

Matrix Completion

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Overview

- 1 What is Matrix Completion?
- 2 Exact Matrix Completion
- 3 Approximate Matrix Completion
- 4 Follow-up Research

Outline

1 What is Matrix Completion?

2 Exact Matrix Completion

3 Approximate Matrix Completion

- Nuclear Norm Minimization
- Low-Rank Matrix Factorization
- Distributed Matrix Completion

4 Follow-up Research

Movie Recommendation

- Websites recommend movies based on users' ratings.
- Users only saw a little part of the movies in the website.
- The ratings in the rating matrix are **very sparse!!!**

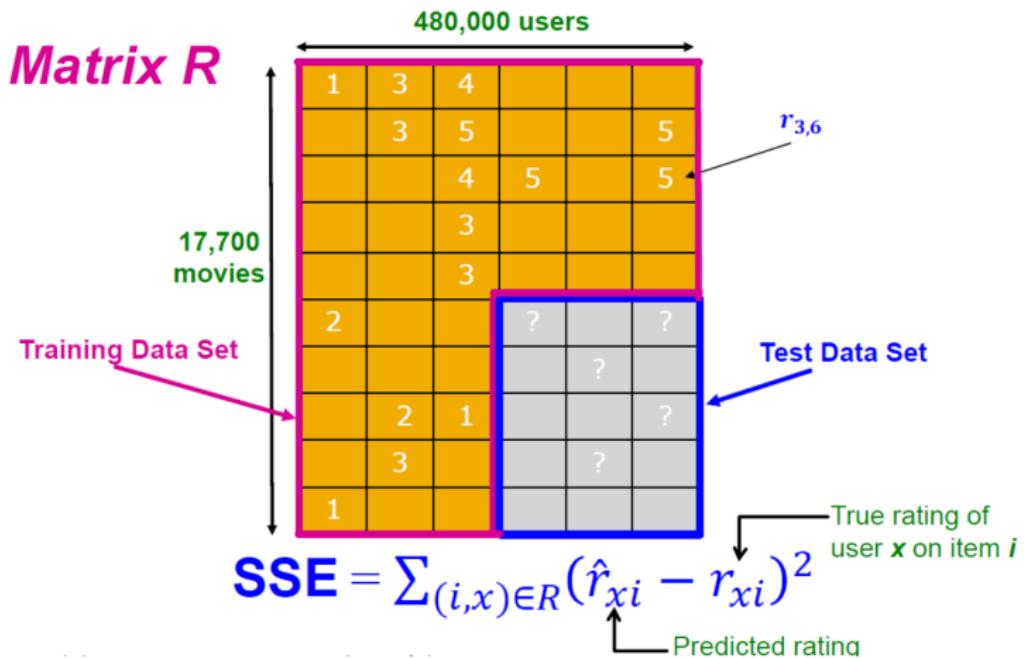


	2			4	5	2.94*
2		4			1	
3		5		2	2.48*	
4	1		5		4	
5		4			2	
6	4	5		1		1.12*

Netflix Prize

- Training data
 - 100 million ratings, 480,000 users, 17,770 movies
 - 6 years of data: 2000-2005
- Testing data
 - Last few ratings of each user (2.8 million)
 - Evaluation criterion – root mean squared error –
$$\text{RMSE} = \sqrt{\sum_{xi} (\hat{r}_{xi} - r_{xi})^2}$$
, where \hat{r}_{xi} and r_{xi} are the predicted and true rating of x on i
 - Netflix Cinematch RMSE: 0.9514
- Competition
 - 2700+ teams
 - \$1 million prize for 10% improvement on Cinematch

Netflix Prize



What is Matrix Completion?

Matrix Completion

Suppose you are given a matrix $M \in \mathbb{R}^{n_1 \times n_2}$ with some given entries $(M_{ij})_{ij \in \Omega}$, where $|\Omega| \ll n_1 n_2$

Problem: How to recover the missing elements in M ?

What is Matrix Completion?

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Suppose you are given a matrix $M \in \mathbb{R}^{n_1 \times n_2}$ with some given entries $(M_{ij})_{ij \in \Omega}$, where $|\Omega| \ll n_1 n_2$

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Lots of applications!!!

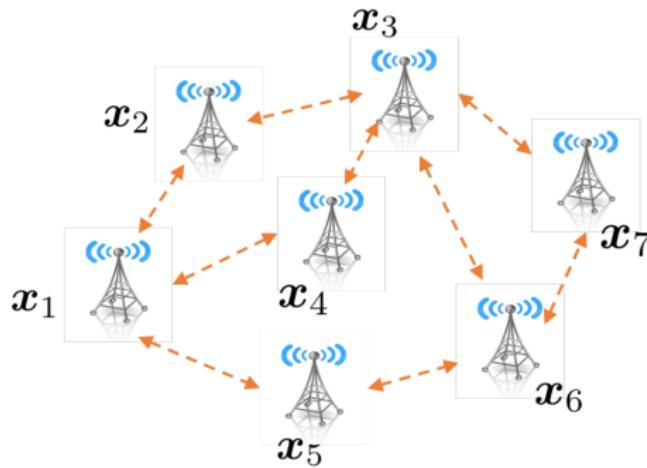
- news personalization
- sensor localization
- link prediction
- imputation
- ...

Application 1: Sensor Localization

- Given n sensors/points $\mathbf{x}_j \in R^3$ ($j = 1, \dots, n$)
- Observe partial information about pairwise distances,

$$D_{i,j} = \|\mathbf{x}_i - \mathbf{x}_j\|^2 = \|\mathbf{x}_i\|^2 + \|\mathbf{x}_j\|^2 - 2\mathbf{x}_i^\top \mathbf{x}_j \quad (1)$$

- Aim:** infer the distances between any pair of locations



Application 1: Sensor Localization

Introduce

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} \in \mathbb{R}^{n \times 3} \quad (2)$$

then the distance matrix $D = [D_{i,j}]_{1 \leq i, j \leq n}$ can be written as

$$D = \underbrace{\mathbf{d}_2 \mathbf{e}^\top + \mathbf{e} \mathbf{d}_2^\top - 2\mathbf{X}\mathbf{X}^\top}_{\text{low rank}} \quad (3)$$

where $\mathbf{d}_2 := [\|\mathbf{x}_1\|^2, \dots, \|\mathbf{x}_n\|^2]^\top$.

Application 1: Sensor Localization

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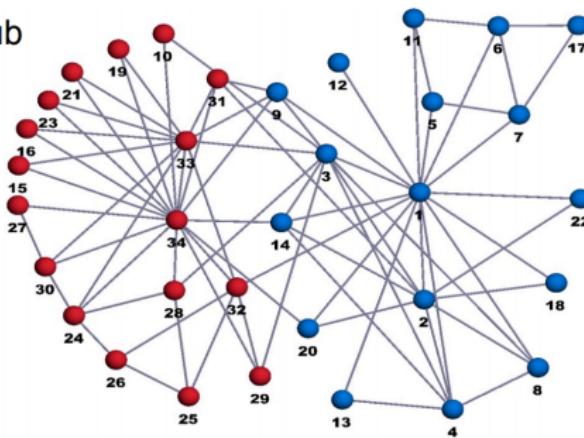
where $\mathbf{d}_2 := [\|\mathbf{x}_1\|^2, \dots, \|\mathbf{x}_n\|^2]^\top$.

rank(D) $\ll n \longrightarrow$ low-rank matrix completion

Application 2: Link Prediction

- Given a snapshot of a network $G = (V, E)$ (e.g., a Facebook social network among users)
- Goal:** predict future possible links between any two users in the network

Zachary Karate Club



<http://ifisc.uib-csic.es/~jramasco/ComplexNets.html>

Application 3: Single-cell RNA-seq Data Imputation

- Given a gene expression matrix M of m genes and n cells
- Dropout:** genes which are expressed even at a relatively high level may be undetected due to technical limitations
- Goal:** impute the dropout events in M

	Cell 1	Cell2	Cell3	Cell4	...
Gene 1	0	0	3	10	
Gene 2	24	0	41	12	
Gene 3	175	284	93	162	
Gene 4	0	0	0	0	
Gene 5	36	0	32	21	
...	

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Matrix Completion Problem

- Given a matrix M with some entries are missing
- Goal:** Complete the matrix M

	1	2	3	4	5	6	7	8	9	10
1		4		2	4					
2	3		3	1			3		3	
3		3	2	3					4	
4			2			4		1	2	5
5	3			3			1			
6			2					3	2	

- In general, it is impossible!!!
- But it can be possible with the **low-rank assumption**

Low-rank Assumption

Low-rank assumption

For a $n_1 \times n_2$ matrix M of rank r , assume that $\min(n_1, n_2) \gg r$.

- Why this assumption is needed?
- Assume M is a rating matrix for example,
 - Only a few factors contribute to anyone's taste or preference
- The matrix only has $(2n - r)r$ degrees of freedom (DoF)
($n = n_1 = n_2$).
- DoF is calculated by counting parameters in the SVD
 - (The number of singular values)
 - + (degree of freedom of left singular vectors)
 - + (degree of freedom of right singular vectors)
 - $= r + ((2n - r - 1) \times r)/2 + ((2n - r - 1) \times r)/2$
- Considerably smaller than n^2 .
 - With the low-rank assumption, DoF is reduced by about $2r/n$.

What Can Go Wrong?

Entire column missing

$$\begin{bmatrix} 1 & 2 & ? & 3 & \dots & 4 \\ 3 & 5 & ? & 4 & \dots & 1 \\ 2 & 5 & ? & 2 & \dots & 5 \end{bmatrix} \quad (4)$$

- No hope of recovery!

Standard solution: Uniform observation model

Assume that the set of s observed entries Ω is drawn uniformly at random:

$$\Omega \sim \text{Unif}(n_1, n_2, s) \quad (5)$$

What Can Go Wrong?

Bad spread of information

$$\mathbf{L} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (6)$$

- Can only recover L if L_{11} is observed

Standard solution: Random orthogonal model

The family $\{u_k\}_{1 \leq k \leq r}$ is selected uniformly at random among all families of r orthonormal vectors, and similarly for the family $\{v_k\}_{1 \leq k \leq r}$. Here u_k and v_k are the left and right singular vectors.

EXACT Matrix Completion

Problem 1.1: Matrix Completion Problem

$$\begin{aligned} & \text{minimize} \quad \text{rank}(X) \\ & \text{subject to } X_{ij} = M_{ij}, \quad (i, j) \in \Omega \end{aligned}$$

- Unfortunately, this problem is NP-hard and non-convex.
 - rank norm is not convex.
- All known algorithms require exponential time to n .

EXACT Matrix Completion

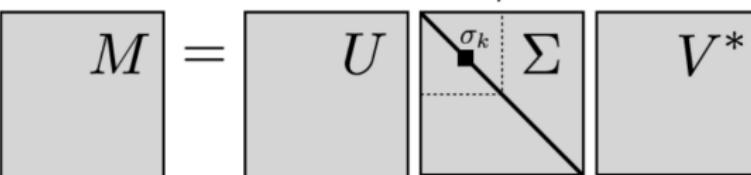
Problem 1.2: Convex Relaxation
[Candes and Recht, 2009]

$$\begin{aligned} & \text{minimize} \quad \|X\|_* \\ & \text{subject to} \quad X_{ij} = M_{ij}, \quad (i, j) \in \Omega \end{aligned}$$

- The nuclear norm $\|X\|_*$ is the **surrogate** of the rank norm.
 - Also, the nuclear norm is a convex function.
 - This heuristic was introduced by [Recht, 2009].

Is Nuclear Norm Relaxation Reasonable?

- Recall that l_1 -norm is the surrogate of l_0 -norm.

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


M = U Σ V^*

$n_1 \times n_2$ $n_1 \times n$ $n \times n$ $n \times n_2$

- Let the vector $\sigma = (\sigma_1, \sigma_2, \dots, \sigma_n)$, σ_i is the i -th singular value of the matrix M .
- The rank norm is the l_0 -norm of the σ vector.
- The nuclear norm is the l_1 -norm of the σ vector.

Connections with Compressed Sensing

General setup

Rank minimization

$$\text{minimize } \text{rank}(X)$$

$$\text{subject to } \mathcal{A}(X) = b$$

Suppose $X = \text{diag}(x)$, $x \in \mathbb{R}^n$

- $\text{rank}(X) = \sum_i \mathbf{1}_{(x_i \neq 0)} = \|x\|_{\ell_0}$
- $\|X\|_* = \sum_i |x_i| = \|x\|_{\ell_1}$

Rank minimization

$$\text{minimize } \|x\|_{\ell_0}$$

$$\text{subject to } Ax = b$$

This is compressed sensing!

Convex relaxation

$$\text{minimize } \|X\|_*$$

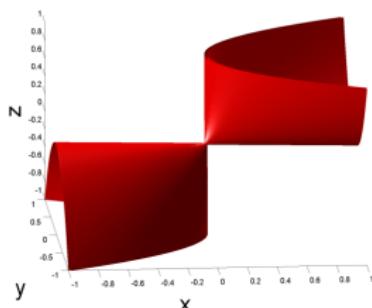
$$\text{subject to } \mathcal{A}(X) = b$$

Convex relaxation

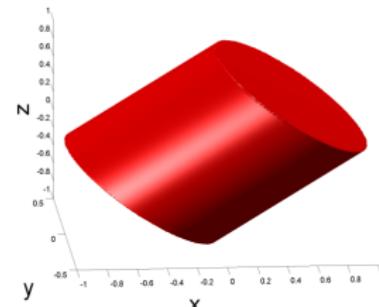
$$\text{minimize } \|x\|_{\ell_1}$$

$$\text{subject to } Ax = b$$

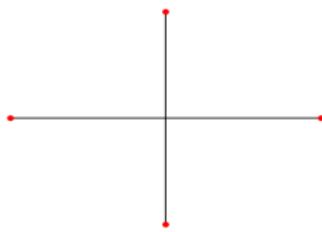
Connections with Compressed Sensing



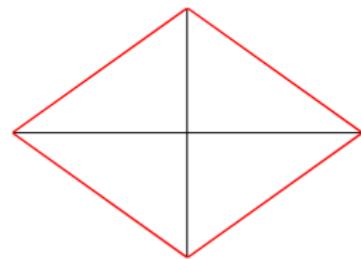
Rank penalty



Nuclear norm



ℓ_0 norm



ℓ_1 norm

Exact Unique Recovery Theorem

- If we want to recover an incomplete matrix, some assumptions are necessary.
- In fact, if some gentle conditions are met, this matrix can be recovered exactly and uniquely [Candes and Recht, 2009].
 - $M: n_1 \times n_2$ matrix of rank r , $n = \max(n_1, n_2)$, $m = |\Omega|$.

Theorem 1.1 (General)

- M obeys the random orthogonal model
- With uniformly random sampling assumption

Then, \exists constants C, c such that if

$$m \geq Cn^{5/4}r \log n$$

the minimizer to the **Problem 1.2** is unique and equal to M with probability at least $1 - cn^{-3}$.

Exact Unique Recovery Theorem

- For the low-rank case, a tighter bound is given.

Theorem 1.1 (Low-rank)

if $r \leq n^{1/5}$, the recovery is exact with same probability provided that

$$m \geq Cn^{6/5}r \log n$$

How to Solve the Nuclear Norm Minimization?

- Convex Relaxation to Matrix Completion Problem (Nuclear Norm Minimization) can be solved by the **Semi-definite Programming (SDP)**
- Let SVD of matrix $X = U\Sigma V^*$
- Define $W_1 = U\Sigma U^*$, $W_2 = V\Sigma V^*$, $X' = \begin{bmatrix} W_1 & X \\ X^* & W_2 \end{bmatrix}$
- Under above settings, the following properties satisfy:
 - $\|X\|_* = \|W_1\|_* = \|W_2\|_*$
 - $X' \succeq 0$ (positive semidefinite matrix),
$$\therefore X' = \begin{bmatrix} U \\ V \end{bmatrix} \Sigma \begin{bmatrix} U \\ V \end{bmatrix}^* = \left(\begin{bmatrix} U \\ V \end{bmatrix} \sqrt{\Sigma} \right) \left(\begin{bmatrix} U \\ V \end{bmatrix} \sqrt{\Sigma} \right)^* \succeq 0$$
 - \forall symmetric matrix X , $\text{trace}(X) = \|X\|_*$

How to Solve the Nuclear Norm Minimization?

- Therefore, the **Problem 1.2** can be reduced to

Reduced form of nuclear norm minimization

$$\begin{aligned} & \text{minimize} \quad \text{trace}(X') \\ & \text{subject to } \mathcal{P}_\Omega(X) = \mathcal{P}_\Omega(M), X' \succeq 0 \end{aligned}$$

- $X' = \begin{bmatrix} W_1 & X \\ X^* & W_2 \end{bmatrix}$
- $\text{trace}(X') = \text{trace}(W_1) + \text{trace}(W_2) = \|X\|_* + \|X\|_* = 2\|X\|_*$

Now, the reduced form can be solved by SDP

- Many algorithms solving SDP have been proposed

How to Solve the Nuclear Norm Minimization?

- However, the off-the-shelf algorithms (such as interior point methods) are not directly amenable to large problems of this kind with over a million unknown entries.
- A faster and less memory-required algorithm is needed.

Singular Value Thresholding (SVT) Algorithm

- We consider the nuclear norm minimization problem,

$$\begin{aligned} & \underset{X}{\text{minimize}} && \|X\|_* \\ & \text{subject to} && \mathcal{P}_\Omega(X) = \mathcal{P}_\Omega(M) \end{aligned}$$

with optimization variable $X \in R^{n_1 \times n_2}$.

- The SVT algorithm [Cai et al., 2010] can be stated as,

Singular Value Thresholding (SVT)

1. Input $\tau \geq 0$, $\{\delta_k\}_{k \geq 1}$, $Y^0 = 0$
2. $X^k = \mathcal{S}_\tau(Y^{k-1})$
3. $Y^k = Y^{k-1} + \delta_k \mathcal{P}_\Omega(M - X^k)$

- \mathcal{S}_τ is the shrinkage operator.
- What's the meaning of the iteration?

Shrinkage Operator

For a matrix $Y \in \mathbb{R}^{n_1 \times n_2}$, consider:

$$\min_{X \in \mathbb{R}^{m \times n}} \tau \|X\|_* + \frac{1}{2} \|X - Y\|_F^2$$

The optimal solution is:

$$X := S_\tau(Y) = U \text{Diag}(s_\tau(\sigma)) V^\top$$

- SVD: $Y = U \text{Diag}(\sigma) V^\top$
- $s_\tau(\sigma) = \max(\sigma - \tau, 0)$
- $S_\tau(Y)$ is a trade-off between minimize the rank and the distance with Y .

How to Understand SVT?

$$\begin{cases} \mathbf{X}^k = \mathcal{S}_\tau(\mathbf{Y}^{k-1}) \\ \mathbf{Y}^k = \mathbf{Y}^{k-1} + \delta_k \mathcal{P}_\Omega(\mathbf{M} - \mathbf{X}^k) \end{cases}$$

The meaning of the iterations is obvious,

- **Proximity Optimization**

- The first step is a trade-off between minimize the rank of X^k and the distance with Y^k .
- Only needs a SVD on a sparse matrix!!!

- **Gradient Descent**

- The second step is a projected gradient descent step, so Y^k is gradually close to M .
- Y^k is always sparse and easy to store.

Convergence Analysis

Theorem 3.1 [Cai et al., 2010]

The sequence $\{X^k\}$ generated by the Proximal gradient iterations converges to some $X^* \in \mathcal{X}^*$, where \mathcal{X}^* is the optimal solution set.

Do We Need Exact Matrix Completion?

- We have recovered the matrix M with the SVT algorithm by solving:

$$\begin{aligned} & \text{minimize} && \|X\|_* \\ & \text{subject to} && P_\Omega(X) = P_\Omega(M) \end{aligned}$$

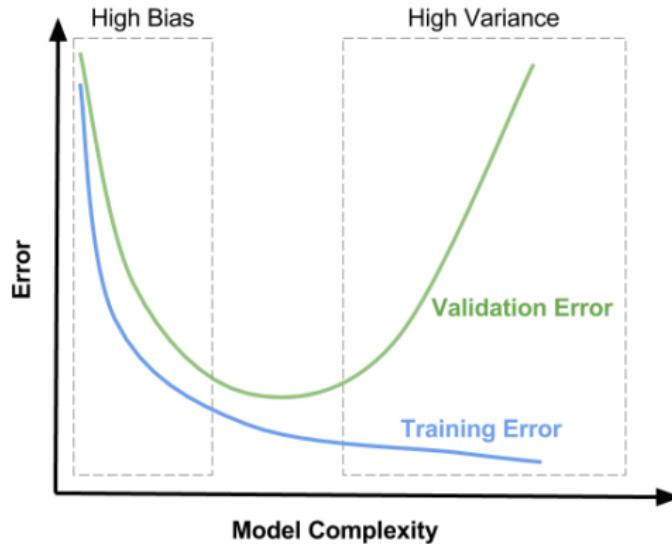
- $X = M$ in every observed entry
- But in real-life, there is always noise — fitting training data exactly incurs added variance
- Introduce bias to decrease variance like,

$$\begin{aligned} & \text{minimize} && \|X\|_* \\ & \text{subject to} && \|P_\Omega(M) - P_\Omega(X)\|_F \leq \delta \end{aligned}$$

where δ is a little positive number

Bias-Variance Trade-Off

- Low bias may incur high variance!!!



- We only need Approximate Matrix Completion!

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Noise Assumption

Noise Assumption

For the observed $n_1 \times n_2$ matrix M of rank r , assume $M = X + E$, where X is the true data and E is the noise.

- Why this assumption is needed?
- For example in recommendation system,
 - We usually rate the movies only with scores 1-5
 - Our rating are influenced seriously by our mood
 - In many situations, we want to give a score between 3-4, for 3.6
 - Our rating are not that real
- Similar in other applications

Matrix Completion with Noise

SVT algorithm solves:

$$\begin{aligned} & \text{minimize} && \|X\|_* \\ & \text{subject to} && P_\Omega(M) = P_\Omega(X) \end{aligned}$$

there is always noise

$$M = X + E$$

Relax the constraint

[Mazumder et al., 2010]

$$\begin{aligned} & \text{minimize} && \|X\|_* \\ & \text{subject to} && \|P_\Omega(M) - P_\Omega(X)\|_F \leq \delta \end{aligned}$$

- First order algorithm to solve via a sparse SVD.
- No-noise reconstruction model seems too rigid.
- In real-life, there is noise - fitting training data exactly incurs added variance.
- Introduce bias to decrease variance.

The Lagrange Form

For a matrix $M_{n_1 \times n_2}$, let $\Omega \subset \{1, \dots, n_1\} \times \{1, \dots, n_2\}$ denote the indices of observed entries, let's consider the following problem:

$$\begin{aligned} & \underset{X}{\text{minimize}} && \|X\|_* \\ & \text{subject to} && \sum_{(i,j) \in \Omega} (X_{ij} - M_{ij})^2 \leq \delta \end{aligned} \tag{*}$$

Equivalently we can reformulate (*) in the Lagrange form

$$\underset{X}{\text{minimize}} \sum_{(i,j) \in \Omega} (X_{ij} - M_{ij})^2 + \lambda \|X\|_* \tag{**}$$

- Here $\lambda \geq 0$ is a regularization parameter controlling the nuclear norm of the minimizer \hat{Z}_λ of (*);
- There is a 1 – 1 mapping between $\delta \geq 0$ and $\lambda \geq 0$ over their active domains.

Back to Shrinkage Operator

Let (fully observed) $M_{n_1 \times n_2}$ have SVD

$$M = U \cdot \text{diag} [\sigma_1, \dots, \sigma_r] \cdot V^T$$

Consider the convex optimization problem

$$\underset{X}{\text{minimize}} \quad \|M - X\|_F^2 + \lambda \|X\|_*$$

Solution is **shrinkage operator** gets,

$$\mathcal{S}_\lambda(M) := U \cdot \text{diag} [(\sigma_1 - \lambda)_+, \dots, (\sigma_r - \lambda)_+] \cdot V^T$$

Like lasso for SVD: singular values are shrunk to zero, with many set to zero. Smooth version of the best-rank approximation.

Soft-Impute Algorithm

Back to the nuclear norm minimization, in the lagrange form:

$$\underset{X}{\text{minimize}} \|P_{\Omega}(X) - P_{\Omega}(M)\|_F^2 + \lambda \|X\|_*$$

Soft-Impute [Mazumder et al., 2010]

1. Initialize $X^{\text{old}} = 0$ and create a decreasing grid Λ of values $\lambda_0 > \lambda_1 > \dots > \lambda_r > 0$, with $\lambda_0 = \lambda_{\max}(P_{\Omega}(M))$
2. For each $\lambda = \lambda_1, \lambda_2, \dots \in \Lambda$ iterate 2a – 2b till convergence:
 - (2a) Compute $X^{\text{new}} \leftarrow \mathcal{S}_{\lambda}(P_{\Omega}(M) + P_{\Omega}^{\perp}(X^{\text{old}}))$
 - (2b) Assign $X^{\text{old}} \leftarrow X^{\text{new}}$ and go to step (2a)
 - (2c) Assign $\hat{X}_{\lambda} \leftarrow X^{\text{new}}$ and go to 2
 - Output the sequence of solutions $\hat{X}_{\lambda_1}, \dots, \hat{X}_{\lambda_K}$

Soft-Impute: Computational Bottleneck

Obtain the sequence $\{X_k\}$ of guesses

- Soft-Impute:

$$X_{k+1} = \operatorname{argmin}_X \|P_\Omega(M) + P_\Omega^\perp(X_k) - X\|_F^2 + \lambda \|X\|_*$$

- SVT: $X_{k+1} = \operatorname{argmin}_X \|P_\Omega(X_k) - X\|_F^2 + \lambda \|X\|_*$

Computational bottleneck: Soft-Impute requires (low-rank) SVD of completed matrix in iterations:

$$\hat{X}_k = \mathcal{S}_\lambda(P_\Omega(M) + P_\Omega^\perp(X_k))$$

Trick:

$$P_\Omega(M) + P_\Omega^\perp(X_k) = \underbrace{\{P_\Omega(M) - P_\Omega(X_k)\}}_{\text{Sparse}} + \underbrace{X_k}_{\text{Low Rank}}$$

Computational Tricks in Soft-Impute

- Anticipate rank of $\hat{X}_{\lambda_{j+1}}$ based on rank of \hat{X}_{λ_j} , erring on generous side.
- Compute the low-rank SVD of \hat{X}_k using orthogonal QR iterations with Reitz acceleration [Hastie et al., 2015].
- Iterations require left and right multiplications $U' \hat{X}_k$ and $\hat{X}_k V$. Ideal for **Sparse + Low-rank structure**.
- Warm starts: $\mathbf{S}_\lambda(\hat{X}_k)$ provides excellent warm starts (U and V) for $\mathbf{S}_\lambda(\hat{X}_{k+1})$. Likewise \hat{Z}_{λ_j} for $\hat{Z}_{\lambda_{j+1}}$.
- Total cost per iteration $O[(m + n) \cdot r + |\Omega|]$ is less than that of the off-the-shelf methods.

Soft-Impute: Convergence Analysis

Theorem 3.2 [Mazumder et al., 2010]

Take $\lambda > 0$. The sequence of estimates $\{X_k\}$ given by:

$$X_{k+1} = \operatorname{argmin}_Z \|P_{\Omega}(M) + P_{\Omega}^{\perp}(X_k) - X\|_F^2 + \lambda \|X\|_* \quad (7)$$

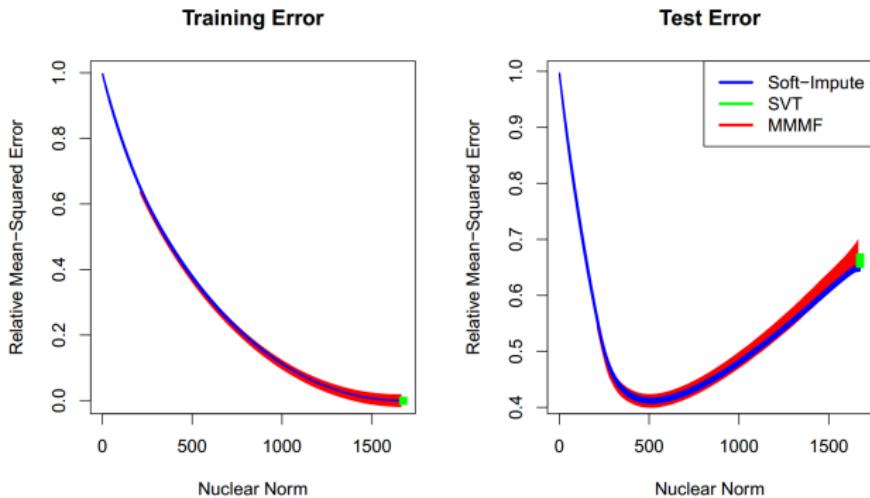
converges to X_{∞} , a fixed point of

$$X = \mathcal{S}_{\lambda} (P_{\Omega}(M) + P_{\Omega}^{\perp}(X))$$

Hence, X_{∞} minimizes

$$f_{\lambda}(X) := \|P_{\Omega}(M) - P_{\Omega}(X)\|_F^2 + \lambda \|X\|_*$$

Experimental Analysis



- MMMF (Maximum Margin Matrix Factorization) is a matrix factorization based method.
- SVT has very poor prediction error.
- Exactly fitting the training data is too rigid and overfitting.

Hard-Impute Algorithm

Let's consider another circumstance where X is low rank and its rank is known a priori,

$$\underset{\text{rank}(X)=r}{\text{minimize}} \|P_{\Omega}(X) - P_{\Omega}(M)\|_F$$

This is not convex in X , but by analogy with Soft-Impute, an iterative algorithm gives good solutions. Replace step:

$$Z^{\text{new}} \leftarrow \mathbf{S}_{\lambda} \left(P_{\Omega}(M) + P_{\Omega}^{\perp}(X^{\text{old}}) \right)$$

with

$$Z^{\text{new}} \leftarrow \mathbf{H}_r \left(P_{\Omega}(M) + P_{\Omega}^{\perp}(X^{\text{old}}) \right)$$

Here $\mathbf{H}_r(X^*)$ is the best rank- r approximation to X^* , i.e. the rank- r truncated SVD approximation.

Discussion

Nuclear norm minimization has many advantages,

- Convex problem
- Global minima

but,

- Storing a big dense matrix needs lots of memory

Since we assume it's a low rank or rank is known a priori, **can we use less memory to store it?**

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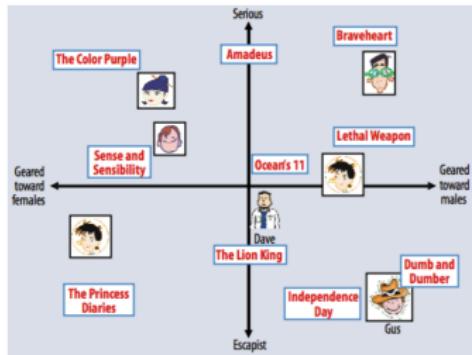
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Latent Factor Models in Recommendation System

Assume that both movies and users live in some low dimensional space describing their properties,

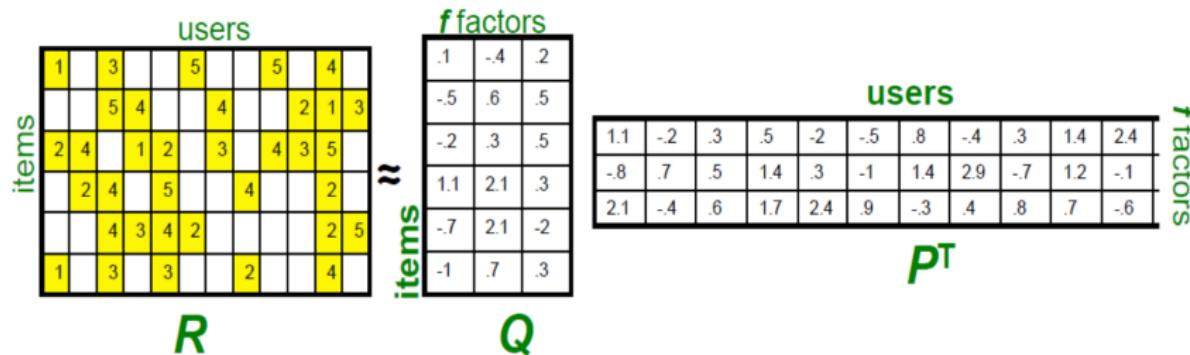
- characters, genres, tastes, ...

Recommend a movie based on its proximity to the user in the latent space.



Latent Factor Models in Recommendation System

- “SVD” on Netflix data: $R \approx Q \cdot P^T$



Latent Factor Models in Recommendation System

- “SVD” on Netflix data: $R \approx Q \cdot P^T$

The diagram shows the decomposition of a rating matrix R into two matrices, Q and P^T , separated by a symbol \approx .

Rating Matrix R : A 6x6 grid representing user-item ratings. The columns are labeled "users" and the rows are labeled "items". Yellow cells indicate known ratings, while white cells indicate missing entries.

Matrix Q : A 6x3 matrix representing user factors. The columns are labeled "factors".

Matrix P^T : A 3x6 matrix representing item factors. The columns are labeled "users".

1	3	5	5	4	
	5	4	4		2
2	4	1	2	3	4
	2	4	5	4	2
	4	3	4	2	
1	3	3	2		4

.1	-.4	.2
-.5	.6	.5
-.2	.3	.5
1.1	2.1	.3
-.7	2.1	-.2
-1	.7	.3

1.1	-.2	.3	.5	-.2	-.5	.8	-.4	.3	1.4	2.4
-.8	.7	.5	1.4	.3	-1	1.4	2.9	-.7	1.2	-.1
2.1	-.4	.6	1.7	2.4	.9	-.3	.4	.8	.7	-.6

- Assume the rating matrix R can be approximated as $Q \cdot P^T$
- R has missing entries
- Hope the reconstruction error to be small on known ratings

Ratings as Products of Factors

- How to estimate the missing rating of user x for item i ?

$$\hat{r}_{ix} = q_i \cdot p_x^T = \sum_f q_{if} p_{xf}$$

where q_i is row i of Q and p_x is column x of P^T .

items

.1	-.4	.2
-.5	.6	.5
-.2	.3	.5
1.1	2.1	.3
-.7	2.1	-.2
-.1	.7	.3

f factors

Q

users

• *f* factors

1.1	-.2	.3	.5	-2	-.5	.8	-.4	.3	1.4	2.4	-.9
-.8	.7	.5	1.4	.3	-1	1.4	2.9	-.7	1.2	-.1	1.3
2.1	-.4	.6	1.7	2.4	.9	-.3	.4	.8	.7	-.6	.1

P^T

What is SVD?

Definition of SVD: if A is a real m -by- n matrix, then there exists $U = [u_1, \dots, u_m] \in \mathbb{R}^{m \times m}$, and $V = [v_1, \dots, v_n] \in \mathbb{R}^{n \times n}$, such that $U^T U = I$, $V^T V = I$ and $U^T A V = \text{diag}(\sigma_1, \dots, \sigma_p) \in \mathbb{R}^{m \times n}$, $p = \min(m, n)$, where $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p \geq 0$.

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Theorem 3

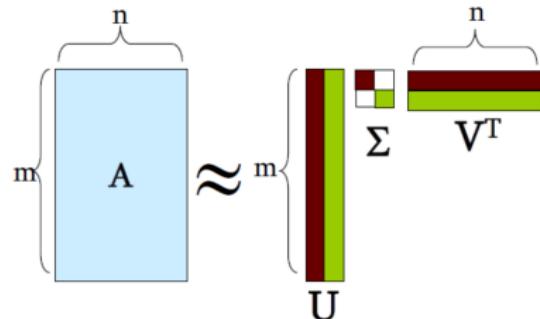
Let the SVD of $A \in \mathbb{R}^{m \times n}$ be given. If $k < r = \text{rank}(A)$ and $A_k = \sum_{i=1}^k \sigma_i u_i v_i^T$, then

$$\min_{\text{rank}(B)=k} \|A - B\|_2 = \|A - A_k\|_2$$

- The theorem says SVD gives a best solution minimizing the mean square error given a certain rank.

What is SVD?

- A : Input data matrix
- U : Left singular vectors
- V : Right singular vectors
- Σ : Singular values
- SVD gives the minimum reconstruction error (SSE)!



$$\min_{U, V, \Sigma} \sum_{ij} (A_{ij} - [U \Sigma V^T]_{ij})^2$$

- In our case, “SVD” on Netflix data: $R \approx Q \cdot P^T$, i.e., $A = R$, $Q = U\Sigma$, $P^T = V^T$
- But, we are not done yet! **R has missing entries!**

Regularized Matrix Factorization

- Minimize SSE on the training data!
- Use specialized methods to find P, Q such that $\hat{r}_{ix} = q_i \cdot p_x^T$

$$\min_{P, Q} \sum_{(i, x) \in \text{training}} (r_{ix} - q_i \cdot p_x^T)^2$$

We don't require cols of P, Q to be orthogonal/unit length.

- P, Q map users/movies to a latent space.

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We don't require cols of P, Q to be orthogonal/unit length.

- P, Q map users/movies to a latent space.
- Add regularization [Srebro et al., 2004]:

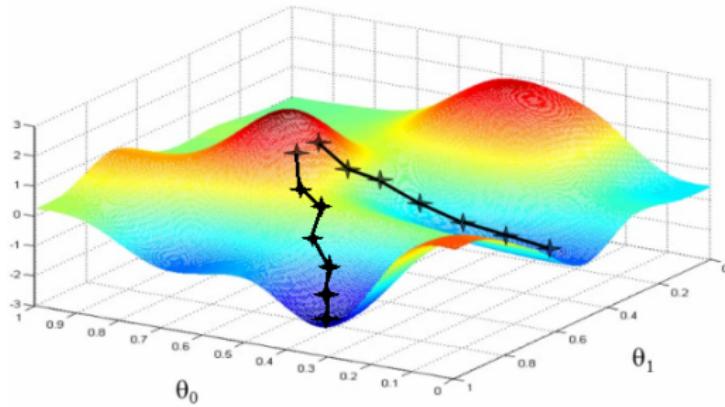
$$\min_{P, Q} \sum_{(i, x) \in \text{training}} (r_{ix} - q_i \cdot p_x^T)^2 + \lambda \left[\sum_i \|q_i\|_2^2 + \sum_x \|p_x\|_2^2 \right]$$

λ is called regularization parameters.

How to Optimize?

$$\min_{P, Q} \sum_{(i, x) \in \text{training}} (r_{ix} - q_i \cdot p_x^T)^2 + \lambda \left[\sum_i \|q_i\|_2^2 + \sum_x \|p_x\|_2^2 \right]$$

- Non-convex, exactly **biconvex**: convex to p or q , but non-convex to (p, q) .
- Lots of local minima, which means initializations are important.



Alternating Least Square (ALS)

Since the problem is convex to P and Q separately, so we can use the alternating least square (ALS) method,

- Repeat

- Fix P and solve $\min_Q \sum_{i \in \text{training}} (r_{ix} - q_i \cdot p_x^T)^2 + \lambda \left[\sum_i \|q_i\|_2^2 \right]$

- Fix Q and solve

$$\min_P \sum_{x \in \text{training}} (r_{ix} - q_i \cdot p_x^T)^2 + \lambda \left[\sum_x \|p_x\|_2^2 \right]$$

Alternating Least Square (ALS)

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- Fix Q and solve

$$\min_P \sum_{x \in \text{training}} (r_{ix} - q_i \cdot p_x^T)^2 + \lambda \left[\sum_x \|p_x\|_2^2 \right]$$

Here, the ALS algorithm is as follows,

$$q_i = \left(\sum_{r_{ix} \in r_{i*}} p_x p_x^T + \lambda I_k \right)^{-1} \sum_{r_{ix} \in r_{i*}} r_{ix} p_x$$

$$p_x = \left(\sum_{r_{ix} \in r_{*x}} q_i q_i^T + \lambda I_k \right)^{-1} \sum_{r_{ix} \in r_{*x}} r_{ix} q_i$$

- Involve inverting a matrix.
- Not only computationally expensive but also numerically unstable.

The Gradient Descent Method

$$\min_{P, Q} F(P, Q) := \sum_{(i, x) \in \text{training}} (r_{ix} - q_i \cdot p_x^T)^2 + \lambda \left[\sum_i \|q_i\|_2^2 + \sum_x \|p_x\|_2^2 \right]$$

Gradient descent:

- Initialize P and Q (using SVD, pretend missing ratings are 0).
- Do gradient descent:

- $P^{k+1} \leftarrow P^k - \tau \nabla_P F(P^k, Q^k)$
- $Q^{k+1} \leftarrow Q^k - \tau \nabla_Q F(P^k, Q^k)$

$$\text{where } (\nabla_Q F)_{if} = -2 \sum_{ix} (r_{ix} - q_i p_x^T) p_{xf} + 2\lambda q_{if}.$$

Computing gradients is slow when the dimension is huge.

The Stochastic Gradient Descent (SGD)

Let q_{if} be entry f of row q_i of matrix Q

$$(\nabla_Q F)_{if} = \sum_{i,x} (-2(r_{ix} - q_i p_x^T) p_{xf} + 2\lambda q_{if}) = \sum_{i,x} \nabla_Q F(r_{ix})$$

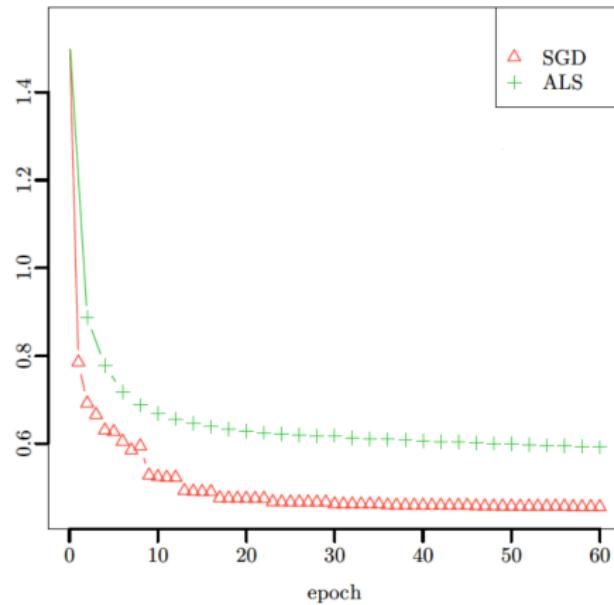
$$(\nabla_P F)_{xf} = \sum_{i,x} (-2(r_{ix} - q_i p_x^T) q_{if} + 2\lambda p_{xf}) = \sum_{i,x} \nabla_P F(r_{ix})$$

Stochastic gradient decent:

- Instead of evaluating gradient over all ratings, evaluate it for each individual rating and make a step
 - $P \leftarrow P - \tau \nabla_P F(r_{ix})$
 - $Q \leftarrow Q - \tau \nabla_Q F(r_{ix})$
- More steps but each step is computed much faster.

Comparison of Different Optimization Algorithms

Small steps! Big Difference!!!



Connections with the Probabilistic Matrix Factorization (PMF)

- PMF [Salakhutdinov, 2008] is a simple probabilistic linear model with the Gaussian observation noise.
- Given the feature vectors for the user and the movie, the distribution of the corresponding rating is:

$$p(r_{ix}|q_i, p_x, \sigma^2) = \mathcal{N}(r_{ix}|q_i p_x^T, \sigma^2)$$

- The user and movie feature vectors are given zero-mean spherical Gaussian priors:

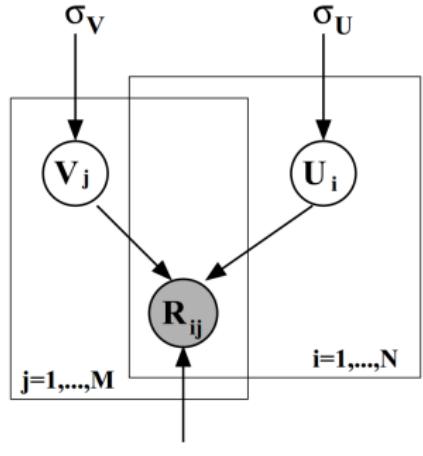
$$p(Q|\sigma_q^2) = \prod_{i=1}^M \mathcal{N}(q_i|0, \sigma_q^2 I), \quad p(P|\sigma_p^2) = \prod_{x=1}^N \mathcal{N}(p_x|0, \sigma_p^2 I)$$

The Graphical Model View for the PMF

- MAP Learning: Maximize the log posterior over movie and user features with fixed hyperparameters.
- Equivalent to minimizing the sum-of-squared-errors with quadratic regularization terms:

$$E = \frac{1}{2} \sum_{i=1}^M \sum_{x=1}^N I_{ix} (r_{ix} - q_i p_x^T)^2 + \frac{\lambda_q}{2} \sum_{i=1}^M \|q_i\|_2^2 + \frac{\lambda_p}{2} \sum_{x=1}^N \|p_x\|_2^2$$

$\lambda_q = \sigma^2 / \sigma_{q'}^2$, $\lambda_p = \sigma^2 / \sigma_{p'}^2$, and $I_{ix} = 1$ if user i rated movie x and is 0 otherwise.



MAP versus Regularized Least-Squares

- MAP under Gaussian Model:

$$E = \frac{1}{2} \sum_{i=1}^N \sum_{x=1}^M \mathbf{I}_{ix} (r_{ix} - q_i p_x^T)^2 + \frac{\lambda_q}{2} \sum_{i=1}^N \|q_i\|_2^2 + \frac{\lambda_p}{2} \sum_{x=1}^M \|p_x\|_2^2$$

- Least-squares matrix completion with L_2 regularization:

$$\min_{Q, P} \frac{1}{2} \sum_{r_{ix}} (q_i \cdot p_x^T - r_{ix})^2 + \frac{\lambda_q}{2} \|Q\|_F^2 + \frac{\lambda_p}{2} \|P\|_F^2$$

- Understanding as a probabilistic model is very useful!
 - Change priors.
 - Incorporate other sources of information or dependencies.

Probabilistic Models on Matrix Factorization

- Imposing different priors on U and V and assuming the underlying distribution of the residual will lead to different models.

$$X = UV + \varepsilon$$

- Probabilistic PCA [Tipping and Bishop, 1997]: isotropic Gaussian prior on V , ε follows i.i.d Gaussian.
- GLAD [Saddiki et al., 2014]: Laplace prior on U and Dirichlet prior on V , ε follows i.i.d Gaussian.
- Probabilistic approaches provide flexible ways to address the uncertain nature of the data!!!

Summary

- In matrix factorization, the matrix is assumed to be low-rank.
- For example, in the recommendation system, we think users' tastes are decided by several features,
 - genders, characters, locations, ...
- Does it make sense to subtract 2 characters?
- Nonnegativity seems to be necessary!!!

Data is often Nonnegative by Nature

- pixel intensities
- amplitude spectra
- occurrence counts
- food or energy consumption
- user scores
- stock market values
- ...

For the sake of interpretability, optimal processing of nonnegative data may call for processing under nonnegativity constraints.

Data is often Nonnegative by Nature

- pixel intensities
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For the sake of interpretability, optimal processing of nonnegative data may call for processing under nonnegativity constraints.

Nonnegative Matrix Factorization (**NMF**) provides an unsupervised linear representation of the data [Lee and Seung, 1999].

NMF vs SVD

Property	NMF	SVD
Formulation	$A = WH$	$A = U \sum V^T$
Optimality (in terms of squared distance)	✗	✓
Speed and robustness	✗	✓
Uniqueness	✗	✓
Sensitivity to initialization	✓	✗
Orthogonality	✗	✓
Sparsity	✓	✗
Non-nongativity	✓	✗
Interpretability	✓	✗

NMF Completion (NMFC)

Model [Xu et al., 2012]:

$$\begin{array}{ll} \min & \|\mathcal{P}_\Omega(XY - M)\|_F \\ \text{s.t.} & X \geq 0, Y \geq 0 \end{array} \iff \begin{array}{l} \min & \frac{1}{2} \|XY - Z\|_F^2 \\ \text{s.t.} & X = U, Y = V \\ & U \geq 0, V \geq 0 \\ & \mathcal{P}_\Omega(Z - M) = 0 \end{array}$$

Augmented Lagrangian function:

$$\begin{aligned} \mathcal{L}_A(X, Y, Z, U, V, \Lambda, \Pi) = & \frac{1}{2} \|XY - Z\|_F^2 + \Lambda \bullet (X - U) + \Pi \bullet (Y - V) \\ & + \frac{\alpha}{2} \|X - U\|_F^2 + \frac{\beta}{2} \|Y - V\|_F^2 \end{aligned}$$

where $A \bullet B := \sum_{i,j} a_{ij} b_{ij}$.

Optimization

Lots of algorithms for NMF have been developed,

- Projected Gradient
- Active Set
- Nesterov's optimal gradient
- Proximal Alternating Non-negative Least Square

The matrix is incomplete. Not all exiting algorithms are applicable.

Optimization

Lots of algorithms for NMF have been developed,

- Projected Gradient
- Active Set
- Nesterov's optimal gradient
- Proximal Alternating Non-negative Least Square

The matrix is incomplete. Not all exiting algorithms are applicable.

- **The Alternating Direction Method of Multipliers (ADMM)**
 - with good robustness of method of multipliers
 - which can support decomposition

Basic Idea of ADMM

- ADMM problem form (with f, g convex),

$$\begin{array}{ll}\text{minimize} & f(x) + g(z) \\ \text{subject to} & Ax + Bz = c\end{array}$$

- 2 sets of variables, with separable objective.
- $L_\rho(x, z, y) = f(x) + g(z) + y^T(Ax + Bz - c) + (\rho/2)\|Ax + Bz - c\|_2^2$
- ADMM:

$$x^{k+1} := \operatorname{argmin}_x L_\rho(x, z^k, y^k) \quad // \text{x-minimization}$$

$$z^{k+1} := \operatorname{argmin}_z L_\rho(x^{k+1}, z, y^k) \quad // \text{z-minimization}$$

$$y^{k+1} := y^k + \rho (Ax^{k+1} + Bz^{k+1} - c) \quad // \text{dual update}$$

ADMM for NMFC

$$\begin{aligned}X_{k+1} &= (Z_k Y_k^T + \alpha U_k - \Lambda_k) (Y_k Y_k^T + \alpha I)^{-1} \\Y_{k+1} &= (X_{k+1}^T X_{k+1} + \beta I)^{-1} (X_{k+1}^T Z_k + \beta V_k - \Pi_k) \\Z_{k+1} &= X_{k+1} Y_{k+1} + \mathcal{P}_\Omega (M - X_{k+1} Y_{k+1}) \\U_{k+1} &= \mathcal{P}_+ (X_{k+1} + \Lambda_k / \alpha) \\V_{k+1} &= \mathcal{P}_+ (Y_{k+1} + \Pi_k / \beta) \\\Lambda_{k+1} &= \mathcal{N}_k + \gamma \alpha (X_{k+1} - U_{k+1}) \\\Pi_{k+1} &= \Pi_k + \gamma \beta (Y_{k+1} - V_{k+1})\end{aligned}$$

where $(\mathcal{P}_+(A))_{ij} = \max\{a_{ij}, 0\}$.

Outline

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2 Exact Matrix Completion

3 Approximate Matrix Completion

- Nuclear Norm Minimization
- Low-Rank Matrix Factorization
- **Distributed Matrix Completion**

4 Follow-up Research

Distributed Matrix Completion

- Real applications can be large,
 - Millions of users, Millions of items, Billions of ratings
 - e.g., Netflix: $\geq 20M$ users, $\geq 20k$ movies, $\geq 4B$ ratings (projected)
- Scalable algorithms are necessary!!!
- Existing MapReduce algorithms, e.g.,
 - DALS [Zhou et al., 2008]
 - DSGD-MR [Gemulla et al., 2011]
 - ASGD [Yun et al., 2013]
 - DSGD++ [Gemulla et al., 2011]
 - ...

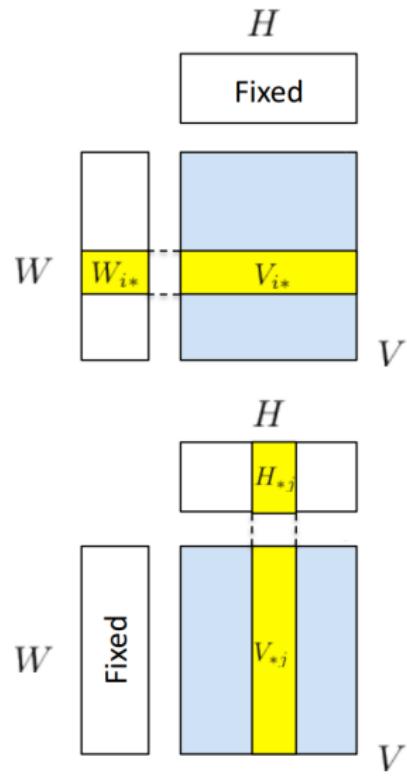
Distributed Alternating Least Squares (DALS)

Alternate

- Fix H optimize for W .
- Fix W optimize for H .
- For each column/row: solve a least squares problem.

Drawbacks

- Slow (cubic in rank).
- Memory intensive (stores data matrix twice).



SGD for Matrix Factorization

- Set $\theta = (W; H)$ and use

$$L(\theta) = \sum_{(i,j) \in Z} L_{ij}(\mathbf{W}_{i*}, \mathbf{H}_{*j})$$

$$L'(\theta) = \sum_{(i,j) \in Z} L'_{ij}(\mathbf{W}_{i*}, \mathbf{H}_{*j})$$

$$\hat{L}'(\theta, z) = N \cdot L'_{i,j_z}(\mathbf{W}_{i_z*}, \mathbf{H}_{*j})$$

where N is all the observed values.

- SGD epoch

- Pick a random entry $z \in Z$
- Compute approximate gradient $\hat{L}'(\theta, z)$
- Update parameters

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

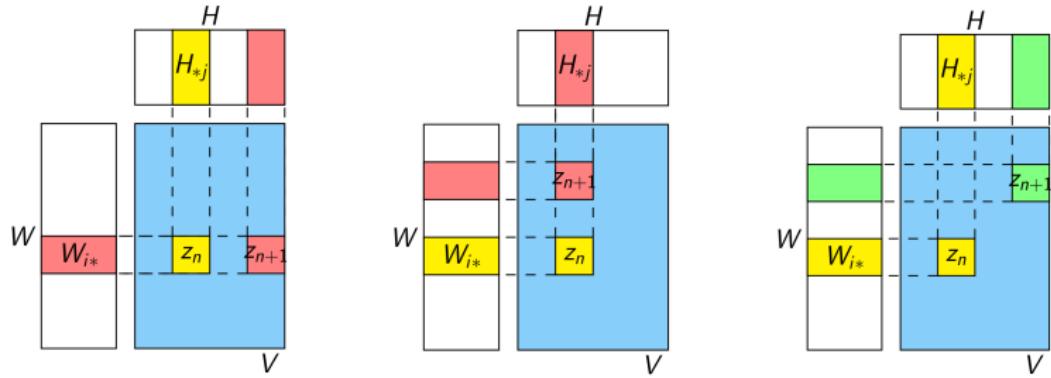
- Repeat N times

Distributed SGD (DSGD)

- SGD steps depend on each other,

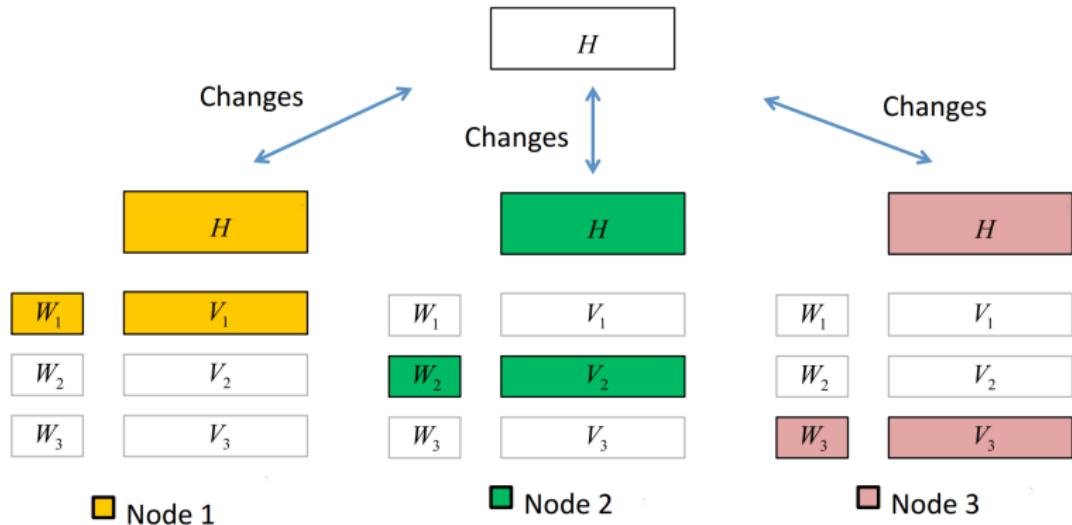
$$\theta_{n+1} = \theta_n - \epsilon_n \hat{L}'(\theta_n)$$

- An SGD step on example $z \in Z$,
 - Reads W_{i_z*} and H_{*j_z}
 - Performs gradient computation $L'_{ij}(W_{i_z*}, H_{*j_z})$
 - Updates W_{i_z*} and H_{*j_z}
- Not all steps are dependent!

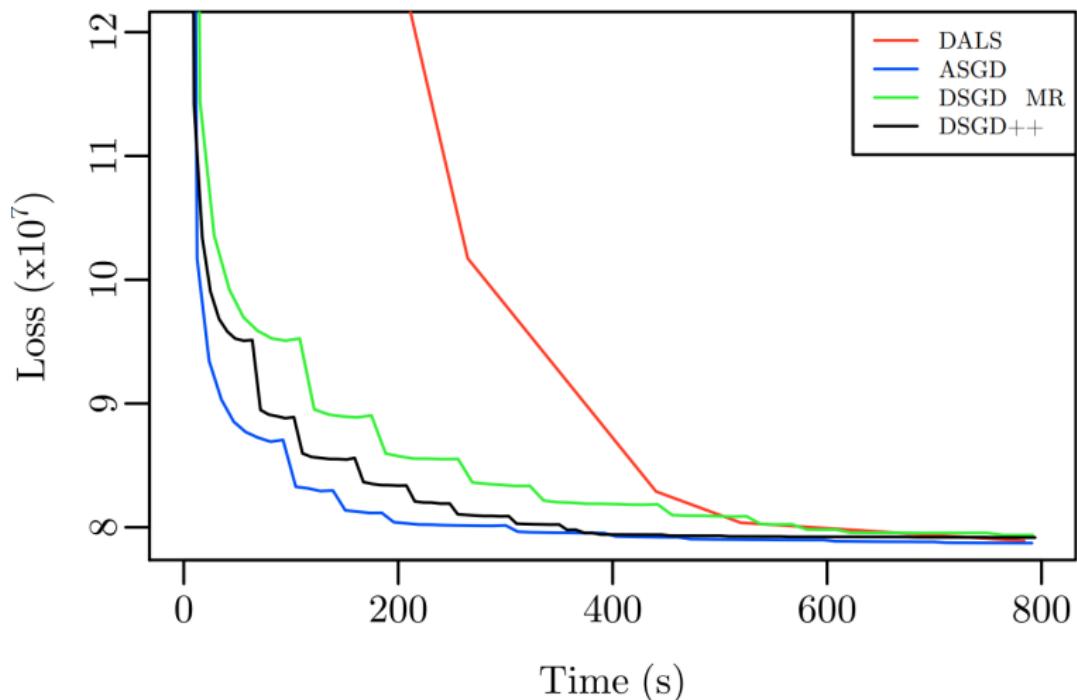


Asynchronous SGD (ASGD)

- Each node works on a local copy of the movie matrix H .
- Local copies are synchronized continuously.



Experiments with Netflix Data



Extended Studies

- There have been lots of techniques and studies on distributed matrix completion,
 - distributed non-negative matrix factorization [[Liu et al., 2016](#)]
 - distributed nuclear norm minimization [[Mardani et al., 2012](#)]
- Because of the variable separation property, ADMM has been adopted in distributed matrix factorization,
 - A distributed NMF with an ADMM algorithm [[Sun and Fevotte, 2014](#)]
 - A stochastic ADMM to matrix factorization [[Yu et al., 2014](#)]
 - ...

Nuclear Norm Minimization vs Direct (Bilinear) Low Rank Solutions

- Nuclear norm minimization:

$$\min_X f(X - M) + \lambda \|X\|_* \quad (*)$$

- convex, global optima, close to truth.
- X is very large, solvers are very slow and non-scalable.
- Low rank approximation:

$$\min_{U,V} f(M - UV^\top) + \frac{\lambda}{2} (\|U\|_F^2 + \|V\|_F^2) \quad (**)$$

- non-convex, many local optima, non-robust.
- less parameters, faster solvers.

Nuclear Norm Minimization vs Direct (Bilinear) Low Rank Solutions

In fact, under some conditions, the local optima of (**) are global optima of (*).

[Boumal et al., 2016]

Let $f(X - M)$ be convex in M , and X^* be an optimal solution of (*) with $\text{rank}(X^*) = k^*$. Then, any solution $X^{**} = UV^\top$ of (**) with $r \geq k^*$ is a solution of (*). [r is the column number of U]

Summary

- Though nuclear norm minimization is convex, it's largely limited by its memory requirements and nonscalable algorithms.
- Matrix Completion based on matrix factorization has made great success in last 10 years!
- Sometimes local minima is good enough for our problem.
- The winner of Netflix Prize win 1000000 dollars relying on matrix factorization.
- Matrix factorization is still very instructive in many domains, e.g., clustering, dimension reduction etc.

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- Link Prediction on Graphs with Deep Learning
- Matrix Completion under Missing Mechanisms

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Build Graphs with Additional Information

- In real problems such as the Netflix task, additional information can be obtained (e.g., users' age, gender, hobbies, education, movies' genre, release year, actors, origin country, etc).
- This additional information can be taken advantage of with **graphs** to encode relationships between users and movies.

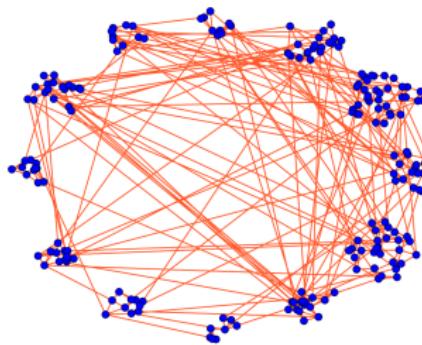


Figure: Graph of users: there will be an edge between two similar-taste users

Graph-regularized Matrix Completion (GMC)

- In matrix completion, we want the reconstructed vectors x_j, x'_j in $X = (x_1, \dots, x_n)$ to be close if $e_{j,j'} \in E_c$.
- Stated differently, we want

$$\sum_{j,j'} w_{jj'}^c \|x_j - x_{j'}\|_2^2 = \text{tr}(XL_cX^\top) = \|X\|_{\mathcal{D},c}^2$$

to be small, where $D_c = \text{Diag}(\sum_{j'=1}^n w_{jj'}^c)$, $L_c = D_c - W_c$ is the Laplacian of the column graph G_c , and $\|\cdot\|_{\mathcal{D},c}$ is the graph Dirichlet semi-norm for columns. Similarly, we can get $\|X\|_{\mathcal{D},r}^2$.

- These smoothness terms can be seen as regularization terms [Benzi et al., 2016]

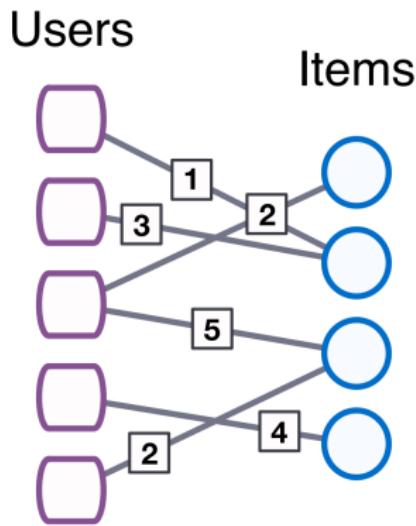
$$\min_X \gamma_n \|X\|_* + \ell(\mathcal{P}_\Omega(X), \mathcal{P}_\Omega(M)) + \frac{\gamma_r}{2} \|X\|_{\mathcal{D},r}^2 + \frac{\gamma_c}{2} \|X\|_{\mathcal{D},c}^2$$

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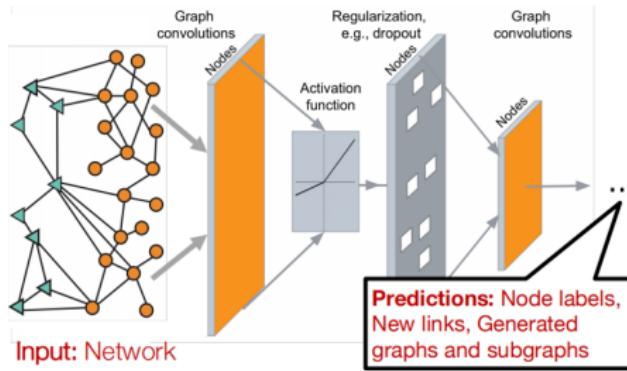
Link Prediction on Graphs

- Undirected weighted graphs can be built among users and items (in the recommendation systems).
- A bipartite graph can also be built between users and items.
- Thus, matrix completion problem can turn to be a **link prediction** problem.



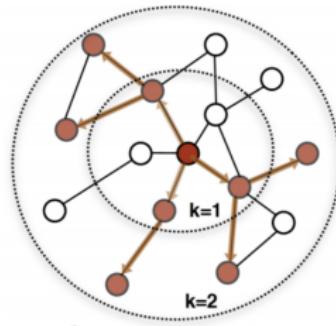
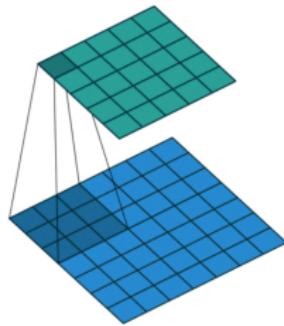
Graph Neural Network (GNN): Deep learning on Graphs

- Graph Neural Networks(GNN) [Scarselli et al., 2009] are designed to solve graphical problem with deep learning.
- Similar structure as deep feedforward neural network: convolution, activation, dropout...
- Convolution and output functions need to be designed specifically according to the data and the task.



Graph Convolutional Networks

- Define Graph Convolutional Networks (GCN) like CNN [Kipf and Welling, 2016].
- In CNN, convolutional operations are sliding on a rectangular tensor.
- In GCN, convolutional are sliding on the vertexes, where kernel covering all the neighbor vertexes.



- The above picture depicts when the kernel size is 1 and 2.

Graph Convolutional Networks

- Graph convolution: nodes aggregate information from their neighbors.
- Every vertex can be encoded into a representation vector with multi-layer graph convolution.
- In the Netflix task, one get the users and movies representation U and V respectively.

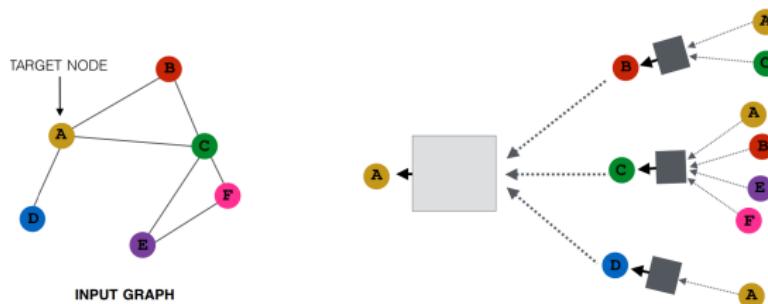


Figure: 2-order convolution: all 2 unit distance nodes information flows into the central node

What's the Output?

- Now we get users and movies representations U and V .
- How to predict the weighted edges between them?
- A commonly used activation function in link prediction is a little like softmax,

$$p(\check{M}_{ij} = r) = \frac{e^{u_i^T Q_r v_j}}{\sum_{s \in R} e^{u_i^T Q_s v_j}}$$

- In the Netflix task, r is 1-5.

Graph Convolutional Matrix Completion

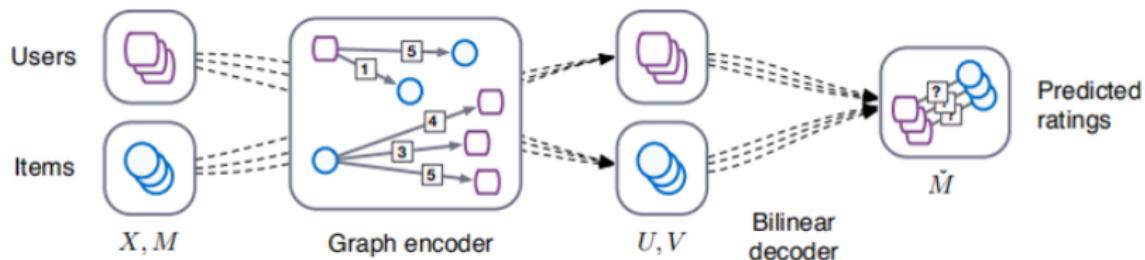


Figure: structure of graph neural network in link prediction

- Matrix Factorization is limited by its expressive ability, failing to mine deep information in the data.
- Graph Neural Network achieves the state-of-the-art results [Berg et al., 2017].

Outline

- 1 What is Matrix Completion?
- 2 Exact Matrix Completion
- 3 Approximate Matrix Completion
- 4 Follow-up Research
 - Graph-regularized Matrix Completion
 - Link Prediction on Graphs with Deep Learning
 - Matrix Completion under Missing Mechanisms

Matrix Completion under Missing Mechanisms

- Most existing studies adopt a uniform observation mechanism.
- This leads to significant simplifications, and enables the domain to move forward rapidly with various theoretical breakthroughs.
- However, uniform mechanism is often unrealistic.
- Several studies have been devoted to relaxing such an restrictive assumption by adopting other missing structures.

Non-uniform Missing Mechanisms

- Why non-uniform Missing Mechanism is necessary?
- In movie recommender system,
 - users tend to rate movies that they prefer or dislike most, while often remain silent to other movies.
- In the online merchandising,
 - users may purchase certain items regularly without often rating them, but evaluate products that they rarely buy with a higher chance.
- Similar to the latent factor model, it is reasonable to believe that the missingness is also governed by a small and possibly different set of hidden factors.

How to Model the Missing Mechanism?

- In matrix completion setting, for the $(i; j)$ -th entry, define the sampling indicator $w_{ij} = 1$ if it's observed, and 0 otherwise.
- As for the sampling mechanism, we adopt a Bernoulli model where w_{ij} are independent Bernoulli random variables with observation probabilities θ_{ij} , collectively denoted by a matrix Θ ,

$$\Theta := (\theta_{ij})_{i,j=1}^{n_1, n_2} \in (0, 1)^{n_1 \times n_2}$$

- Similar to the latent factor model, it is also believed Θ is low-rank.

Low-rank Modeling of Θ

- There have been lots of studies on how to model the missing mechanism Θ .
 - [Srebro and Salakhutdinov, 2010] utilize an independent row and column sampling mechanism, leading to a rank-1 structure for Θ .
 - [Cai et al., 2016] consider a block structure for Θ and hence M can be regarded as a special case of the low-rank modeling.
 - [Mao et al., 2018] consider Θ is dependent on some hidden factors, which reflects situations when obvious covariates are unknown or not available.
 - Still a hot area currently ...

Weighted Loss Function

- Once we get the probability matrix Θ , we induce the weighted nuclear norm minimization loss,

$$\min_X \|\Theta \circ (X - M)\|_2 + \lambda \|X\|_*$$

- Or weighted low rank matrix factorization loss,

$$\min_X \|\Theta \circ (M - WH)\|_2 + \lambda (\|W\|_2 + \|H\|_2)$$

- Thus, attention will be focused on the entries with high probability!!!
- Optimization is similar to the original problem.

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