Randomized SVD

CSCI 4360/6360 Data Science II

Singular Value Decomposition (SVD)

• Given a (any!) matrix M, which is n x m, it can be represented as

$$M = U\Sigma V^T$$

- *U*: *n x n*, unitary matrix (orthogonal)
- Σ : $n \times m$, diagonal matrix of singular values
- V^T : $m \times m$, unitary matrix (orthogonal)

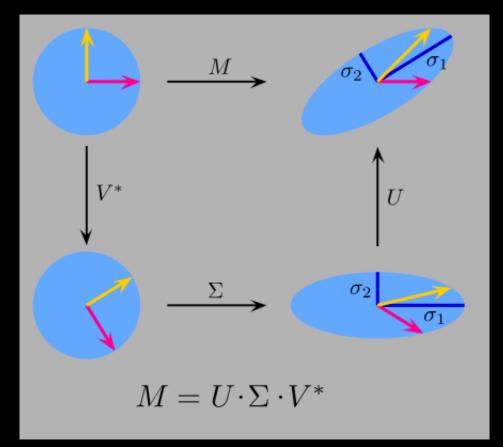
SVD

$$\mathbf{A}_{[m \times n]} = \mathbf{U}_{[m \times r]} \Sigma_{[r \times r]} (\mathbf{V}_{[n \times r]})^{T}$$

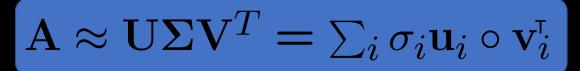
- A: Input data matrix
 - m x n matrix (e.g., m documents, n terms)
- U: Left singular vectors
 - *m* x *r* matrix (*m* documents, *r* concepts)
- Σ: Singular values
 - r x r diagonal matrix (strength of each 'concept')
 (r: rank of the matrix A)
- V: Right singular vectors
 - *n* x *r* matrix (*n* terms,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

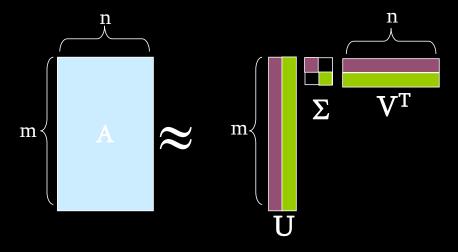
Singular Value Decomposition (SVD)

- Columns of *U* and *V* are orthonormal bases
- Singular values are the "strength" of each singular vector

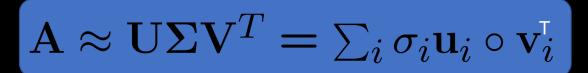


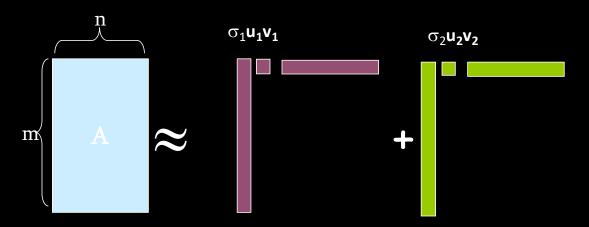
SVD





SVD





σ_i ... scalar

u_i ... vector

v_i ... vector

SVD - Properties

It is **always** possible to decompose a real matrix \boldsymbol{A} into $\boldsymbol{A} = \boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{V}^{\mathsf{T}}$, where

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

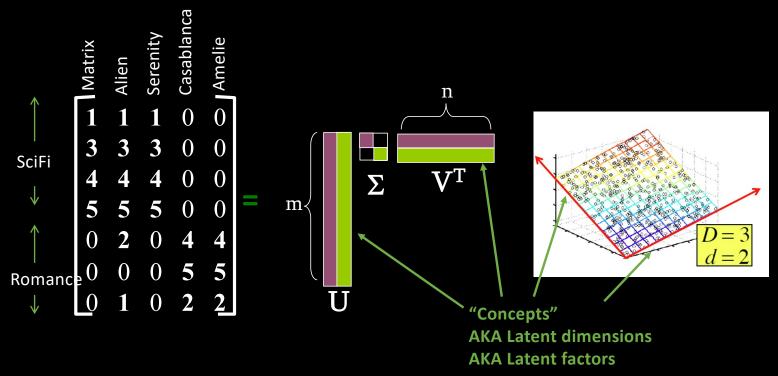
Nice proof of uniqueness: http://www.mpi-inf.mpg.de/~bast/ir-seminar-ws04/lecture2.pdf

Why randomize SVD?

• Runtime

- We're good at generating [pseudo-]random numbers
- Can easily parallelize / distribute matrix algebra
- SVD, like PCA, runs $O(n^3)$, making anything beyond ~10³ infeasible

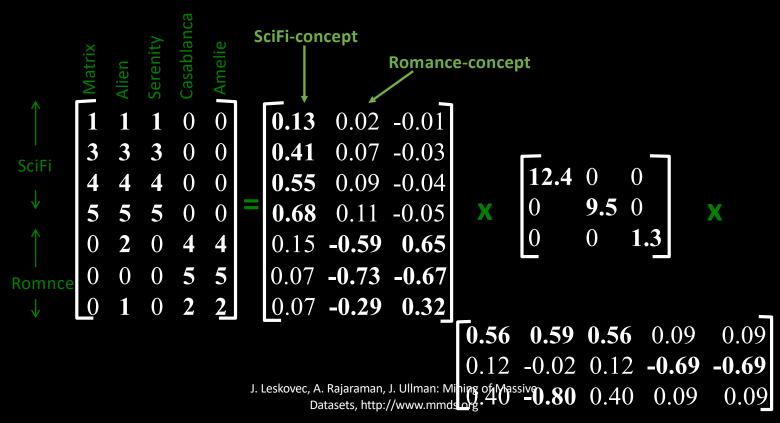
• $A = U \sum V^T$ - example: Users to Movies



J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, http://www.mmds.org

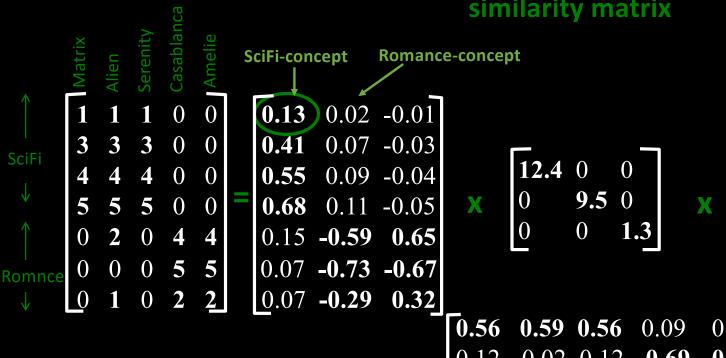
• $A = U \Sigma V^T$ - example: Users to Movies

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• A = U Σ V^T - example:

U is "user-to-concept" similarity matrix



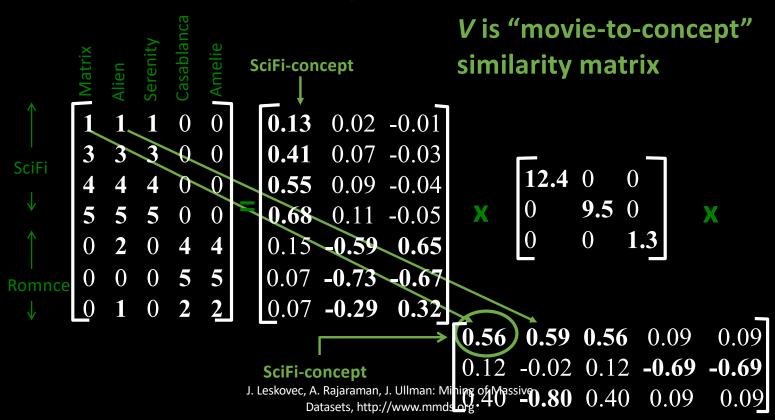
J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive 0.80 0.40 0.09

• $A = U \Sigma V^T$ - example:



J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive 0.80 0.40 0.09

• A = U Σ V^T - example:



'movies', 'users' and 'concepts':

- *U*: user-to-concept similarity matrix
- **V**: movie-to-concept similarity matrix
- Σ: its diagonal elements:
 'strength' of each concept

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

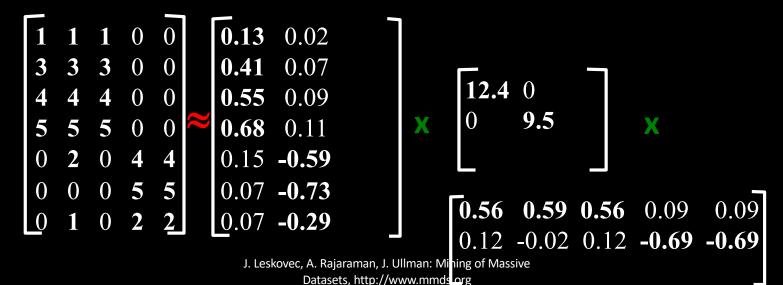
$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 &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

$$\begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \end{bmatrix}$$
I. Leskovec, A. Rajaraman, J. Ullman: Mingr of Massive and Section 1.1 and the property of the section 1.2 and the property of the section 1.2 and the property of the section 1.3 and the property of the section 1.3 and the property of the section 1.3 and the property of the property of the section 1.3 and the property of the proper

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More details

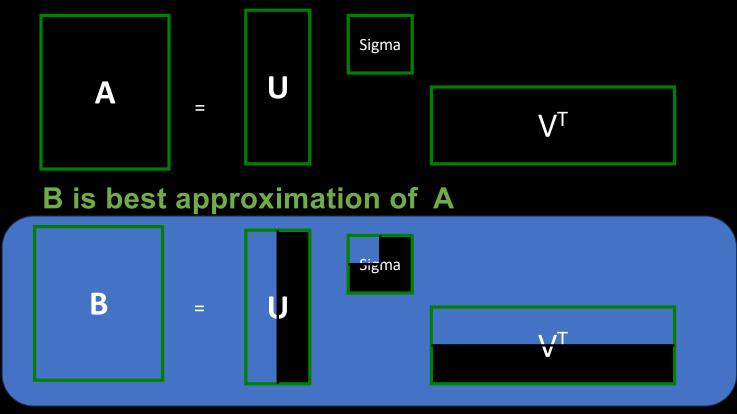
- Q: How exactly is dim. reduction done?
- A: Set smallest singular values to zero

$$\|\mathbf{A} - \mathbf{B}\|_{\mathrm{F}} = \sqrt{\Sigma_{ij} (\mathbf{A}_{ij} - \mathbf{B}_{ij})^2}$$
 is "small"

Frobenius norm:

$$\|\mathbf{M}\|_{\mathbf{F}} = \sqrt{\sum_{ij} \mathbf{M}_{ij}}^2$$

SVD – Best Low Rank Approx.



Relationship to PCA

- SVD can be applied to *any* matrix; PCA only works on symmetric covariance matrices
- However, there is a relationship

$$\begin{split} M^T M &= V \Sigma^T U^T U \Sigma V^T = V (\Sigma^T \Sigma) V^T \\ M M^T &= U \Sigma V^T V \Sigma^T U^T = U (\Sigma \Sigma^T) U^T \end{split}$$

- Columns of V are eigenvectors of M^TM
- Columns of U are eigenvectors of MM^T
- Singular values are square roots of eigenvalues of M^TM or MM^T

SVD: Drawbacks

+Optimal low-rank approximation

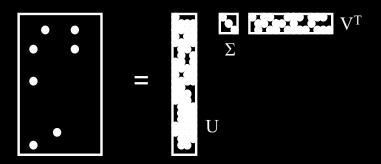
in terms of Frobenius norm

Interpretability problem:

 A singular vector specifies a linear combination of all input columns or rows

-Lack of sparsity:

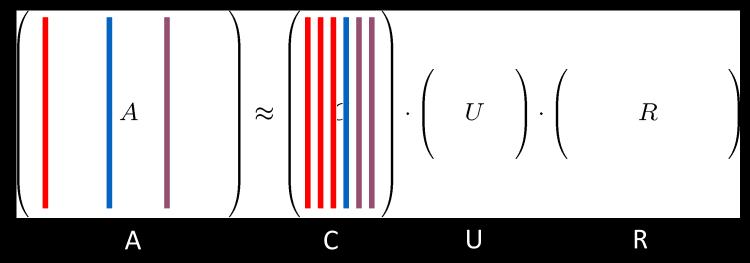
• Singular vectors are dense!



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·U·R||_F small
- "Constraints" on C and R:

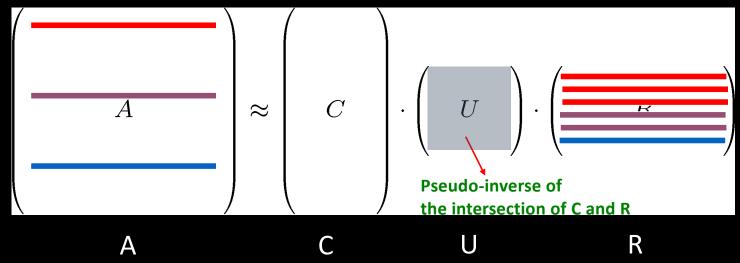


J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, http://www.mmds.org

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CUR: How it Works

Note this is a randomized algorithm; the same column can be sampled more than once

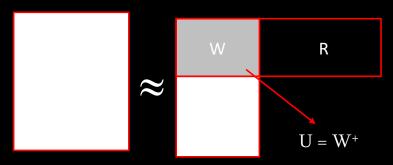
• Sampling columns (similarly for rows):

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

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

Computing U

- Let W be the "intersection" of sampled columns C and rows R
 - Let SVD of W = X Z Y^T
- Then: $U = W^+ = Y Z^+ X^T$
 - Z⁺: reciprocals of non-zero singular values: Z⁺_{ii} =1/ Z_{ii}
 - W⁺ is the "pseudoinverse"



Why pseudoinverse works?

W = X Z Y then W⁻¹ = X⁻¹ Z⁻¹ Y⁻¹
Due to orthonomality
X⁻¹=X^T and Y⁻¹=Y^T
Since Z is diagonal Z⁻¹ = $1/Z_{ii}$ Thus, if **W** is nonsingular,

Thus, if W is nonsingular, pseudoinverse is the true inverse

CUR: Pros & Cons

+ Easy interpretation

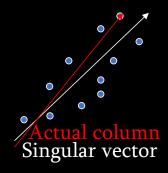
 Since the basis vectors are actual columns and rows

+Sparse basis

 Since the basis vectors are actual columns and rows

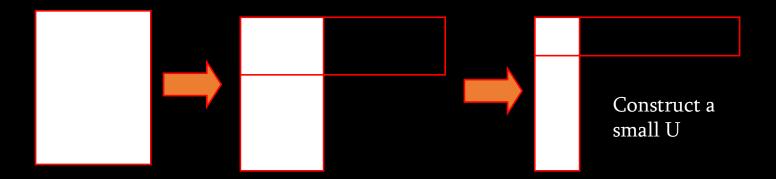
Duplicate columns and rows

Columns of large norms will be sampled many times

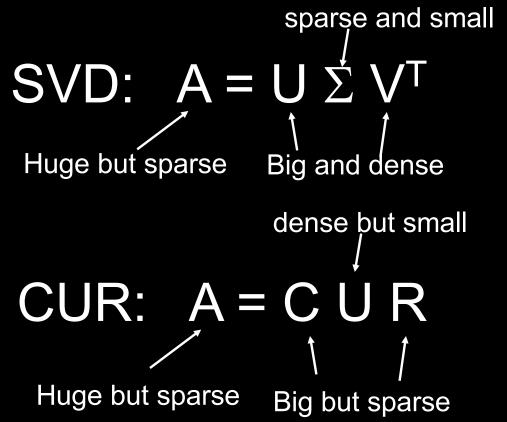


Solution

- If we want to get rid of the duplicates:
 - Throw them away
 - Scale (multiply) the columns/rows by the square root of the number of duplicates



SVD vs. CUR



J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, http://www.mmds.org

Stochastic SVD (SSVD)

- Uses random projections to find close approximation to SVD
- Combination of probabilistic strategies to maximize convergence likelihood
- Easily scalable to *massive* linear systems

Basic goal

- Matrix A
 - Find a low-rank approximation of A
 - Basic dimensionality reduction





Approximating range of A

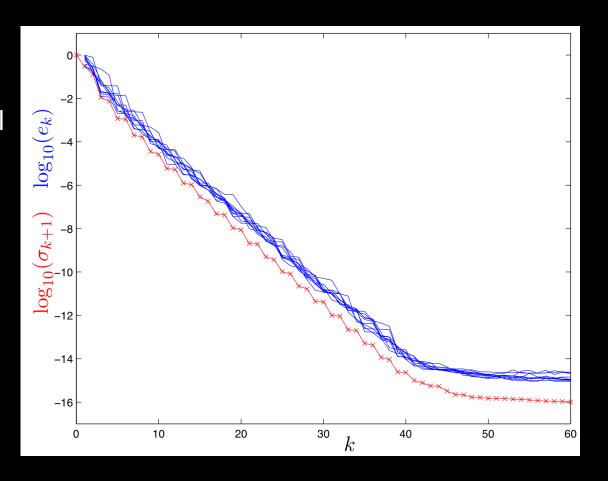
- INPUT: *A*, *k*, *p*
- OUTPUT: Q
- 1. Draw Gaussian n x k test matrix Ω
- 2. Form product $Y = A\Omega$
- 3. Orthogonalize columns of $Y \rightarrow Q$

Approximating SVD of A

- INPUT: Q
- OUTPUT: Singular vectors *U*
- 1. Form k x n matrix $B = Q^TA$
- 2. Compute SVD of B = $\hat{U}\Sigma V^T$
- 3. Compute singular vectors $U = Q\hat{U}$

Empirical Results

- 1000x1000 matrix
- Several runs of empirical results (blue) to theoretical lower bound (red)
- Error seems to be systemic



Power iterations

• Affects decay of eigenvalues / singular values



$$\mathsf{Y} = (\mathsf{A}\,\mathsf{A}^*)^q\,\mathsf{A}\,\mathsf{\Omega}$$

Power iterations

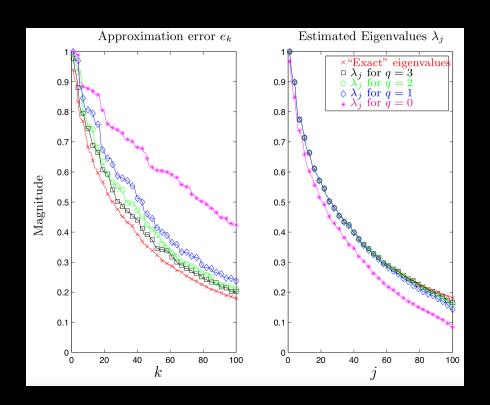
$$\mathbb{E}\|\mathsf{A} - \mathsf{Q}\mathsf{Q}^{\mathsf{T}}\mathsf{A}\|_{2} \le \left(1 + \sqrt{\frac{k}{p-1}}\right)\sigma_{k+1} + \frac{e\sqrt{k+p}}{p} \cdot \left(\sum_{j>k}\sigma_{j}^{2}\right)^{1/2}$$

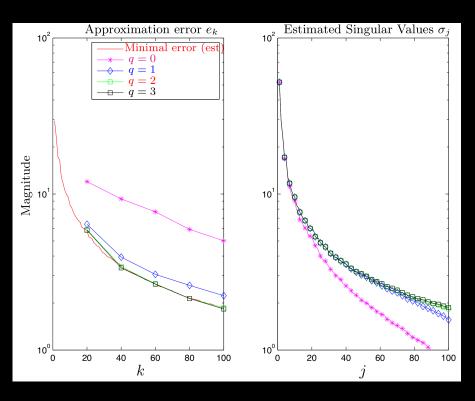
$$\le \left[1 + \frac{4\sqrt{k+p}}{p-1} \cdot \sqrt{\min\{m,n\}}\right]\sigma_{k+1}$$

$$= C \cdot \sigma_{k+1}.$$

Upshot: after only a single power iteration, the error is proportional to the *next* [uncomputed] singular value (times a constant *C*).

Empirical Results





Why does this work?

• Three primary reasons:

1. Johnson-Lindenstrauss Lemma

• Low-dimensional embeddings preserve pairwise distances

$$(1-arepsilon)\|u-v\|^2 \leq \|f(u)-f(v)\|^2 \leq (1+arepsilon)\|u-v\|^2$$

2. Concentration of measure

 Geometric interpretation of classical idea: regular functions of independent random variables rarely deviate far from their means

3. Preconditioning

- Condition number: how much change in output is produced from change in input (relation to #1)
- Q matrix lowers condition number while preserving overall system

$$\kappa = rac{|\lambda_{ ext{max}}|}{|\lambda_{ ext{min}}|}$$

Summary

- Relationship of SVD and PCA
 - PCA: eigenvectors and eigenvalues of the covariance matrix (or kernel matrix, for Kernel PCA)
 - SVD: Low-rank approximation for *any* matrix

• CUR

- Randomly sample columns of data matrix A to use as basis
- Interpretable and sparse, but potentially oversample high-magnitude columns

SVD via SGD

- Reframe SVD as a matrix completion problem
- Use SGD in alternating least-squares to infer "missing" components

SSVD

- Full-blown Johnson-Lindenstrauss exploitation
- Use random projections to approximate SVD to high accuracy
- Requires some empirical tweaks (oversampling, power iterations)

References

- "Randomized methods for computing low-rank approximations of matrices", https://amath.colorado.edu/faculty/martinss/Pubs/2012_halko_dissertation.pdf
- "CUR decomposition for compression and compressed sensing of large-scale traffic data", https://dspace.mit.edu/openaccess-disseminate/1721.1/86879



Large-Scale Matrix Factorization with Distributed Stochastic Gradient Descent

Rainer Gemulla

talk pilfered from →



Peter J. Haas Yannis Sismanis Erik Nijkamp







Collaborative Filtering

- Problem
 - Set of users
 - Set of items (movies, books, jokes, products, stories, ...)
 - ► Feedback (ratings, purchase, click-through, tags, ...)
- Predict additional items a user may like
 - ▶ Assumption: Similar feedback ⇒ Similar taste
- Example

$$Avatar \quad The \ Matrix \quad Up$$

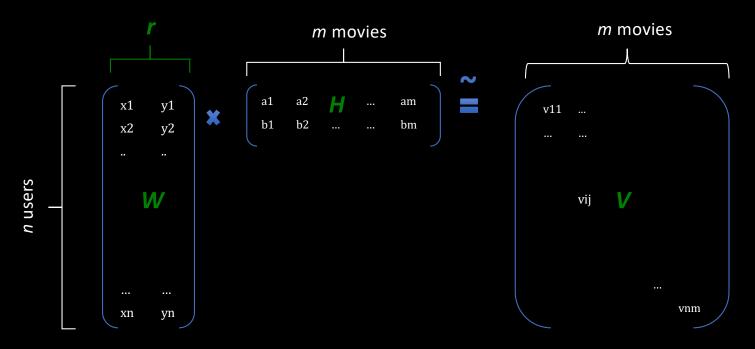
$$Alice \quad ? \quad 4 \quad 2$$

$$Bob \quad 2 \quad ?$$

$$Charlie \quad 5 \quad ? \quad 3$$

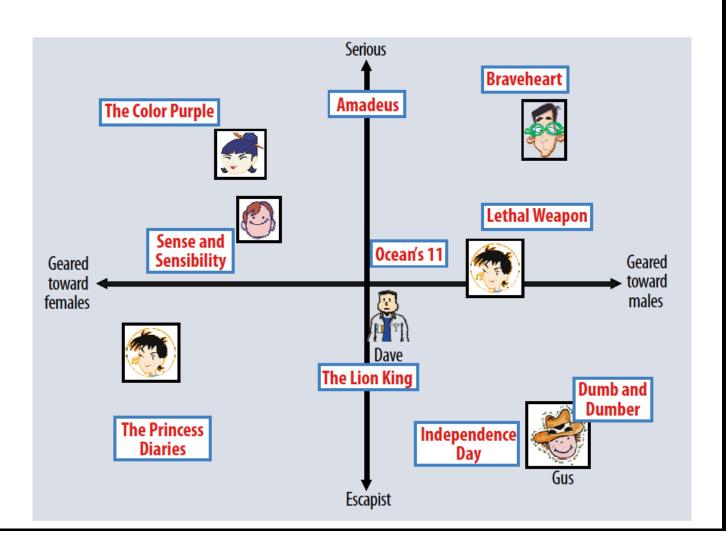
► Netflix competition: 500k users, 20k movies, 100M movie ratings, 3M question marks

Recovering latent factors in a matrix



V[i,j] = user i's rating of movie j

Semantic Factors (Koren et al., 2009)



Latent Factor Models

▶ Discover latent factors (r = 1)

	A vatar (2.24)	The Matrix (1.92)	Up (1.18)
Alice (1.98)		4 (3.8)	2 (2.3)
Bob (1.21)	3 (2.7)	2 (2.3)	
Charlie (2.30)	5 (5.2)		3 (2.7)

► Minimum loss

$$\min_{\mathbf{W},\mathbf{H}} \sum_{(i,j) \in Z} (\mathbf{V}_{ij} - [\mathbf{W}\mathbf{H}]_{ij})^2$$

Latent Factor Models

▶ Discover latent factors (r = 1)

	Avatar (2.24)	The Matrix (1.92)	Up (1.18)
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Bob (1.21)	3 (2.7)	2 (2.3)	? (1.4)
Charlie (2.30)	5 (5.2)	? (4.4)	3 (2.7)

► Minimum loss

$$\min_{\mathbf{W}, \mathbf{H}, \mathbf{u}, \mathbf{m}} \sum_{(i,j) \in Z} (\mathbf{V}_{ij} - \mu - \mathbf{u}_i - \mathbf{m}_j - [\mathbf{W}\mathbf{H}]_{ij})^2 + \lambda (\|\mathbf{W}\| + \|\mathbf{H}\| + \|\mathbf{u}\| + \|\mathbf{m}\|)$$

► Bias, regularization

Matrix factorization as SGD

require that the loss can be written as

$$L = \sum_{(i,j) \in Z} l(oldsymbol{V}_{ij}, oldsymbol{W}_{i*}, oldsymbol{H}_{*j})$$

Algorithm 1 SGD for Matrix Factorization

Require: A training set Z, initial values W_0 and H_0 while not converged do {step}

Select a training point $(i, j) \in Z$ uniformly at random.

$$\boldsymbol{W}'_{i*} \leftarrow \boldsymbol{W}_{i*} - \epsilon_n N \frac{\partial}{\partial \boldsymbol{W}_{i*}} l(\boldsymbol{V}_{ij}, \boldsymbol{W}_{i*}, \boldsymbol{H}_{*j})$$

$$\boldsymbol{H}_{*j} \leftarrow \boldsymbol{H}_{*j} - \epsilon_n N \frac{\partial}{\partial \boldsymbol{H}_{*j}} l(\boldsymbol{V}_{ij}, \boldsymbol{W}_{i*}, \boldsymbol{H}_{*j})$$

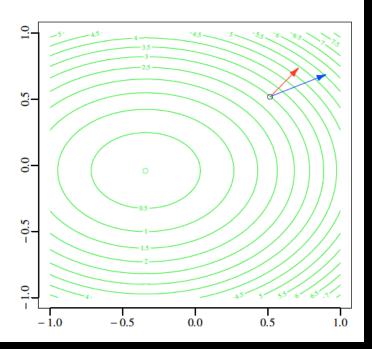
$$oldsymbol{W}_{i*} \leftarrow oldsymbol{W}_{i*}'$$

end while

why does this work?

Stochastic Gradient Descent

- ▶ Find minimum θ^* of function L
- ▶ Pick a starting point θ_0
- ▶ Approximate gradient $\hat{L}'(\theta_0)$

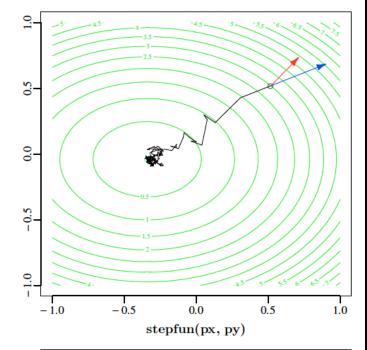


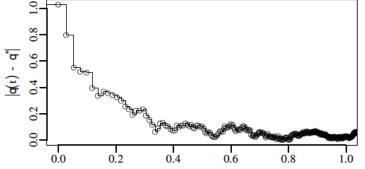
Stochastic Gradient Descent

- ▶ Find minimum θ^* of function L
- ▶ Pick a starting point θ_0
- Approximate gradient $\hat{L}'(\theta_0)$
- ▶ Jump "approximately" downhill
- ► Stochastic difference equation

$$\theta_{n+1} = \theta_n - \epsilon_n \hat{\mathcal{L}}'(\theta_n)$$

 Under certain conditions, asymptotically approximates (continuous) gradient descent





Why does this work?

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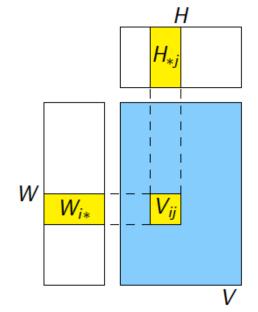
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Key Claim

require that the loss can be written as

$$L = \sum_{(i,j) \in Z} l(oldsymbol{V}_{ij}, oldsymbol{W}_{i*}, oldsymbol{H}_{*j})$$



$$\frac{\partial}{\partial \boldsymbol{W}_{i'k}}L_{ij}(\boldsymbol{W},\boldsymbol{H}) = \begin{cases} 0 & \text{if } i \neq i' \\ \frac{\partial}{\partial \boldsymbol{W}_{ik}}l(\boldsymbol{V}_{ij},\boldsymbol{W}_{i*},\boldsymbol{H}_{*j}) & \text{otherwise} \end{cases}$$

$$\frac{\partial}{\partial \boldsymbol{H}_{kj'}}L_{ij}(\boldsymbol{W},\boldsymbol{H}) = \begin{cases} 0 & \text{if } j \neq j' \\ \frac{\partial}{\partial \boldsymbol{H}_{kj}}l(\boldsymbol{V}_{ij},\boldsymbol{W}_{i*},\boldsymbol{H}_{*j}) & \text{otherwise} \end{cases}$$

Checking the claim

$$\frac{\partial}{\partial \boldsymbol{W}_{i*}}L(\boldsymbol{W},\boldsymbol{H}) = \frac{\partial}{\partial \boldsymbol{W}_{i*}} \sum_{(i',j) \in Z} L_{i'j}(\boldsymbol{W}_{i'*},\boldsymbol{H}_{*j}) = \sum_{j \in Z_{i*}} \frac{\partial}{\partial \boldsymbol{W}_{i*}} L_{ij}(\boldsymbol{W}_{i*},\boldsymbol{H}_{*j}),$$

where
$$Z_{i*} = \{j \colon (i,j) \in Z\}.$$

$$rac{\partial}{\partial oldsymbol{H}_{*j}}L(oldsymbol{W},oldsymbol{H}) = \sum_{i \in Z_{*j}} rac{\partial}{\partial oldsymbol{W}_{*j}} L_{ij}(oldsymbol{W}_{i*},oldsymbol{H}_{*j}),$$

where
$$Z_{*j} = \{ i : (i, j) \in Z \}.$$

Think for SGD for logistic regression

- LR loss = compare y and \hat{y} = dot(w,x)
- similar but now update w (user weights) and x (movie weight)

Stochastic Gradient Descent on Netflix Data

