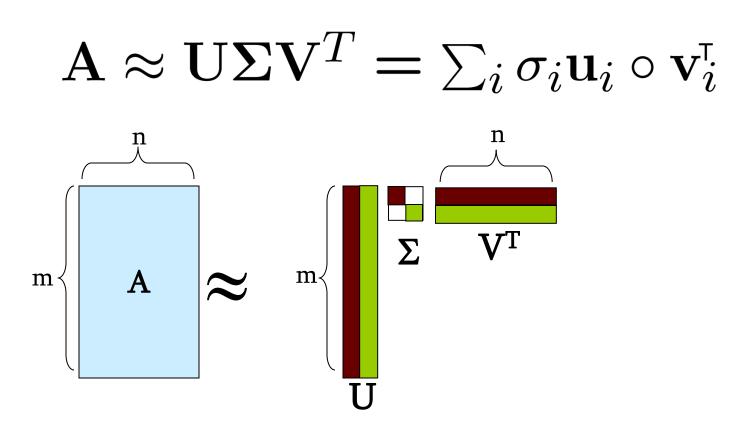
U and V are column-orthonormal (so  $V^T$  has orthonormal rows)

 $\Sigma$  is a diagonal matrix

#### Facts About SVD

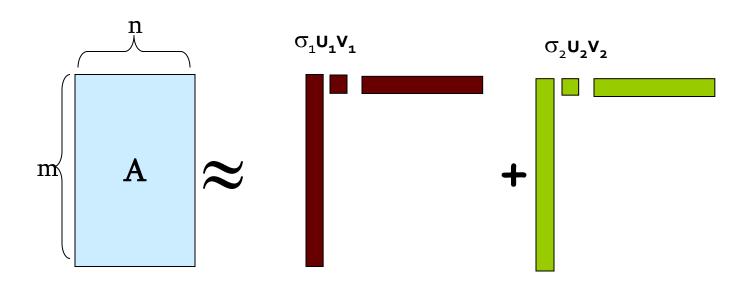
- The values of  $\Sigma$  along the diagonal are called the *singular values*.
- It is always possible to decompose M exactly, if r is the rank of M.
- But usually, we want to make r much smaller, and we do so by setting to 0 the smallest singular values.
  - Which has the effect of making the corresponding columns of U and V useless, so they may as well not be there.

#### Linkage Among Components of U, V, $\Sigma$



# Each Singular Value Affects One Column of U and V

$$\mathbf{A} pprox \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T = \sum_i \sigma_i \mathbf{u}_i \circ \mathbf{v}_i^{\mathsf{T}}$$



If we set  $\sigma_2 = 0$ , then the green columns may as well not exist.

 $\sigma_i$  ... scalar  $u_i$  ... vector  $v_i$  ... vector

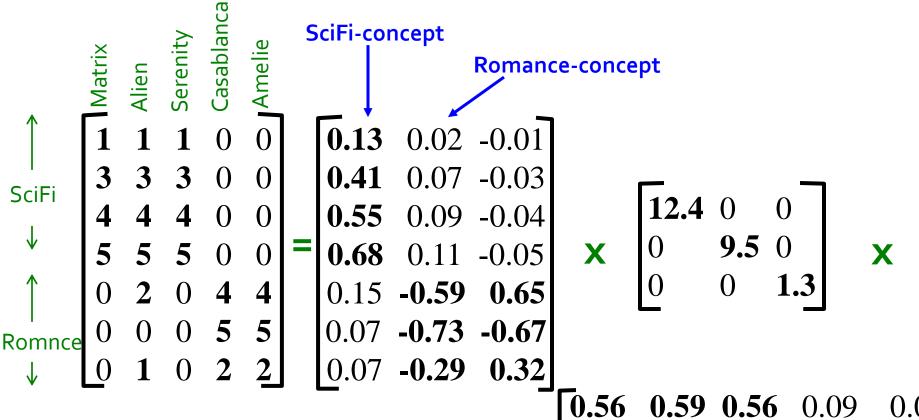
#### Jure's Example Decomposition

- The following is Example 11.9 from MMDS.
- It modifies the simpler Example 11.8, where a rank-2 matrix can be decomposed exactly into a 7-by-2 U and a 5-by-2 V.

#### ■ A = U $\Sigma$ V<sup>T</sup> - example: Users to Movies

	Matrix	Alien	Sereni	Casabl	Ameli				
	1	1	1	0	0		0.13	0.02	-0.0
l SciFi	3	3	3	0	0		0.41	0.02 0.07	-0.0
<b>↓</b>	4	4	4	0	0		0.55	0.09	-0.0
<b>V</b>	5	5	5	0	0	=	0.68	0.11 <b>-0.59</b>	-0.0
	0	2	0	4	4				
ा Romnce	0	0	0	5	5		0.07	-0.73	-0.6
$\downarrow$	0	1	0	2	2		0.07	-0.29	0.3

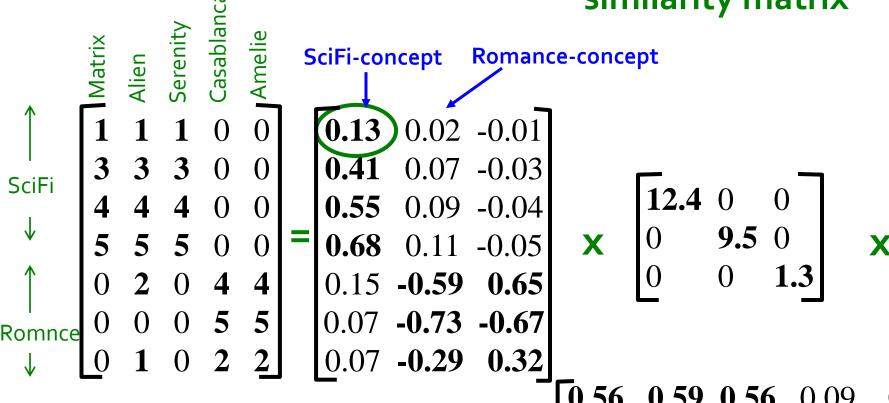
#### - $A = U \Sigma V^T$ - example: Users to Movies



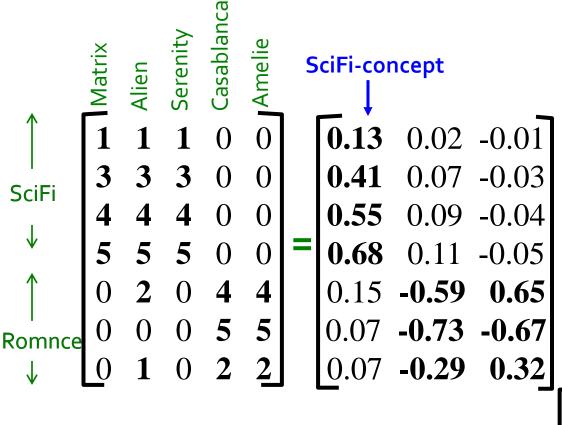
12 -0.02 0.12 **-0.69 -0.69** 40 **-0.80** 0.40 0.09 0.09

#### • $A = U \Sigma V^T$ - example:

*U* is "user-to-concept" similarity matrix



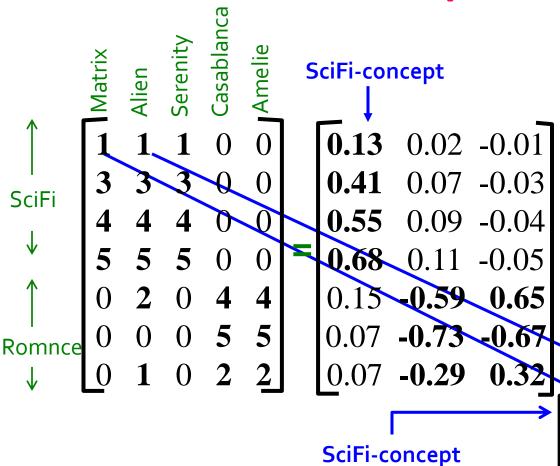
#### • $A = U \Sigma V^T$ - example:



\*\*strength" of the SciFi-concept

(12.4) 0 0 0 0 0 9.5 0 0 0 1.3

#### • $A = U \Sigma V^T$ - example:



V is "movie-to-concept" similarity matrix

$$\begin{array}{c|cccc}
\mathbf{12.4} & 0 & 0 \\
0 & \mathbf{9.5} & 0 \\
0 & 0 & \mathbf{1.3}
\end{array}$$

**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

3

#### Lowering the Dimension

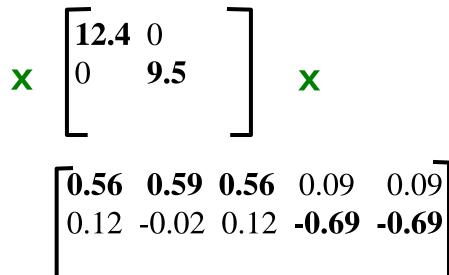
- Q: How exactly is dimensionality reduction done?
- A: Set smallest singular values to zero

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## Lowering the Dimension

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

```
      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
```

 $\approx$ 

```
      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
```

# Frobenius Norm and Approximation Error

- The Frobenius norm of a matrix is the square root of the sum of the squares of its elements.
- The error in an approximation of one matrix by another is the Frobenius norm of the difference.
  - Same as the RMSE.
- Important fact: The error in the approximation of a matrix by SVD, subject to picking r singular values, is minimized by zeroing all but the largest r singular values.

#### Energy

- So what's a good value for r?
- 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.
- 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.
- But also dropping 9.5 leaves us with too little.

## Finding Eigenpairs

- We want to describe how the SVD is actually computed.
- Essential is a method for finding the principal eigenvalue (the largest one) and the corresponding eigenvector of a symmetric matrix.
  - M is symmetric if m<sub>ij</sub> = m<sub>ji</sub> for all i and j.
- Start with any "guess eigenvector" x<sub>0</sub>.
- Construct  $\mathbf{x}_{k+1} = \mathbf{M}\mathbf{x}_k / ||\mathbf{M}\mathbf{x}_k||$  for k = 0, 1,...
  - | | | ... | | denotes the Frobenius norm.
- Stop when consecutive  $\mathbf{x}_k$ 's show little change.

# **Example: Iterative Eigenvector**

$$M = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} \quad x_0 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\frac{Mx_0}{\|Mx_0\|} = \frac{3}{5} / \sqrt{34} = \frac{0.51}{0.86} = x_1$$

$$\frac{Mx_1}{\|Mx_1\|} = \frac{2.23}{3.60} / \sqrt{17.93} = \frac{0.53}{0.85} = x_2$$

# Finding the Principal Eigenvalue

- Once you have the principal eigenvector  $\mathbf{x}$ , you find its eigenvalue  $\lambda$  by  $\lambda = \mathbf{x}^T \mathbf{M} \mathbf{x}$ .
- In proof:  $\mathbf{x}\lambda = \mathbf{M}\mathbf{x}$  for this  $\lambda$ , since  $\mathbf{x} \mathbf{x}^T \mathbf{M}\mathbf{x} = \mathbf{M}\mathbf{x}$ .
  - Why?  $\mathbf{x}$  is a unit vector, so  $\mathbf{x} \mathbf{x}^T = 1$ .
- **Example:** If we take  $\mathbf{x}^{T} = [0.54, 0.87]$ , then  $\lambda =$

$$\begin{bmatrix} 0.53 & 0.85 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} = 4.25$$

## Finding More Eigenpairs

- Eliminate the portion of the matrix M that can be generated by the first eigenpair,  $\lambda$  and  $\mathbf{x}$ .
- $\mathbf{M}^* := \mathbf{M} \lambda \mathbf{x} \mathbf{x}^\mathsf{T}.$
- Recursively find the principal eigenpair for M\*, eliminate the effect of that pair, and so on.
- Example:

$$M* = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} -4.25 \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} [0.53 \ 0.85] = \begin{bmatrix} -0.19 \ 0.09 \ 0.09 \end{bmatrix}$$

#### How to Compute the SVD

- Start by supposing  $M = U\Sigma V^{T}$ .
- $M^{\mathsf{T}} = (\mathsf{U}\Sigma\mathsf{V}^{\mathsf{T}})^{\mathsf{T}} = (\mathsf{V}^{\mathsf{T}})^{\mathsf{T}}\Sigma^{\mathsf{T}}\mathsf{U}^{\mathsf{T}} = \mathsf{V}\Sigma\mathsf{U}^{\mathsf{T}}.$ 
  - 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 function.
- $M^{\mathsf{T}}M = V\Sigma U^{\mathsf{T}}U\Sigma V^{\mathsf{T}} = V\Sigma^{2}V^{\mathsf{T}}.$ 
  - Why? U is orthonormal, so U<sup>T</sup>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  $\Sigma$ .
- $M^{\mathsf{T}}MV = V\Sigma^{2}V^{\mathsf{T}}V = V\Sigma^{2}.$ 
  - Why? V is also orthonormal.

# Computing the SVD –(2)

- Starting with  $M^TMV = V\Sigma^2$ , note that therefore the i-th column of V is an eigenvector of  $M^TM$ , and its eigenvalue is the i-th element of  $\Sigma^2$ .
- Thus, we can find V and  $\Sigma$  by finding the eigenpairs for  $M^TM$ .
  - Once we have the eigenvalues in  $\Sigma^2$ , we can find the singular values by taking the square root of these eigenvalues.
- Symmetric argument, starting with MM<sup>T</sup>, gives us U.

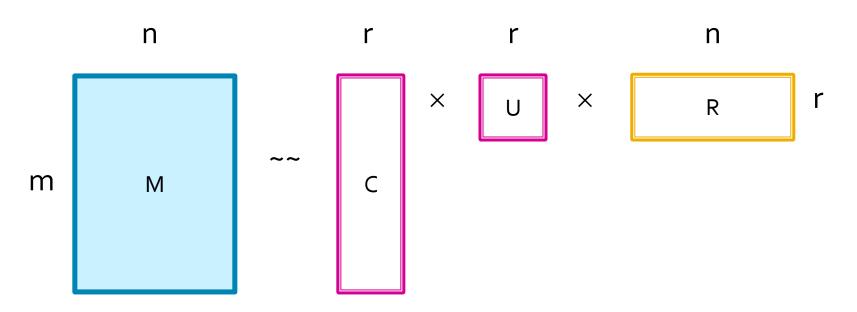
# **CUR Decomposition**

The Sparsity Issue Picking Random Rows and Columns

# **Sparsity**

- It is common for the matrix M that we wish to decompose to be very sparse.
- But U and V from a UV or SVD decomposition will not be sparse even so.
- CUR decomposition solves this problem by using only (randomly chosen) rows and columns of M.

## Form of CUR Decomposition



r chosen as you like.

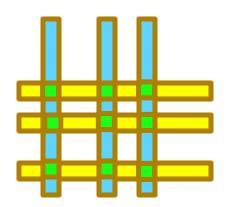
C = randomly chosen columns of M.

R = randomly chosen rows of M

U is tricky – more about this.

#### Construction of U

- U is r-by-r, so it is small, and it is OK if it is dense and complex to compute.
- Start with W = intersection of the r columns chosen for C and the r rows chosen for R.
- Compute the SVD of W to be  $X\Sigma Y^T$ .
- Compute  $\Sigma^+$ , the *Moore-Penrose inverse* of  $\Sigma$ .
  - Definition, next slide.
- $U = Y(\Sigma^+)^2 X^T.$



#### **Moore-Penrose Inverse**

- If  $\Sigma$  is a diagonal matrix, its More-Penrose inverse is another diagonal matrix whose i-th entry is:
  - $1/\sigma$  if  $\sigma$  is not 0.
  - 0 if  $\sigma$  is 0.
- Example:

#### Which Rows and Columns?

- To decrease the expected error between M and its decomposition, we must pick rows and columns in a nonuniform manner.
- The *importance* of a row or column of M is the square of its Frobinius 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.