CSC 411: Introduction to Machine Learning

CSC 411 Lecture 18: Matrix Factorizations

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- Today we consider another generalization, matrix factorizations
    - view PCA as a matrix factorization problem
    - extend to matrix completion, where the data matrix is only partially observed
    - extend to other matrix factorization models, which place different kinds of structure on the factors

PCA as Matrix Factorization

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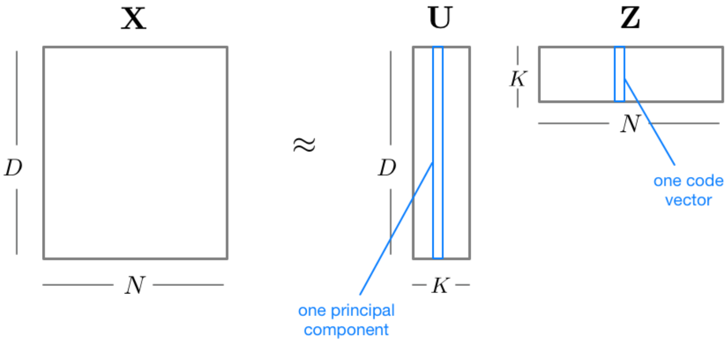
  - We transpose our usual convention for data matrices (for some parts of this lecture).
- Writing the squared error in matrix form

$$\sum_{i=1}^{N} \|\mathbf{x}^{(i)} - \mathbf{U}\mathbf{z}^{(i)}\|^2 = \|\mathbf{X} - \mathbf{UZ}\|_F^2$$

- Recall that the **Frobenius norm** is defined as $\|\mathbf{A}\|_F^2 = \sum_{i,j} a_{ij}^2$.

PCA as Matrix Factorization

- So PCA is approximating $\mathbf{X} \approx \mathbf{UZ}$.



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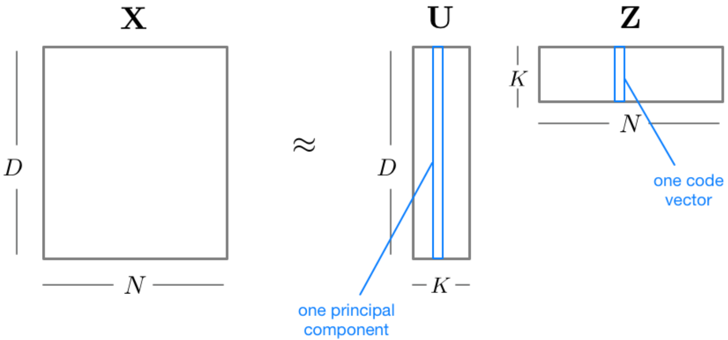

- Based on the sizes of the matrices, this is a rank-K approximation.
- Since $\mathbf{U}$ was chosen to minimize reconstruction error, this is the *optimal* rank-K approximation, in terms of $||\mathbf{X} - \mathbf{UZ}||_F^2$.

PCA vs. SVD (optional)

This has a close relationship to the **Singular Value Decomposition (SVD)** of $\mathbf{X}$. This is a factorization

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$$

Properties:

- $\mathbf{U}$, $\mathbf{\Sigma}$, and $\mathbf{V}^\top$ provide a real-valued matrix factorization of $\mathbf{X}$, an $m \times n$ matrix.
- $\mathbf{U}$ is a $m \times m$ matrix with orthonormal columns $\mathbf{U}^\top\mathbf{U} = I_m$, where I_m is the $m \times m$ identity matrix.
- $\mathbf{V}$ is an orthonormal $n \times n$ matrix, $\mathbf{V}^\top\mathbf{V} = I_n$.
- $\mathbf{\Sigma}$ is a $m \times n$ diagonal matrix, with non-negative singular values, $\sigma_1, \sigma_2, \ldots, \sigma_{\min\{m,n\}}$, on the diagonal, where the singular values are conventionally ordered from largest to smallest.

It's possible to show that the first n singular vectors correspond to the first n principal components; more precisely, $\mathbf{Z} = \mathbf{U}\mathbf{\Sigma}$

PCA vs. SVD (optional)

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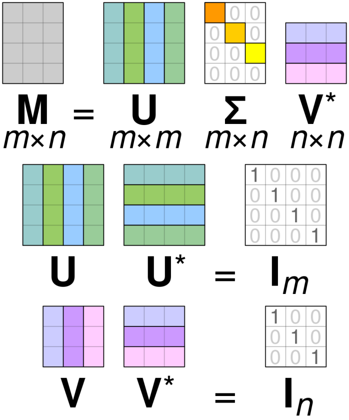

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  - 1) Consider when **X** is only partially observed.
    - A sparse 1000×1000 matrix with 50,000 observations (only 5% observed).
    - A rank 5 approximation requires only 10,000 parameters, so it's reasonable to fit this.
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    - Unfortunately, no closed form solution.
  - 2) Impose structure on the factors. We can get lots of interesting models this way.

Recommender systems: Why?

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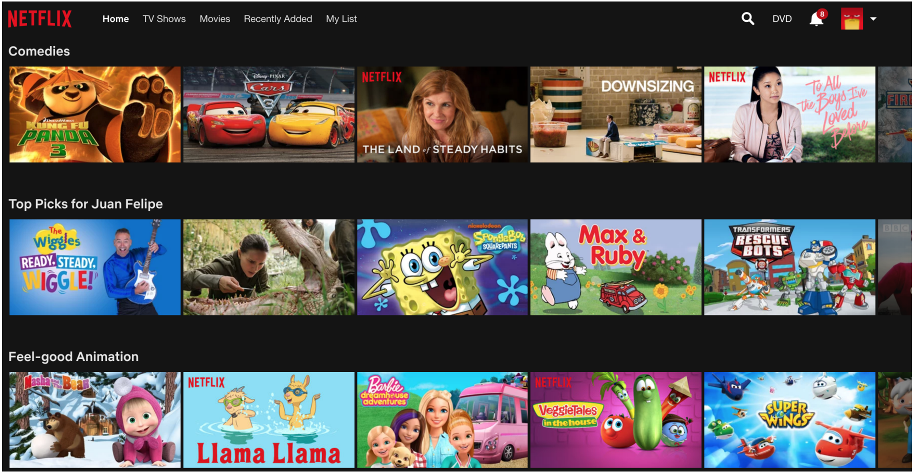
Recommender systems suggest items of interest and enjoyment to people based on their preferences

Some recommender systems in action



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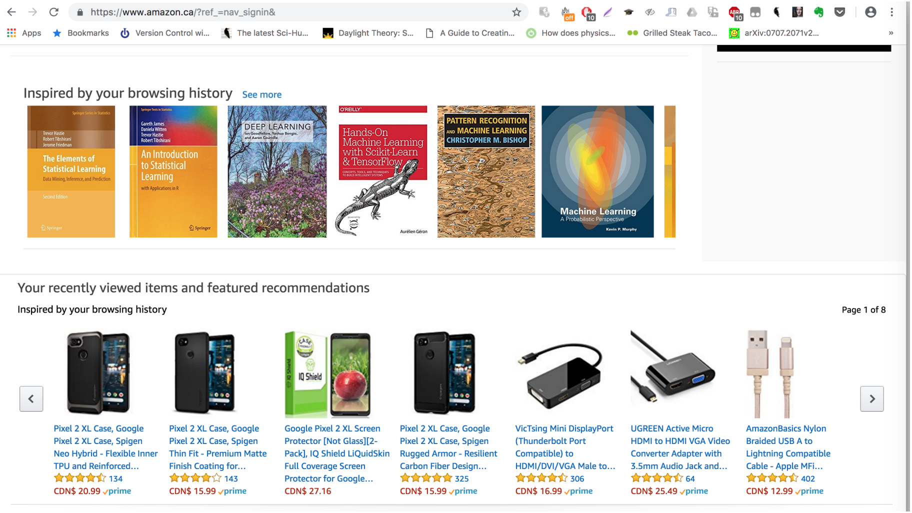

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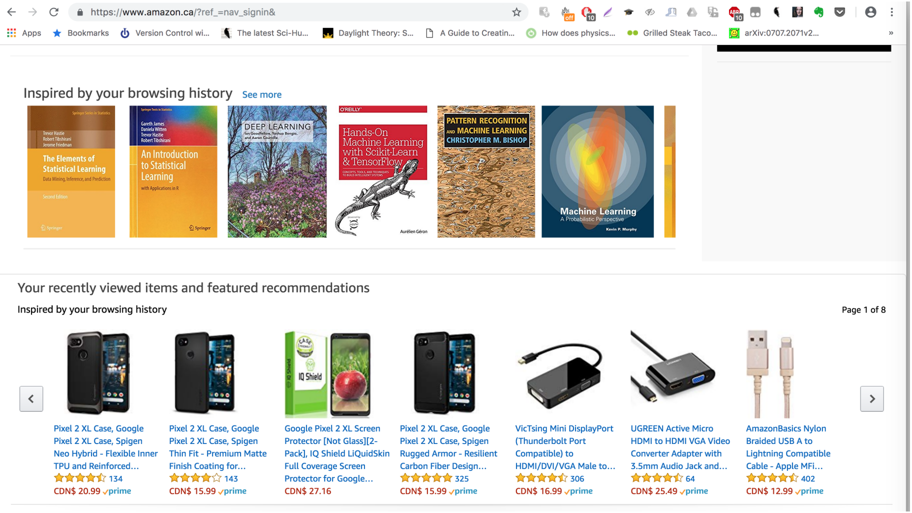

Ideally recommendations should combine global and session interests, look at your history if available, should adapt with time, be coherent and diverse, etc.

The Netflix problem

Movie recommendation: Users watch movies and rate them as good or bad.

User	Movie	Rating
	Thor	★ ☆ ☆ ☆ ☆
	Chained	★ ★ ☆ ☆ ☆
	Frozen	★ ★ ★ ☆ ☆
	Chained	★ ★ ★ ★ ☆
	Bambi	★ ★ ★ ★ ★
	Titanic	★ ★ ★ ☆ ☆
	Goodfellas	★ ★ ★ ★ ★
	Dumbo	★ ★ ★ ★ ★
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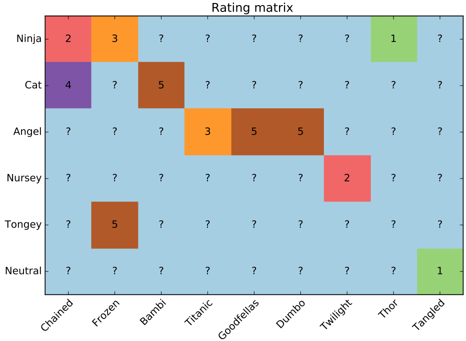
Because users only rate a few items, one would like to infer their preference for unrated items

Matrix completion problem

Matrix completion problem: Transform the table into a N users by M movies matrix $\mathbf{R}$



- **Data**: Users rate some movies. $\mathbf{R}_{\text{user,movie}}$. Very sparse
- **Task**: Finding missing data, e.g. for recommending new movies to users. Fill in the question marks
- **Algorithms**: Alternating Least Square method, Gradient Descent, Non-negative Matrix Factorization, low rank matrix Completion, etc.

Latent factor models

- In our current setting, **latent factor models** attempt to explain the ratings by characterizing both movies and users on a number of factors K inferred from the ratings patterns.
- That is, we seek a representation movies and users as vectors in $\mathbb{R}^K$
- For simplicity, we can associate these factors (i.e. the dimensions of the vectors) with idealized concepts like
  - comedy
  - drama
  - action
  - But also uninterpretable dimensions

Can we use the sparse ratings matrix $\mathbf{R}$ to find these latent factors automatically?

Alternating least squares

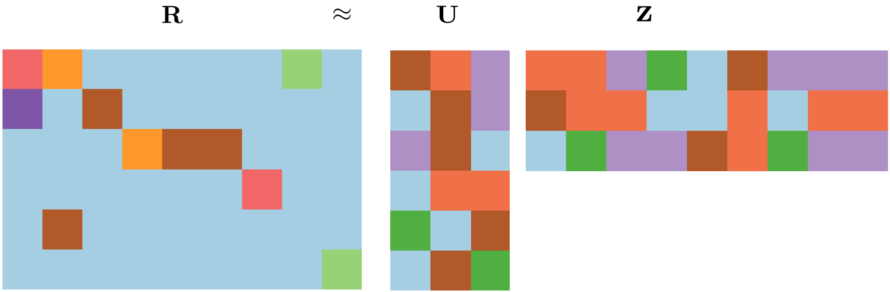
- Let the representation of user n in the K-dimensional space be $\mathbf{u}_n$ and the representation of movie m be $\mathbf{z}_m$
- Assume the rating user n gives to movie m is given by a dot product: $R_{nm} \approx \mathbf{u}_n^T \mathbf{z}_m$
- In matrix form, if:

$$\mathbf{U} = \begin{bmatrix} — & \mathbf{u}_1^\top & — \\ & \vdots & \\ — & \mathbf{u}_N^\top & — \end{bmatrix} \text{ and } \mathbf{Z} = \begin{bmatrix} | & & | \\ \mathbf{z}_1 & \ldots & \mathbf{z}_M \\ | & & | \end{bmatrix}$$

  then: $\mathbf{R} \approx \mathbf{UZ}$

- This is a matrix factorization problem!

Approach: Matrix factorization methods



Alternating least squares

- Let $O = \{(n, m) : \text{ entry } (n, m) \text{ of matrix } R \text{ is observed}\}$
- Using the squared error loss, a matrix factorization corresponds to solving

$$\min_{\mathbf{U},\mathbf{Z}} \frac{1}{2} \sum_{(n,m)\in O} \left(R_{nm} - \mathbf{u}_n^\top \mathbf{z}_m \right)^2$$

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Alternating Least Squares (ALS): fix **Z** and optimize **U**, followed by fix **U** and optimize **Z**, and so on until convergence.

Alternating least squares

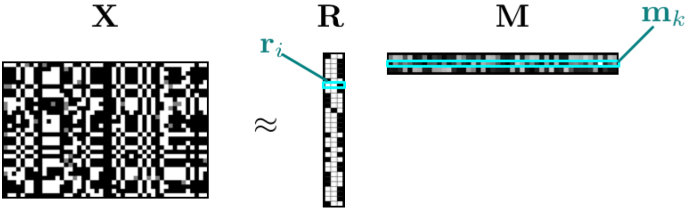
ALS for Matrix Completion algorithm

1. Initialize $\mathbf{U}$ and $\mathbf{Z}$ randomly
2. repeat
3. **for** $n = 1, .., N$ **do**
4. $\mathbf{u}_n = \left(\sum_{m:(n,m)\in O} \mathbf{z}_m \mathbf{z}_m^\top\right)^{-1} \sum_{m:(n,m)\in O} R_{nm} \mathbf{z}_m$
5. **for** $m = 1, .., M$ **do**
6. $\mathbf{z}_m = \left(\sum_{n:(n,m)\in O} \mathbf{u}_n \mathbf{u}_n^\top\right)^{-1} \sum_{n:(n,m)\in O} R_{nm} \mathbf{u}_n$
7. until convergence

See also the paper "Probabilistic Matrix Factorization" in the course readings.

K-Means

- It's possible to view K-means as a matrix factorization.
- Stack the indicator vectors $\mathbf{r}_i$ for assignments into a $N \times K$ matrix $\mathbf{R}$, and stack the cluster centers $\mathbf{m}_k$ into a matrix $K \times D$ matrix $\mathbf{M}$.
- "Reconstruction" of the data (replace each point with its cluster center) is given by $\mathbf{RM}$.



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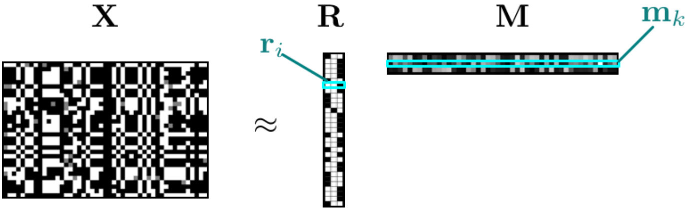
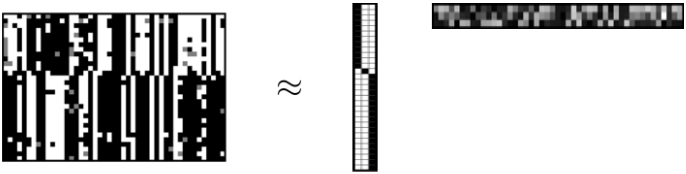


- K-means distortion function in matrix form:

$$\sum_{n=1}^{N} \sum_{k=1}^{K} r_k^{(n)} ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2 = ||\mathbf{X} - \mathbf{RM}||_F^2$$

K-Means

- Can sort by cluster for visualization:



Co-clustering (optional)

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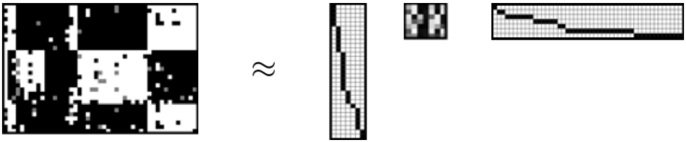
- **Co-clustering** clusters both the rows and columns of a data matrix, giving a block structure.
- We can represent this as the indicator matrix for rows, times the matrix of means for each block, times the indicator matrix for columns



Sparse Coding

- **Efficient coding hypothesis**: the structure of our visual system is adapted to represent the visual world in an efficient way
  - E.g., be able to represent sensory signals with only a small fraction of neurons having to fire (e.g. to save energy)

Sparse Coding

- **Efficient coding hypothesis**: the structure of our visual system is adapted to represent the visual world in an efficient way
  - E.g., be able to represent sensory signals with only a small fraction of neurons having to fire (e.g. to save energy)
- Olshausen and Field fit a **sparse coding** model to natural images to try to determine what's the most efficient representation.
- They didn't encode anything specific about the brain into their model, but the learned representations bore a striking resemblance to the representations in the primary visual cortex

Sparse Coding

- This algorithm works on small (e.g. 20×20) **image patches**, which we reshape into vectors (i.e. ignore the spatial structure)
- Suppose we have a dictionary of **basis functions** $\{\mathbf{a}_k\}_{k=1}^K$ which can be combined to model each patch

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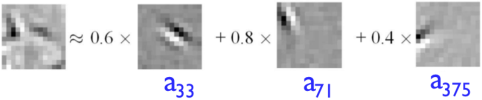
- Suppose we have a dictionary of **basis functions** $\{\mathbf{a}_k\}_{k=1}^K$ which can be combined to model each patch
- Each patch is approximated as a linear combination of a small number of basis functions:

$$x = \sum_{k=1}^{K} s_k \mathbf{a}_k = \mathbf{A}\mathbf{s}$$

- This is an **overcomplete** representation, in that typically $K > D$ (e.g. more basis functions than pixels)
- The requirement that $\mathbf{s}$ is sparse makes things interesting

Sparse Coding



$$\mathbf{x} \approx \sum_{k=1}^{K} s_k \mathbf{a}_k = \mathbf{A}\mathbf{s}$$

Since we use only a few basis functions, **s** is a sparse vector.

Sparse Coding

- We'd like choose **s** to accurately reconstruct the image, but encourage sparsity in **s**.
- What cost function should we use?

Sparse Coding

- We'd like choose $\mathbf{s}$ to accurately reconstruct the image, but encourage sparsity in $\mathbf{s}$.
- What cost function should we use?
- Inference in the sparse coding model:

$$\min_{\mathbf{s}} ||\mathbf{x} - \mathbf{A}\mathbf{s}||^2 + \beta||\mathbf{s}||_1$$

- Here, β is a hyperparameter that trades off reconstruction error vs. sparsity.
- There are efficient algorithms for minimizing this cost function (beyond the scope of this class)

Sparse Coding: Learning the Dictionary

- We can learn a dictionary by optimizing both $\mathbf{A}$ and $\{\mathbf{s}_i\}_{i=1}^N$ to trade off reconstruction error and sparsity

$$\min_{\{\mathbf{s}_i\},\mathbf{A}} \quad \sum_{i=1}^{N} \left\|\mathbf{x} - \mathbf{A}\mathbf{s}_i\right\|^2 + \beta\|\mathbf{s}_i\|_1$$

$$\text{subject to} \quad \|\mathbf{a}_k\|^2 \leq 1 \text{ for all } k$$

- Why is the normalization constraint on $\mathbf{a}_k$ needed?

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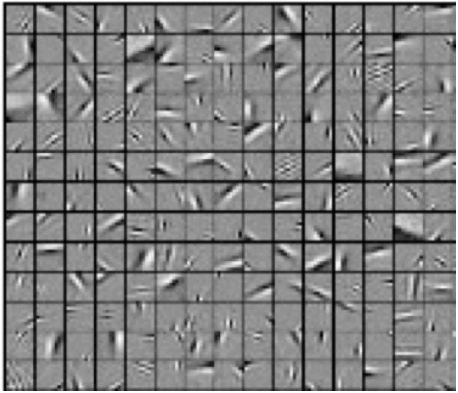
- Why is the normalization constraint on $\mathbf{a}_k$ needed?
- Reconstruction term can be written in matrix form as $\|\mathbf{X} - \mathbf{AS}\|_F^2$, where $\mathbf{S}$ combines the $\mathbf{s}_i$ as columns
- Can fit using an alternating minimization scheme over $\mathbf{A}$ and $\mathbf{S}$, just like K-means, EM, low-rank matrix completion, etc.

Sparse Coding: Learning the Dictionary

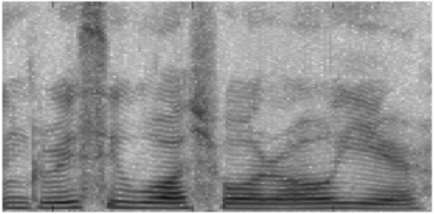
- Basis functions learned from natural images:



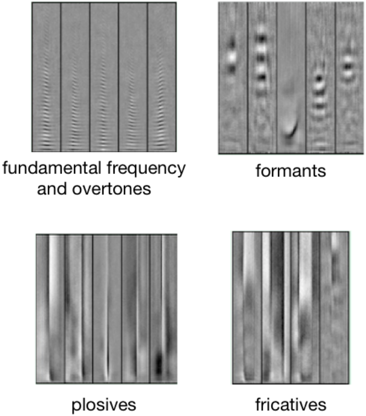
Sparse Coding: Learning the Dictionary

- The sparse components are oriented edges, similar to what a conv net learns
- But the learned dictionary is much more diverse than the first-layer conv net representations: tiles the space of location, frequency, and orientation in an efficient way
- Each basis function has similar response properties to cells in the primary visual cortex (the first stage of visual processing in the brain)

Applying sparse coding to speech signals:



example speech spectrogram (log amplitude)



(Grosse et al., 2007, "Shift-invariant sparse coding for audio classification")

Summary

- PCA can be viewed as fitting the optimal low-rank approximation to a data matrix.
- Matrix completion is the setting where the data matrix is only partially observed
  - Solve using ALS, an alternating procedure analogous to EM
- PCA, K-means, co-clustering, sparse coding, and lots of other interesting models can be viewed as matrix factorizations, with different kinds of structure imposed on the factors.