Dimensionality Reduction

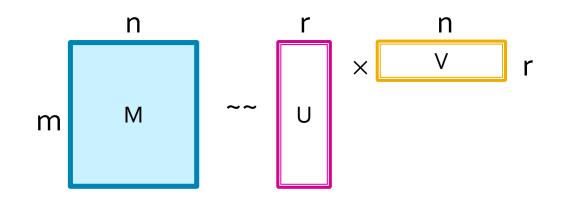
UV Decomposition Singular-Value Decomposition CUR Decomposition

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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.

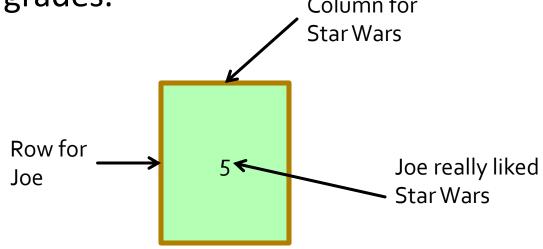


Why Is That Even Possible?

- 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.
 - "Latent" factors may explain the relationship.
 - 2. Matrices that are really a relation (as in a relational database).
 - The columns may not really be independent.

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: types of courses.
 - Sue is good at computer science, and CS246 is a CS course.

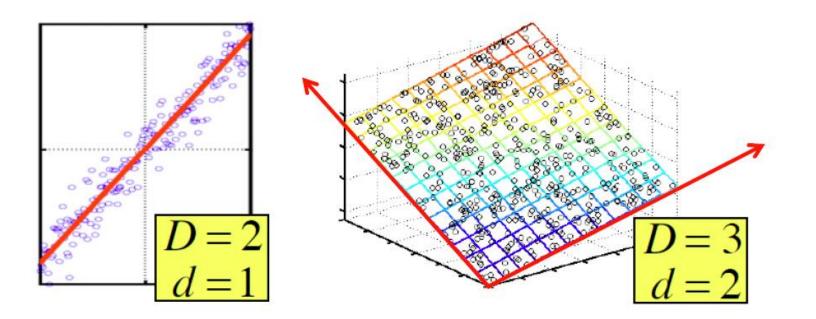
Matrices as Relational Data

- 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

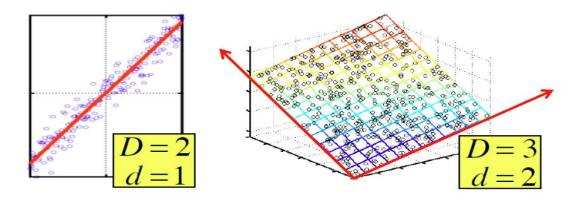
Star	Mass	Luminosity	Color	Age
Sun	1.0	1.0	Yellow	4.6B
Alpha Centauri	1.1	1.5	Yellow	5.8B
Sirius A	2.0	25	White	0.25B
		Th	ne matrix	

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



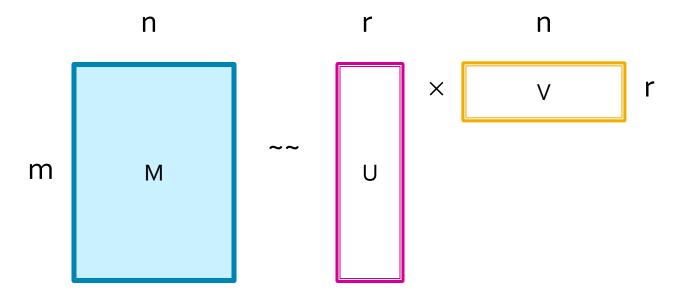
Intuition

- 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 that variance is really low.



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.



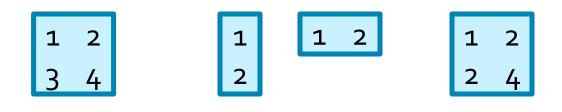
Latent Factors

- This decomposition works well if r is the number of "hidden factors" that explain the matrix M.
- Example: m_{ij} is the rating person i gives to movie j; u_{ik} measures how much person i likes genre k; v_{kj} 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 affect which choice of U and V is best.

Example: RMSE



M U V P RMSE = sqrt((0+0+1+0)/4) sqrt(0.25) = 0.5

 1
 2
 1
 2
 1
 2

 3
 4
 3
 3
 3
 6

 M
 U
 V
 P

RMSE = sqrt((0+0+0+4)/4) sqrt(1.0) = 1.0

Ouestion for Thought: Are either of these the best choice?

Optimizing U and V

- Pick r, the number of latent factors.
- Think of U and V as composed of variables, u_{ik} and v_{kj}.
- Express the RMSE as (the square root of)

$$\mathsf{E} = \Sigma_{ij} (\mathsf{m}_{ij} - \Sigma_k \mathsf{u}_{ik} \mathsf{v}_{kj})^2$$

 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.

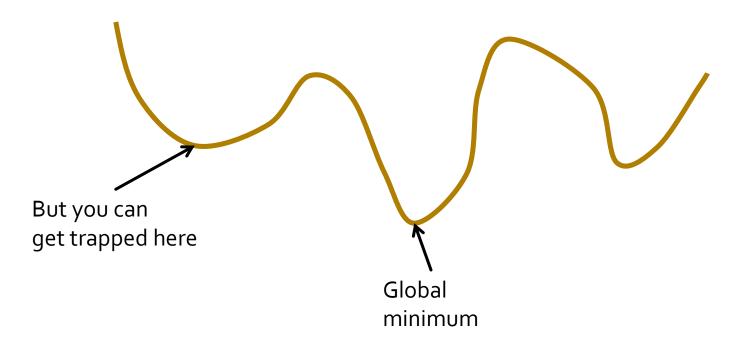
Important point: Go only a small distance, because E is not linear, so following the derivative too far gets you off-course.

What if M is Missing Entries?

- Ignore the error term for m_{ij} if that value is "unknown."
- Example: in a person-movie matrix, most movies are not rated by most people, so measure the error only for the known ratings.
 - To be covered by Jure in mid-February.

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.

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.
 - Trivial sum = all coefficients are 0.
- Example: Exist two independent rows.
 - In fact, no row is a multiple of another in this example.
- But **any** 3 rows are dependent.
 - Example: First + third twice the second = [0,0,0].
- Similarly, the 3 columns are dependent.
- Therefore, rank = 2.

4 5

8

6

17

Important Fact About Rank

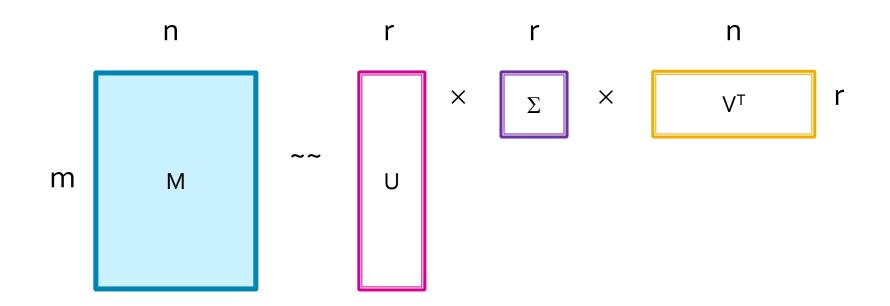
- If a matrix has rank r, then it can be decomposed exactly into matrices whose shared dimension is r.
- Example, in Sect. 11.3 of MMDS, of a 7-by-5 matrix with rank 2 and an exact decomposition into a 7-by-2 and a 2-by-5 matrix.

Orthonormal Bases

- Vectors are orthogonal if their dot product is 0.
- Example: [1,2,3].[1,-2,1] = 1*1 + 2*(-2) + 3*1 = 1-4+3 = 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.

3/√116	1/2	7/√116	1/2
3/√116	-1/2	7/√116	-1/2
7/√116	1/2	-3/√116	-1/2
7/√116	-1/2	-3/√116	1/2

Form of SVD



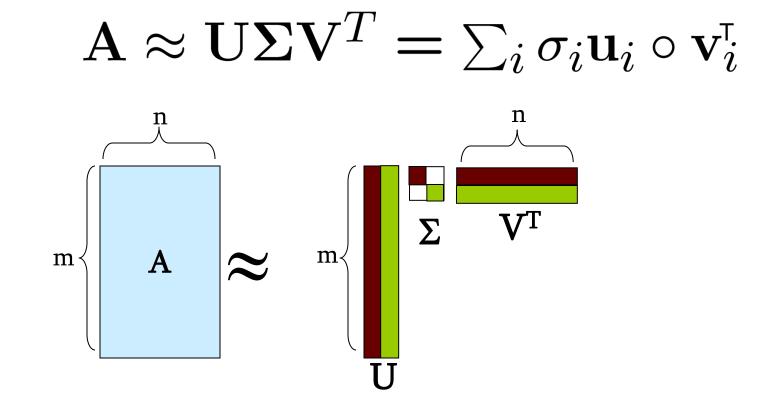
Special conditions:

U and V are column-orthonormal (so V^T has orthonormal rows) Σ is a diagonal matrix

Facts About SVD

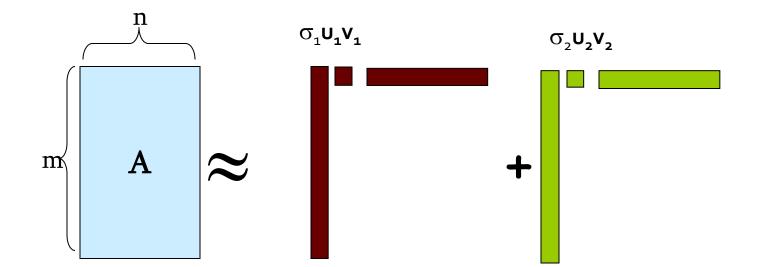
- The values of Σ along the diagonal are called the singular values.
- It is always possible to decompose M exactly, if r is the rank of M.
- But usually, we want to make r much smaller than the rank, and we do so by setting to 0 the smallest singular values.
 - Which has the effect of making the corresponding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

Linkage Among Components of U, V, Σ



Each Singular Value Affects One Column of U and V

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

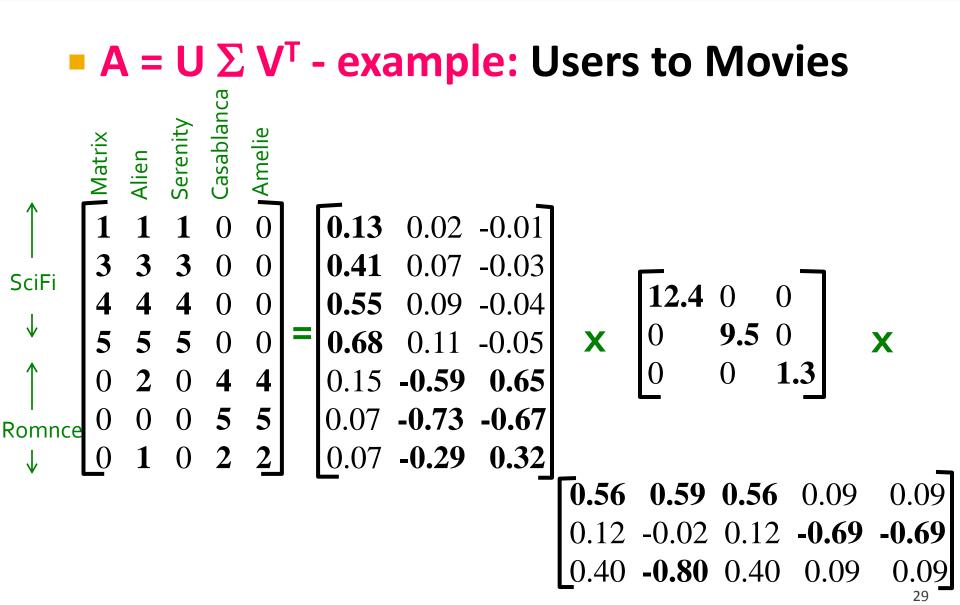


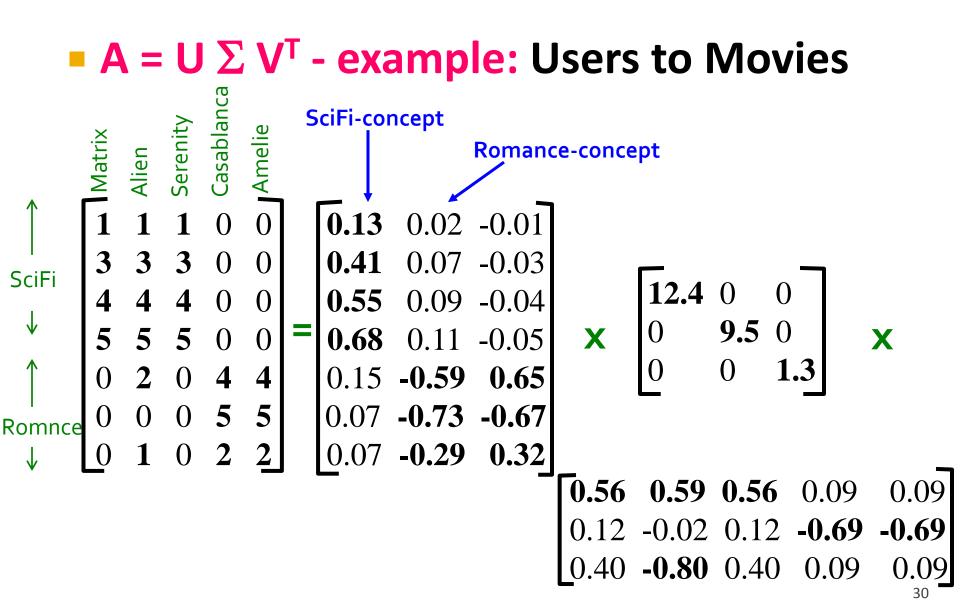
If we set $\sigma_2 = 0$, then the green columns may as well not exist.

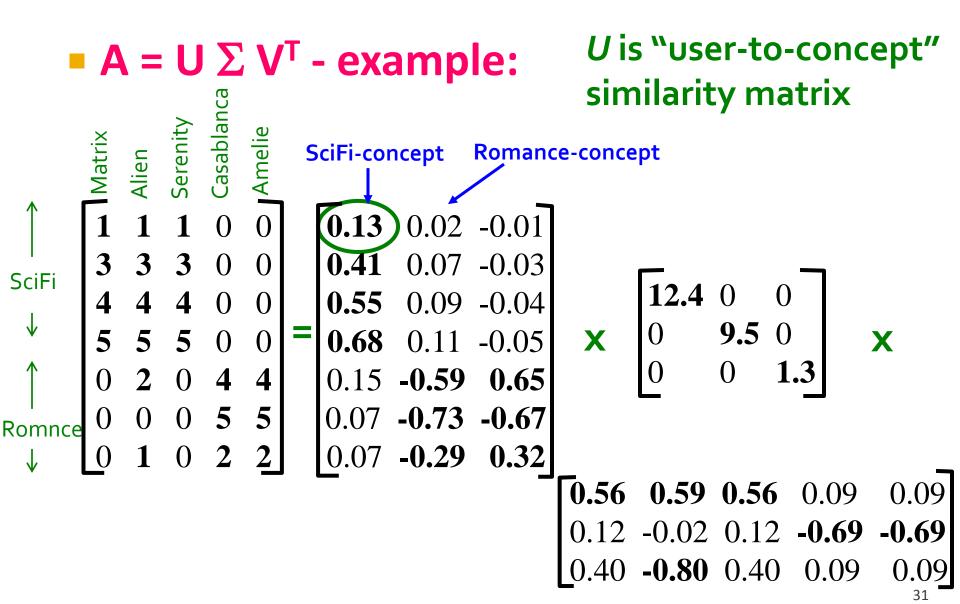
 $\sigma_i \dots$ scalar $u_i \dots$ vector $v_i \dots$ vector

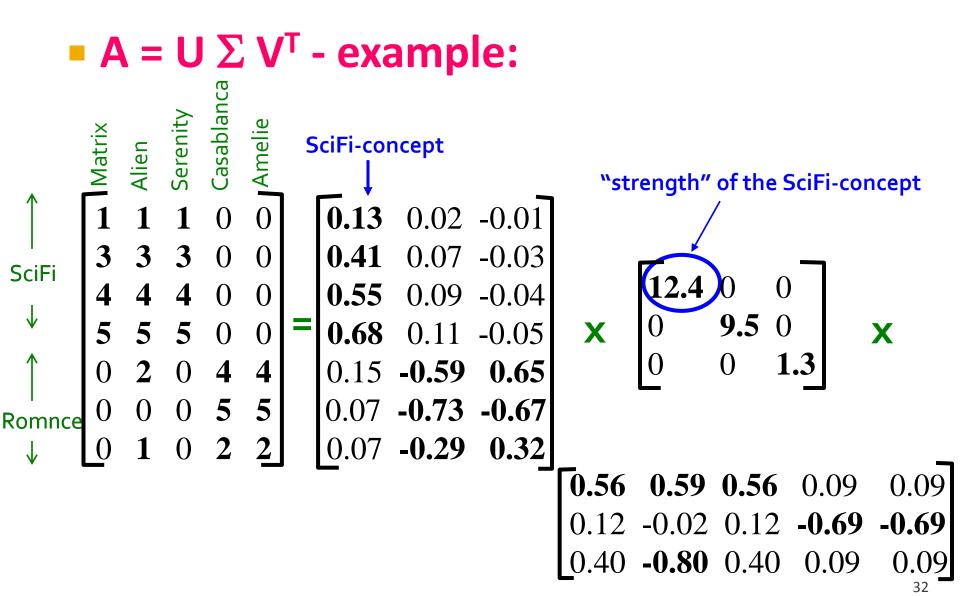
Jure's Example Decomposition

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.





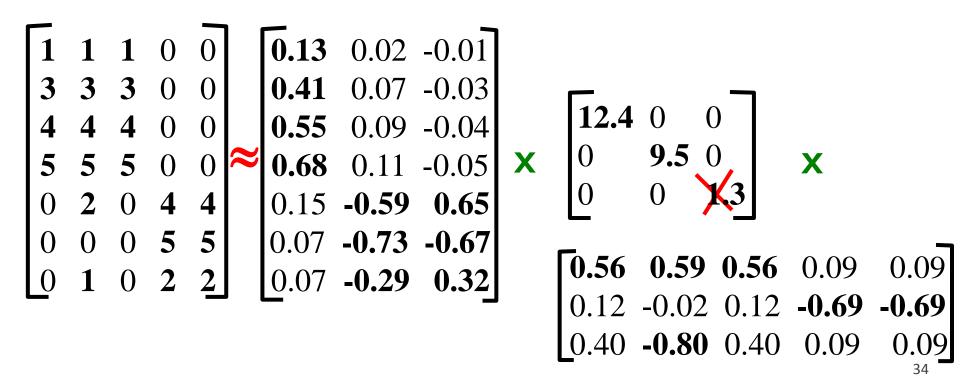




```
• A = U \Sigma V^T - example:
                Casablanca
                                              V is "movie-to-concept"
             Serenity
                    Amelie
      Matrix
                                             similarity matrix
                        SciFi-concept
         Alien
             1
                    0
                          0.13
                                0.02 -0.01
                0
             3
                                      -0.03
                 0
                    0
                          0.41
                                 0.07
SciFi
                                                    12.4
                                                          0
                          0.55
                                0.09
                                      -0.04
                    \mathbf{0}
 \downarrow
                                                    0 9.5 0
       5
             5 0
                                               Χ
                          Q.68
                                 0.11
                                      -0.05
                                                                       Χ
                    0
                                                          0
                                                               1.3
                                                    0
                4
            0
                    4
                                       0.65
       0
                          0.15 -0.59
                5
                   5
          0 0
                          0.07
                                -0.73 -0.67
       0
Romnce
                                       0.32
                    2
                          0.07
                                -0.29
                 2
                                           →[0.56)
                                                    0.59 0.56
                                                                0.09
                                                                        0.09
                                                    -0.02 0.12 -0.69 -0.69
                          SciFi-concept
                                                    -0.80 0.40
                                                                0.09
```

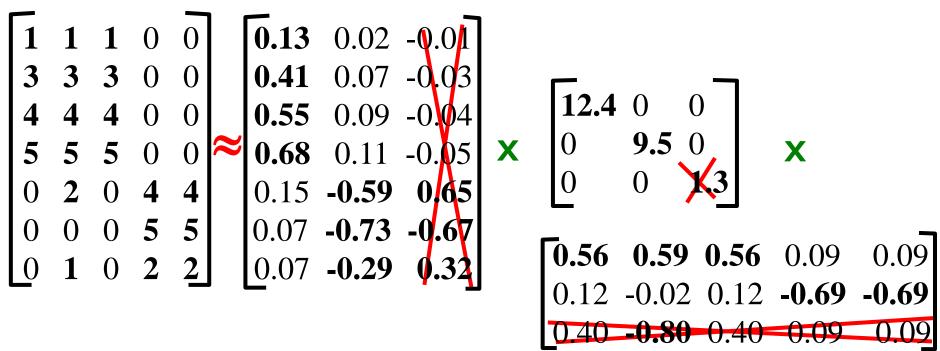
Lowering the Dimension

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



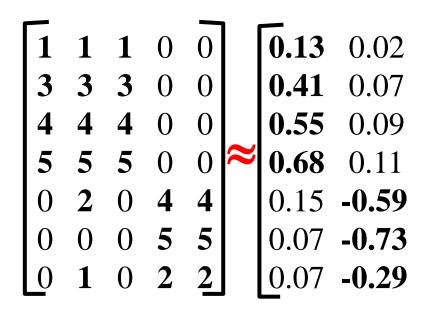
Lowering the Dimension

- Q: How exactly is dimensionality reduction done?
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Lowering the Dimension

- Q: How exactly is dimensionality reduction done?
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x $\begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix}$ **x** $\begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \end{bmatrix}$

Lowering the Dimension

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

$\boxed{1}$	1	1	0	0		0.92	0.95	0.92	0.01	0.01
3	3	3	0	0		2.91	3.01	2.91	-0.01	-0.01
4			-	-		3.90	4.04	3.90	0.01	0.01
5	5	5	0	0	*	4.82	5.00	4.82	0.03	0.03
0	2	0	4	4		0.70	0.53	0.70	4.11	4.11
0	0	0	5	5		-0.69	1.34	-0.69	4.78	4.78
0	1	0	2	2		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.



- 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_{ii} = m_{ii} for all i and j.
- Start with any "guess eigenvector" x₀.
- Construct $\mathbf{x}_{k+1} = M\mathbf{x}_k / ||M\mathbf{x}_k||$ for k = 0, 1,...
 - I ||...|| denotes the Frobenius norm.
- Stop when consecutive x_k's show little change.

Example: Iterative Eigenvector

$$M = \frac{1}{2} \frac{2}{3} \quad \mathbf{x}_{0} = \frac{1}{1}$$

$$\frac{M\mathbf{x}_{0}}{\|M\mathbf{x}_{0}\|} = \frac{3}{5} /\sqrt{34} = \frac{0.51}{0.86} = \mathbf{x}_{1}$$

$$\frac{M\mathbf{x}_{1}}{\|M\mathbf{x}_{1}\|} = \frac{2.23}{3.60} /\sqrt{17.93} = \frac{0.53}{0.85} = \mathbf{x}_{2}$$

Finding the Principal Eigenvalue

- Once you have the principal eigenvector **x**, you find its eigenvalue λ by $\lambda = \mathbf{x}^T \mathbf{M} \mathbf{x}$.
- In proof: we know $\mathbf{x}\lambda = \mathbf{M}\mathbf{x}$ if λ 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 $\lambda =$

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

Finding More Eigenpairs

- Eliminate the portion of the matrix M that can be generated by the first eigenpair, λ 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 $M = U\Sigma V^{T}$.
- $M^{\mathsf{T}} = (U\Sigma V^{\mathsf{T}})^{\mathsf{T}} = (V^{\mathsf{T}})^{\mathsf{T}}\Sigma^{\mathsf{T}}U^{\mathsf{T}} = V\Sigma U^{\mathsf{T}}.$
 - 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^TU is an identity matrix.
 - Also note that Σ^2 is a diagonal matrix whose i-th element is the square of the i-th element of Σ .
- $\mathsf{M}^{\mathsf{T}}\mathsf{M}\mathsf{V} = \mathsf{V}\Sigma^{2}\mathsf{V}^{\mathsf{T}}\mathsf{V} = \mathsf{V}\Sigma^{2}.$
 - Why? V is also orthonormal.

Computing the SVD –(2)

- Starting with (M^TM)V = VΣ², note that therefore the i-th column of V is an eigenvector of M^TM, and its eigenvalue is the i-th element of Σ².
- Thus, we can find V and Σ by finding the eigenpairs for M^TM.
 - Once we have the eigenvalues in Σ², we can find the singular values by taking the square root of these eigenvalues.
- Symmetric argument, starting with MM^T, gives us U.

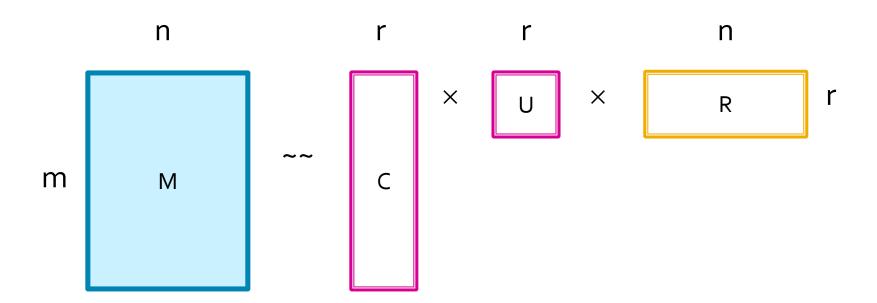
CUR Decomposition

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

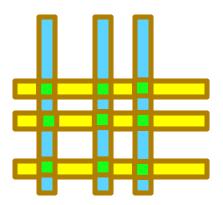


r chosen as you like.

- 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 Σ^+ , the *Moore-Penrose inverse* of Σ .
 - Definition, next slide.
- $U = Y(\Sigma^+)^2 X^T$.



Moore-Penrose Inverse

- If Σ is a diagonal matrix, its More-Penrose inverse is another diagonal matrix whose i-th entry is:
 - 1/σ if σ is not 0.
 - 0 if σ 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.