Matrix Factorization Methods

Irwin King, Baichuan Li, and Tom Chao Zhou
Joint work with Guang Ling

Department of Computer Science & Engineering The Chinese University of Hong Kong

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Outline

- Introduction
- Singular Value Decomposition
- Probabilistic Matrix Factorization
- Mon-negative Matrix Factorization
- Demonstration



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The Netflix Problem

- Netflix database
 - About half a million users
 - About 18,000 movies
- People assign ratings to movies
- A sparse matrix





The Netflix Problem

- Netflix database
 - Over 480,000 users
 - About 18,000 movies
 - Over 100,000,000 ratings
- People assign ratings to movies
- A sparse matrix
 - Only 1.16% of the full matrix is observed



The Netflix Problem

- Netflix database
 - About half a million users
 - About 18,000 movies
- People assign ratings to movies
- A sparse matrix

[x		X		X
 	X			X
X		X		
X				Χ
L		X	X	Χ.

Challenge

Complete the "Netflix Matrix"

Many such problems: collaborative filtering, partially filled out surveys ...



Matrix Completion

- Matrix $X \in \mathbb{R}^{N \times M}$
- Observe subset of entries
- Can we guess the missing entries?

$$\begin{bmatrix} x & ? & x & ? & x \\ ? & x & ? & ? & x \\ x & ? & x & ? & ? \\ x & ? & ? & ? & x \\ ? & ? & x & x & x \end{bmatrix}$$



Matrix Completion

- Matrix $X \in \mathbb{R}^{N \times M}$
- Observe subset of entries
- Can we guess the missing entries?

Everyone would agree this looks impossible.

$$\begin{bmatrix} x & ? & x & ? & x \\ ? & x & ? & ? & x \\ x & ? & x & ? & ? \\ x & ? & ? & ? & x \\ ? & ? & x & x & x \end{bmatrix}$$



Massive High-dimensional Data

Engineering/scientific applications

Unknown matrix often has (approx.) low rank.



Images





Videos



High-dimensionality but often low-dimensional structure



Web data

Recovery Algorithm

Observation

Try to recover a lowest complexity (rank) matrix that agrees with the observation.

Recovery by minimum complexity (assuming no noise)

minimize
$$\operatorname{rank}(\hat{X})$$
 subject to $\hat{X}_{ii} = X_{ii}$ $(i,j) \in \mathcal{Q}_{obs}$



Recovery Algorithm

Observation

Try to recover a lowest complexity (rank) matrix that agrees with the observation.

Recovery by minimum complexity

minimize
$$\operatorname{rank}(\hat{X})$$
 subject to $\hat{X}_{ii} = X_{ii} \quad (i,j) \in \mathcal{Q}_{obs}$

- NP hard: not feasible for N > 10!
- Resort to other approaches
 - Select a low rank K, and approximate X by a rank K matrix \hat{X} .



Low Rank Factorization

- Assume X can be recovered by a rank K matrix \hat{X}
- Then \hat{X} can be factorized into the product of $U \in \mathbb{R}^{K \times N}$, $V \in \mathbb{R}^{K \times M}$

$$\hat{X} = U^T V.$$

• Define \mathcal{E} to be a loss function

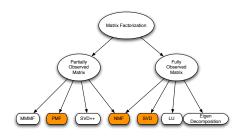
Recovery by rank K matrix

$$\begin{array}{ll} \text{minimize} & \sum_{i,j \in \mathcal{Q}_{obs}} \mathcal{E}(\hat{X}_{ij} - X_{ij}) \\ \\ \text{subject to} & \hat{X} = U^T V \end{array}$$





Overview of Matrix Factorization Methods



- Some methods are traditional mathematical way of factorizing a matrix.
 - SVD, LU, Eigen Decomposition
- Some methods are used to factorize partially observed matrix.
 - PMF, SVD++, MMMF
- Some methods have multiple applications.
 - NMF in image processing
 - NMF in collaborative filtering



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Singular Value Decomposition

Singular Value Decomposition

The Singular Value Decomposition (SVD) of an $N \times M$ matrix A is a factorization of the form

$$A = U\Sigma V^*$$

- V^* is the conjugate transpose of V.
- $U \in \mathbb{R}^{N \times N}$ is unitary matrix, i.e. $UU^* = I$.
- $\Sigma \in \mathbb{R}^{N \times M}$ is rectangular diagonal matrix with real entries.
- $V^* \in \mathbb{R}^{M \times M}$ is unitary matrix, i.e. $VV^* = I$.



SVD v.s. Eigen Decomposition

Singular Value Decomposition

The Singular Value Decomposition (SVD) of an $N \times M$ matrix A is a factorization of the form

$$A = U\Sigma V^*$$

- Diagonal entries of Σ are called singular values of A.
- Columns of *U* and *V* are called left singular vectors and right singular vectors of *A*, respectively.
- The singular values Σ_{ii} s are arranged in descending order in Σ .



SVD v.s. Eigen Decomposition

Singular Value Decomposition

The Singular Value Decomposition (SVD) of an $N \times M$ matrix A is a factorization of the form

$$A = U\Sigma V^*$$

• The left singular vectors of A are eigenvectors of AA^* , because

$$AA^* = (U\Sigma V^*)(U\Sigma V^*)^* = U\Sigma \Sigma^T U^*$$

• The right singular vectors of A are eigenvectors of A^*A , because

$$A^*A = (U\Sigma V^*)^*(U\Sigma V^*) = V\Sigma^T\Sigma V$$

• The singular values of A are the square roots of eigenvalues of both AA^* and A^*A .

SVD as Low Rank Approximation

Low Rank Approximation

$$\operatorname{argmin}_{\tilde{A}} \quad \|A - \tilde{A}\|_{Fro}$$
s.t. $\operatorname{Rank}(\tilde{A}) = r$

SVD gives the optimal solution.

Solution (Eckart-Young Theorem)

Let $A = U\Sigma V^*$ be the SVD for A, and $\tilde{\Sigma}$ is the same as Σ by keeping the largest r singular values. Then,

$$\tilde{A} = U\tilde{\Sigma}V^*$$

is the solution to the above problem.

SVD as Low Rank Approximation

Solution (Eckart-Young Theorem)

Let $A = U\Sigma V^*$ be the SVD for A, and $\tilde{\Sigma}$ is the same as Σ by keeping the largest r singular values. Then,

$$\tilde{A} = U\tilde{\Sigma}V^*$$

is the solution to the above problem.

- It works when A is fully observed.
- What if A is only partially observed?



Low Rank Approximation for Partially Observed Matrix

Low Rank Approximation for Partially Observed Matrix

$$\operatorname{argmin}_{ ilde{A}} \qquad \sum_{i=1}^{N} \sum_{j=1}^{M} I_{ij} (A_{ij} - \tilde{A}_{ij})^2$$
 s.t. $\operatorname{\mathsf{Rank}}(ilde{A}) = r$

- I_{ij} is the indicator that equals 1 if A_{ij} is observed and 0 otherwise.
- We consider only the observed entries.
- A natural probabilistic extension of the above formulation is Probabilistic Matrix Factorization.



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- A popular collaborative filtering (CF) method
- Follow the low rank matrix factorization framework



Collaborative Filtering

Collaborative Filtering

The goal of collaborative filtering (CF) is to infer user preferences for items given a large but incomplete collection of preferences for many users.

- For example:
 - Suppose you infer from the data that most of the users who like "Star Wars" also like "Lord of the Rings" and dislike "Dune".
 - Then if a user watched and liked "Star Wars" you would recommend him/her "Lord of the Rings" but not "Dune".
- Preferences can be explicit or implicit:
 - Explicit preferences
 - Ratings assigned to items
 - Facebook "Like", Google "Plus"
 - Implicit preferences
 - Catalog browse history
 - Items rented or bought by users



Collaborative Filtering vs. Content Based Filtering

- Collaborative Filtering
 - User preferences are inferred from ratings
 - Item features are inferred from ratings
 - Cannot recommend new items
 - Very effective with sufficient data

- Content Based Filtering
 - Analyze the content of the item
 - Match the item features with users preferences
 - Item features are hard to extract
 - Music, Movies
 - Can recommend new items



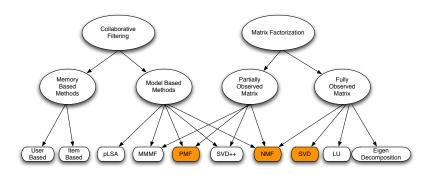
CF as Matrix Completion

 CF can be viewed as a matrix completion problem Items

- Task: given a user/item matrix with only a small subset of entries present, fill in (some of) the missing entries.
- PMF approach: low rank matrix factorization.

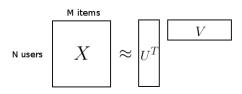


Collaborative Filtering and Matrix Factorization



- Collaborative filtering can be formulated as a matrix factorization problem.
- Many matrix factorization methods can be used to solve collaborative filtering problem.
- The above is only a partial list.

Notations



- Suppose we have M items, N users and integer rating values from 1 to D.
- Let ijth entry of X, X_{ij} , be the rating of user i for item j.
- $U \in \mathbb{R}^{K \times N}$ is latent user feature matrix, U_i denote the latent feature vector for user i.
- $V \in \mathbb{R}^{K \times M}$ is latent item feature matrix, V_j denote the latent feature vector for item j.

Matrix Factorization: the Non-probabilistic View

To predict the rating given by user i to item j,

$$\hat{R}_{ij} = U_i^T V_j = \sum_k U_{ik} V_{jk}$$

- Intuition
 - The item feature vector can be viewed as the input.
 - The user feature vector can be viewed as the weight vector.
 - The predicted rating is the output.
 - Unlike in linear regression, where inputs are fixed and weights are learned, we learn both the weights and the input by minimizing squared error.
 - The model is symmetric in items and users.



- PMF is a simple probabilistic linear model with Gaussian observation noise.
- Given the feature vectors for the user and the item, the distribution of the corresponding rating is:

$$P(R_{ij}|U_i,V_j,\sigma^2) = \mathcal{N}(R_{ij}|U_i^TV_j,\sigma^2)$$

 The user and item feature vectors adopt zero-mean spherical Gaussian priors:

$$P(U|\sigma_U^2) = \prod_{i=1}^N \mathcal{N}(U_i|\mathbf{0}, \sigma_U^2\mathbf{I})$$

$$P(V|\sigma_V^2) = \prod_{j=1}^M \mathcal{N}(V_j|\mathbf{0}, \sigma_V^2\mathbf{I})$$



- Maximum A Posterior (MAP): Maximize the log-posterior over user and item features with fixed hyperparameters.
- MAP is equivalent to minimizing the following objective function:

$$\mathcal{E} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{M} I_{ij} (R_{ij} - U_i^T V_j)^2 + \frac{\lambda_U}{2} \sum_{i=1}^{N} \|U_i\|_{Fro}^2 + \frac{\lambda_V}{2} \sum_{j=1}^{M} \|V_j\|_{Fro}^2$$



$$\mathcal{E} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{M} I_{ij} (R_{ij} - U_i^T V_j)^2 + \frac{\lambda_U}{2} \sum_{i=1}^{N} \|U_i\|_{Fro}^2 + \frac{\lambda_V}{2} \sum_{j=1}^{M} \|V_j\|_{Fro}^2$$

- $\lambda_U = \sigma^2/\sigma_U^2$, $\lambda_V = \sigma^2/\sigma_V^2$ and I_{ij} is indicator of whether user i rated item j.
- First term is the sum-of-squared-errors.
- Second and third term are quadratic regularization term to avoid over-fitting problem.



$$\mathcal{E} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{M} I_{ij} (R_{ij} - U_i^T V_j)^2 + \frac{\lambda_U}{2} \sum_{i=1}^{N} \|U_i\|_{Fro}^2 + \frac{\lambda_V}{2} \sum_{j=1}^{M} \|V_j\|_{Fro}^2$$

- Non-convex problem, global minima generally not achievable
- Alternating update U and V, fix one while updating the another
- Use gradient descent

$$U_i \leftarrow U_i - \eta \frac{\partial \mathcal{E}}{\partial U_i}; \qquad \frac{\partial \mathcal{E}}{\partial U_i} = \sum_{j=1}^M I_{ij} (U_i^T V_j - R_{ij}) V_j + \lambda_U U_i$$

$$V_j \leftarrow V_j - \eta \frac{\partial \mathcal{E}}{\partial V_j}; \qquad \frac{\partial \mathcal{E}}{\partial V_j} = \sum_{i=1}^N I_{ij} (U_i^T V_j - R_{ij}) U_i + \lambda_V V_j$$

$$\mathcal{E} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{M} I_{ij} (R_{ij} - U_i^T V_j)^2 + \frac{\lambda_U}{2} \sum_{i=1}^{N} \|U_i\|_{Fro}^2 + \frac{\lambda_V}{2} \sum_{j=1}^{M} \|V_j\|_{Fro}^2$$

- If all ratings were observed, the objective reduces to the SVD objective in the limit of prior variances going to infinity.
- PMF can be viewed as a probabilistic extension of SVD.



A trick to improve stability

- Map ratings to [0,1] by $(R_{ii}-1)/(D-1)$
- Pass $U_i^T V_i$ through logistic function

$$g(x) = \frac{1}{1 + \exp(-x)}$$

$$\mathcal{E} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{M} I_{ij} (R_{ij} - g(U_i^T V_j))^2 + \frac{\lambda_U}{2} \sum_{i=1}^{N} \|U_i\|_{Fro}^2 + \frac{\lambda_V}{2} \sum_{i=1}^{M} \|V_j\|_{Fro}^2$$



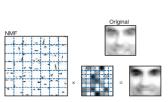
Outline

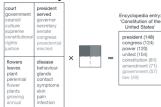
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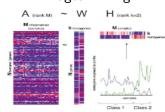
Non-negative Matrix Factorization

NMF is a popular method that is widely used in:





Images Mining



Metagenes Study

Text Mining



Collaborative Filtering



Non-negative Matrix Factorization

- NMF fits in the low rank matrix factorization framework with additional non-negativity constraints.
- NMF can only factorize a Non-negative matrix $A \in \mathbb{R}^{N \times M}$ into basis matrix $W \in \mathbb{R}^{N \times K}$ and weight matrix $H \in \mathbb{R}^{K \times M}$

$$A \approx WH$$

s.t.
$$W, H \geq \mathbf{0}$$



Interpretation with NMF

- Columns of W are the underlying basis vectors, i.e., each of the M columns of A can be built from K columns of W.
- Columns of *H* give the weights associated with each basis vector.

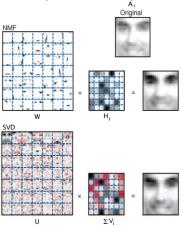
$$Ae_1 = WH_{*1} = [W_1]H_{11} + [W_2]H_{21} + \cdots + [W_K]H_{K1}$$

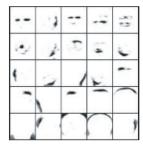
• $W, H \ge 0$ commands additive parts-based representation.



NMF in Image Mining

Additive parts-based representation







NMF in Image Mining

• In image processing, we often assume Poisson Noise

NMF Poisson Noise

min
$$\sum_{i,j} (A_{ij} \log \frac{A_{ij}}{[WH]_{ij}} - A_{ij} + [WH]_{ij})$$
s.t.
$$W, H > \mathbf{0}$$

 Objective function can be changed to other form, the non-negative constraint is more important than the form of the objective function

NMF Gaussian Noise

min
$$||A - WH||_{Fro}^2$$

s.t. $W, H > \mathbf{0}$

Inference of NMF

NMF Gaussian Noise

min
$$||A - WH||_{Fro}^2$$

s.t. $W, H > \mathbf{0}$

- Convex in W or H. but not both.
- Global min generally not achievable.
- Many number of unknowns: NK for W and MK for H



Inference of NMF

NMF Gaussian Noise

min
$$||A - WH||_{Fro}^2$$

s.t. $W, H > \mathbf{0}$

Alternating gradient descent can get a local minima

$$F = \|A - WH\|_{Fro}^2$$

MF

Algorithm 1 Alternating gradient descent

$$W \leftarrow \operatorname{abs}(\operatorname{randn}(N, K))$$

$$H \leftarrow \mathsf{abs}(\mathsf{randn}(M,K))$$

$$\textbf{for } i=1: \textit{MaxIteration } \textbf{do}$$

$$H \leftarrow H - \eta \frac{\partial F}{\partial H}, H \leftarrow H. * (H \ge 0)$$

$$W \leftarrow W - \eta \frac{\partial F}{\partial W}, \ H \leftarrow W. * (W \ge 0)$$



end for

Alternating Gradient Descent

```
\begin{split} & W \leftarrow \mathsf{abs}(\mathsf{randn}(N,K)) \\ & H \leftarrow \mathsf{abs}(\mathsf{randn}(M,K)) \\ & \textbf{for } i = 1 : \textit{MaxIteration do} \\ & \quad H \leftarrow H - \eta \frac{\partial F}{\partial H}, \ H \leftarrow H.*(H \geq 0) \\ & \quad W \leftarrow W - \eta \frac{\partial F}{\partial W}, \ H \leftarrow W.*(W \geq 0) \\ & \textbf{end for} \end{split}
```

- Pros
 - works well in practice
 - speedy convergence
 - 0 elements not locked
- Cons
 - ad hoc nonnegativity: negative elements are set to 0
 - ad hoc sparsity: negative elements are set to 0
 - no convergence theory



Inference of NMF

```
\begin{split} & W \leftarrow \mathsf{abs}(\mathsf{randn}(N,K)) \\ & H \leftarrow \mathsf{abs}(\mathsf{randn}(M,K)) \\ & \textbf{for } i = 1 : \textit{MaxIteration do} \\ & H \leftarrow H - \eta \frac{\partial F}{\partial H}, \ H \leftarrow H.* (H \geq 0) \\ & W \leftarrow W - \eta \frac{\partial F}{\partial W}, \ H \leftarrow W.* (W \geq 0) \\ & \textbf{end for} \end{split}
```

Observation

By choosing suitable η , we can change the additive update rule to multiplicative update rule. Non-negativity of W,H is guaranteed by the initial non-negativity. Ad hoc non-negativity is no longer needed.



NMF Gaussian Noise

min
$$||A - WH||_{Fro}^2$$

s.t. $W, H > \mathbf{0}$

Algorithm 2 Multiplicative update rule

$$W \leftarrow \operatorname{abs}(\operatorname{randn}(N,K))$$

 $H \leftarrow \operatorname{abs}(\operatorname{randn}(M,K))$
for $i=1$: MaxIteration do
 $H \leftarrow H.*(W^TA)./(W^TWH+10^{-9})$
 $W \leftarrow W.*(AH^T)./(WHH^T+10^{-9})$
end for

• Non-negativity is guaranteed.



Inference of NMF

NMF Poisson Noise

min
$$\sum_{i,j} (A_{ij} \log \frac{A_{ij}}{[WH]_{ij}} - A_{ij} + [WH]_{ij})$$
s.t.
$$W, H \ge \mathbf{0}$$

Algorithm 3 Multiplicative update rule

```
W \leftarrow \operatorname{abs}(\operatorname{randn}(N,K))

H \leftarrow \operatorname{abs}(\operatorname{randn}(M,K))

for i=1: MaxIteration do

H \leftarrow H.*(W^T(A./(WH+10^{-9})))./W^Tee^T

W \leftarrow W.*((A./(WH+10^{-9}))H^T)./ee^TH^T

end for
```



Multiplicative Update Rule

- Pros
 - Convergence theory: guaranteed to converge to fixed point
 - ullet Good initialization of W, H speeds convergence and gets to better fixed point
- Cons
 - Fixed point may be local min or saddle point
 - Slow: many matrix multiplications at each iteration
 - 0 elements locked



Properties of NMF

- Basis vectors W_i are not orthogonal
- $W_k, H_k \ge 0$ have immediate interpretation
 - EX: large w_{ij} 's \Rightarrow basis vector W_i is mostly about terms j
 - EX: h_{i1} denotes how much sample i is pointing in the "direction" of topic vector W_1

$$Ae_1 = WH_{*1} = [W_1]H_{11} + [W_2]H_{21} + \cdots + [W_K]H_{K1}$$

• NMF is algorithm-dependent: W, H not unique



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- Application of PMF in Collaborative Filtering is used.
- Required Packages:
 - Python version 2.7
 - NumPy
 - SciPy
 - Matplotlib
- Script provided: pmf.py
 - Code credit: Danny Tarlow
 - Available at http://blog.smellthedata.com/2009/06/netflix-prizetribute-recommendation.html



Required Packages

```
NumPy
    http://numpy.scipy.org/
SciPy
    http://www.scipy.org/
Matplotlib
    http://matplotlib.sourceforge.net/users/installing.html
```



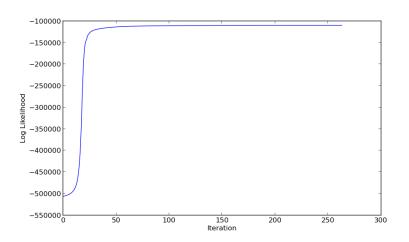
- Install all the required packages
- Run the script "python pmf.py"

What the script does?

100 users' partial ratings on 100 items is simulated. 30% of the rating matrix is observed. Then PMF algorithm is performed on the generated dataset using a factorization dimension 5. When the learning is done, the convergency of the log-likelihood, user features, item features and predicted ratings are plotted.

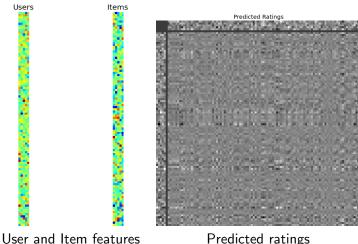


Figure: Convergency of the loglikelihood













- Application of NMF in image processing is used.
- Required Packages:
 - Python version 2.7
 - Python Image Library (PIL)
 - Python Matrix Factorization Module (PyMF)
 - NumPy
 - SciPy



Required Packages

```
Python Image Library (PIL)
    http://www.pythonware.com/products/pil/index.htm
Python Matrix Factorization Module (PyMF)
    http://code.google.com/p/pymf/
NumPy
    http://numpy.scipy.org/
SciPy
    http://www.scipy.org/
```



- Install all the required packages
- Run the script "python nmfdemo.py"

What the script does?

 $2429\ 19 \times 19$ face image is loaded into a matrix "data", one column per image. NMF is then performed on "data". The original image and the recovered image placed side by side is saved in folder "recover".



Figure: 49 Basis Images (normalized)



Original Recovered









QA

Thanks for your attention!



Some of the slides are modified from materials:

http://videolectures.net/site/normal_dl/tag=623106/mlss2011_candes_lowrank_01.pdf http://www.cs.toronto.edu/~hinton/csc2515/notes/pmf_tutorial.pdf http://langvillea.people.cofc.edu/NISS-NMF.pdf

