# Algorithm Foundations of Data Science and Engineering

## Lecture 9: Matrix Factorization

YANHAO WANG

DaSE @ ECNU
(for course related communications)
yhwang@dase.ecnu.edu.cn

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# Outline

# Motivation

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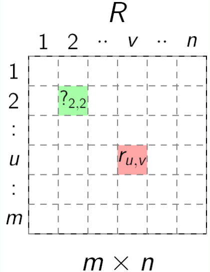
For recommender systems: a group of users give ratings to some items.

| User | Item | Rating |
|---|---|---|
| 1 | 5 | 100 |
| 1 | 10 | 80 |
| 1 | 13 | 30 |
| 2 | 10 | 50 |
| ... | ... | ... |
| $u$ | $v$ | $r$ |
| ... | ... | ... |

# Matrix with missing value



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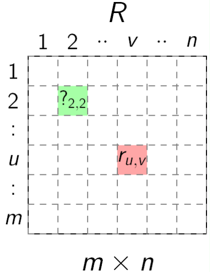


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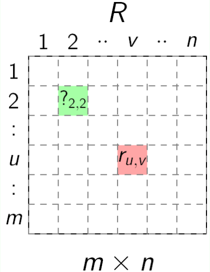


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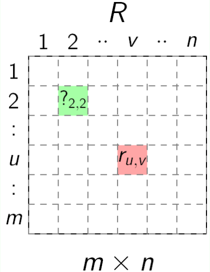


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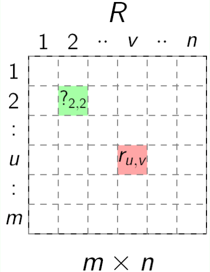


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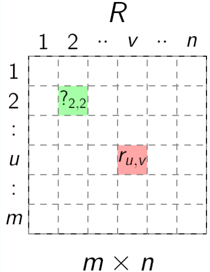


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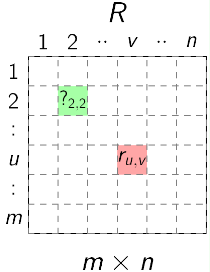


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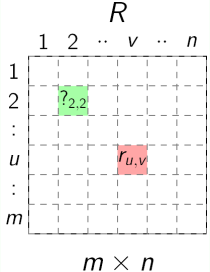


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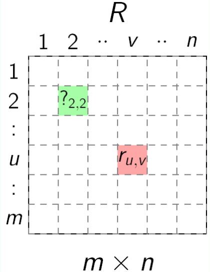


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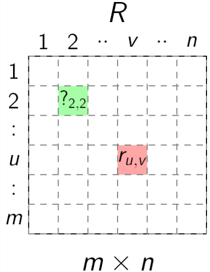


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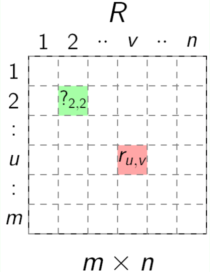


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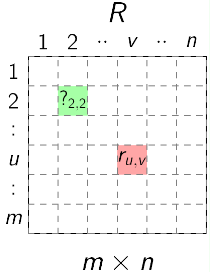


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The given matrix can be used to model the online user behaviors.

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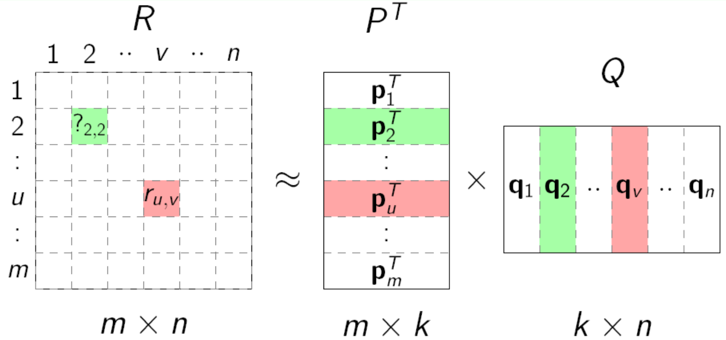

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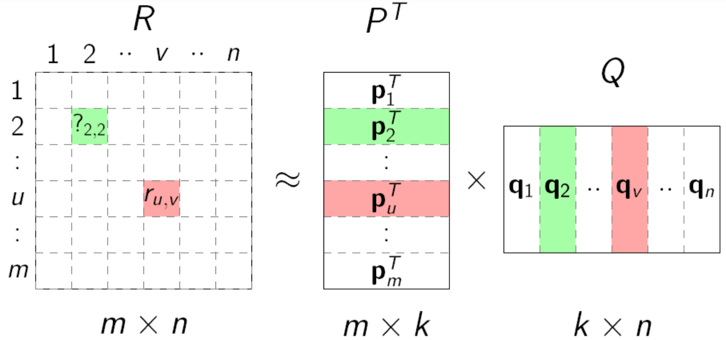


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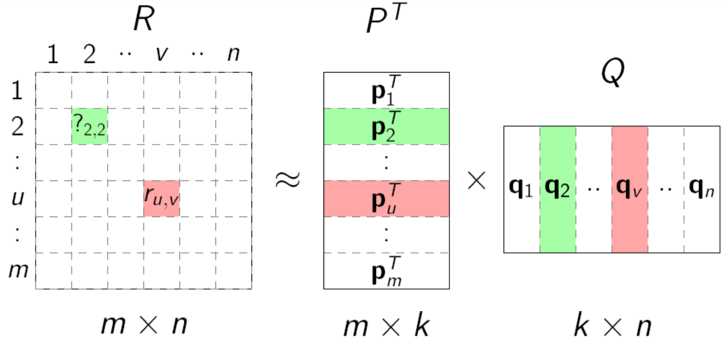


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- $r_{u,v} = \mathbf{p}_u^T \mathbf{q}_v$.

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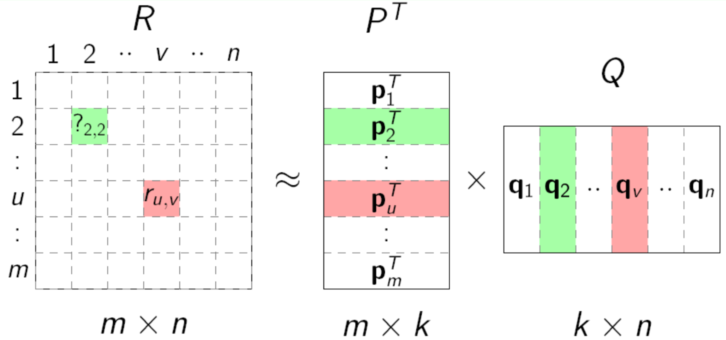


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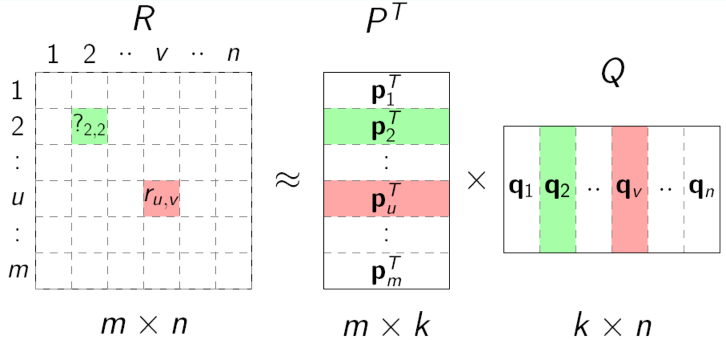


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The approach is called matrix factorization, i.e., $R_{n \times m} \approx P_{n \times k} \cdot Q_{k \times m}$

# Optimization

Much of supervised machine learning can be written as an optimization problem

$$\min_{\mathbf{x}} \sum_{i=1}^{N} f(\mathbf{x}; y_i)$$

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  - Convex optimization: the easy case;
  - Non-convex optimization: NP-hard in general, includes deep learning.

# Outline

# Convex functions

**Definition**

Function $f(x)$ is a convex function if $\forall \alpha \in [0, 1]$,

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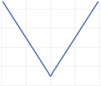

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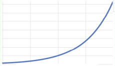

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Examples of convex functions

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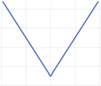

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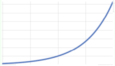

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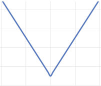

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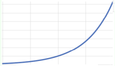

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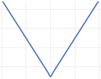

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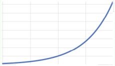

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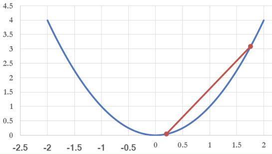

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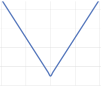

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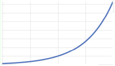

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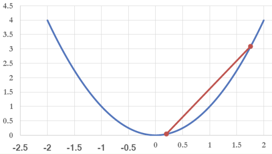


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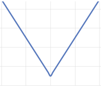

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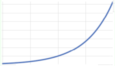

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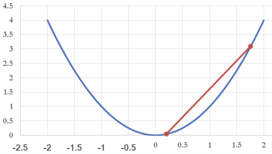


Any line segment we draw between two points lies above the curve.
Every local minimum is a global minimum.

## Properties of convex functions

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- Compositions of convex functions are **NOT** generally convex, except for convex nondecreasing functions.

$$h(x) = f(g(x)) \text{ (Neural nets are like this)};$$

For example, if $f(x) = e^{-x}$ on $[0, \infty)$, then $f$ is convex, but $f \circ f$ is concave.

# Outline

# Gradient descent

## Problem formulation

Consider unconstrained, smooth convex optimization

$$\min_{\mathbf{x}} f(\mathbf{x})$$

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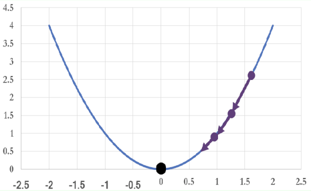
## Gradient descent algorithm

1: Pick a starting point $\mathbf{x}^{(0)} \in \mathbb{R}^n$;
2: For $k = 1, 2, \cdots$;
3: $\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} - \lambda \cdot \nabla f(\mathbf{x}^{(k-1)})$;
where $\lambda$ is the step size.



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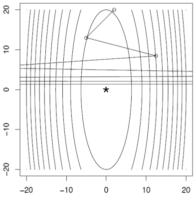


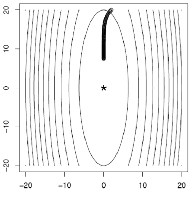

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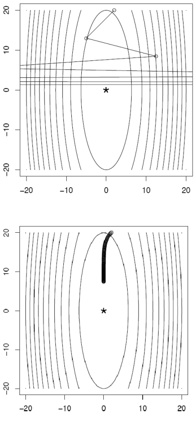


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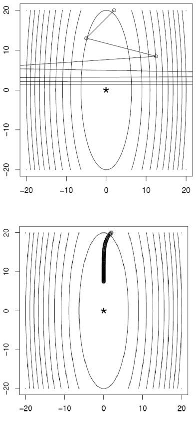


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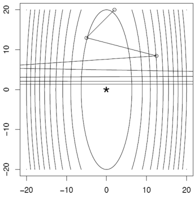


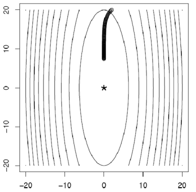


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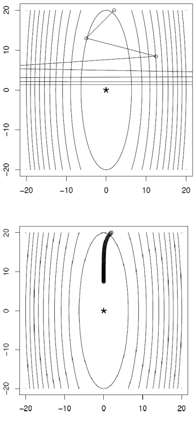


(Refer to [a])

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- Simply take a large value of $\lambda$, it will slowly converge (after 8 iterations).
- It can also be slow if $\lambda$ is to small (after 100 iterations).
- When $f$ is additionally Lipschitz continuous with constant $L > 0$, the gradient descent has convergence rate $O(1/k)$, i.e., to get $f(\mathbf{x}^{(k)}) - f^* \leq \epsilon$, we need $O(\frac{1}{\epsilon})$ iterations.

[a] https://www.cs.rochester.edu/u/jliu/CSC-576/class-note-10.pdf

## The problem with Gradient descent

In many machine learning task, the cost function can be written as

$$h(\mathbf{x}) = \sum_{i=1}^{N} f(\mathbf{x}; y_i),$$

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If we want to scale up to huge datasets, so how can we do this? (Refer to [a])

[a] http://www.cs.cornell.edu/courses/cs6787/2017fa/Lecture1.pdf

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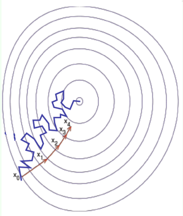
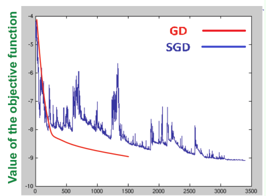
- Can SGD converge using just one example to estimate the gradient?

# SGD VS. GD

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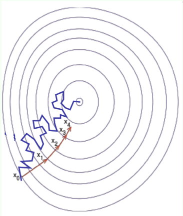

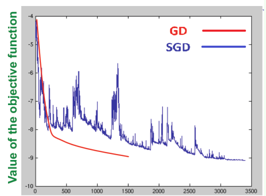


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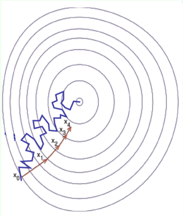


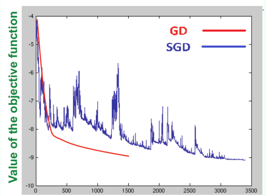


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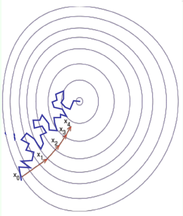


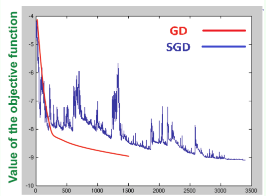


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- In practice, SGD is much faster!

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- Thus, the objective function is equal to the sum of the squares of the entries in the residual matrix $R - PQ^T$.
- This objective function can be viewed as a quadratic loss function, which quantifies the loss of accuracy in estimating the matrix $R$ with the use of low-rank factorization.

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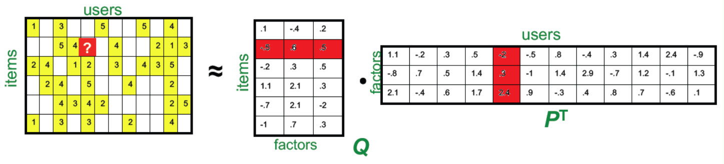
- Now, we have to find a way to obtain $P$ and $Q$.

# Matrix factorization Cont'd

## Example



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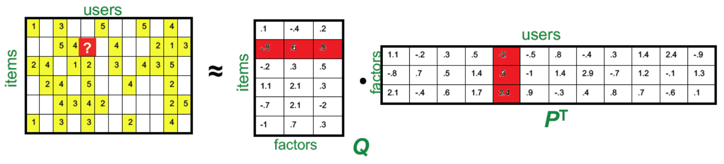


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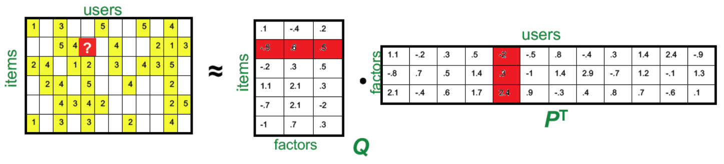


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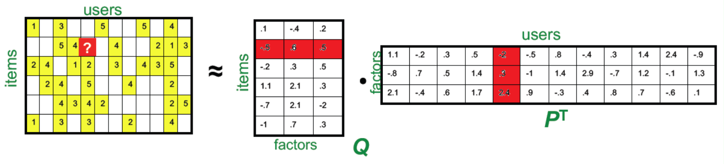


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The estimating error can be

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## Problem formulation

### Formal definition

$$J = \min_{P,Q} \frac{1}{2} \sum_{(u,i)\in\mathcal{K}} (r_{ui} - \mathbf{p}_u^T \mathbf{q}_i)^2,$$

where $r_{ui}$ is the known rating of user $u$ for item $i$, $\widehat{u}_{ui} = \mathbf{p}_u^T \mathbf{q}_i$ is the predicted rating given by user $u$ for item $i$, and the set of all user-item pair $(u, i)$, which are observed in $R$, be denoted by $\mathcal{K}$, i.e., $\mathcal{K} = \{(u, i) | r_{ui} \text{ is observed}\}$.

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# Batch gradient descent algorithm

## Estimate parameters iteratively

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- Subsequently, the updates can be computed as follows:
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# Outline

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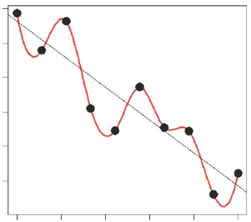

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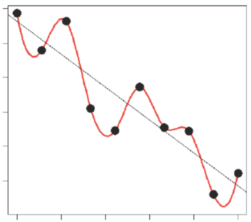

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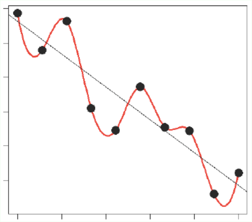

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- Regularization is a common approach to address the problem.

## Regularization

$$\min_{q^*,p^*} J = \frac{1}{2}\Big[\sum_{(u,i)\in\mathcal{K}} (r_{ui} - q_i^T p_u)^2 + \lambda(\|Q\|^2 + \|P\|^2)\Big],$$

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# Incorporating user and item biases

## Loss function

$$J = \frac{1}{2}\Big[\sum_{(u,i)\in\mathcal{K}} (r_{ui} - b_i - b_u - q_i^T p_u)^2 + \lambda(\|Q\|^2 + \|P\|^2 + \|b_u\|^2 + \|b_i\|^2)\Big]$$

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  - $p_{u(k+1)} = b_u$ and $p_{u(k+2)} = 1, \forall u \in \{1, 2, \cdots, n\}$
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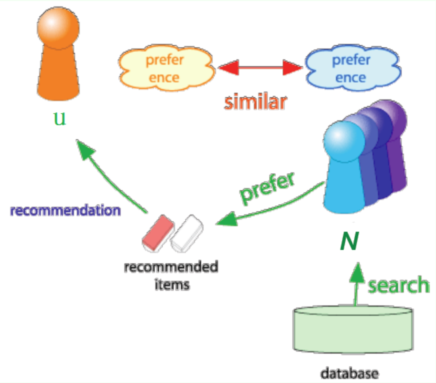
$$s.t. (k+2)\text{th column of } \widetilde{P} \text{ contains only 1s}$$

$$(k+1)\text{th column of } \widetilde{Q} \text{ contains only 1s}$$

# Outline

# Motivation of collaborative filtering



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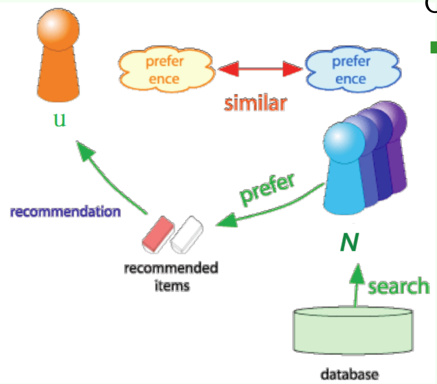


Consider user $U$

- Find set $S$ of other users whose ratings are "similar" to $u'$s ratings.

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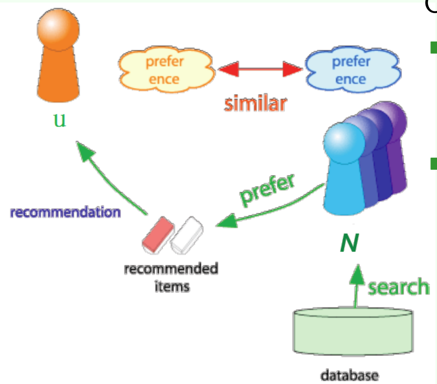


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- Estimate $u'$s ratings based on ratings of users in $S$.

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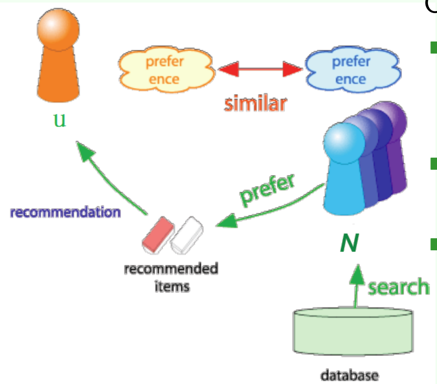


Consider user $U$

- Find set $S$ of other users whose ratings are "similar" to $u'$s ratings.
- Estimate $u'$s ratings based on ratings of users in $S$.
- Question: how to evaluate whose ratings are "similar" to $u'$s ratings.

# MF for collaborative filtering

## Problem formulation

$$J = \min_{P,Q} \frac{1}{2} \sum_{(u,i)\in\mathcal{K}} (r_{ui} - \mathbf{p}_u^T \mathbf{q}_i)^2 + \frac{\gamma}{2} \sum_{(u,v)\in\mathcal{U}} s_{uv} \|\mathbf{p}_u - \mathbf{p}_v\|_2^2,$$

where $r_{ui}$ is the known rating of user $u$ for item $i$, $\widehat{u}_{ui} = \mathbf{p}_u^T \mathbf{q}_i$ is the predicted rating given by user $u$ for item $i$, and $s_{uv}$ is the preference similarity between users $u$ and $v$.

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### Stochastic gradient descent

- $p_{uj}^{(t+1)} \leftarrow p_{uj}^{(t)} + \alpha\big(e_{ui}^{(t)} q_{ji}^{(t)} - \gamma s_{uv} (p_{uj}^{(t)} - p_{vj}^{(t)}) p_{uj}^{(t)}\big).$

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# Non-negative matrix factorization

## Formulation

Define an optimization problem as:

$$\begin{aligned}\text{Minimize } J &= \frac{1}{2}\|R - UV^T\|_F^2 \\ s.t. U &\geq 0 \\ V &\geq 0\end{aligned}$$

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# Solution for NMF

## Iterative algorithm

- $u_{ij}^{(t+1)} \leftarrow \frac{(RV^{(t)})_{ij} u_{ij}^{(t)}}{(U^{(t)} V^{(t)T} V^{(t)})_{ij} + \epsilon}$, $v_{ij}^{(t+1)} \leftarrow \frac{(R^T U^{(t)})_{ij} v_{ij}^{(t)}}{(V^{(t)} U^{(t)T} U^{(t)})_{ij} + \epsilon}$, where $\epsilon$ is a small term, e.g., $10^{-9}$.

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As in the case of other types of matrix factorization, regularization can be used to improve the quality of the underlying solution.

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- The update rules:
  - $u_{ij}^{(t+1)} \leftarrow \max\left\{ \left\lceil \frac{(RV^{(t)})_{ij} - \lambda_1 u_{ij}^{(t)}}{(U^{(t)} V^{(t)T} V^{(t)})_{ij} + \epsilon} \right\rceil u_{ij}^{(t)}, 0 \right\}$
  - $v_{ij}^{(t+1)} \leftarrow \max\left\{ \left\lceil \frac{(R^T U^{(t)})_{ij} - \lambda_2 v_{ij}^{(t)}}{(V^{(t)} U^{(t)T} U^{(t)})_{ij} + \epsilon} \right\rceil v_{ij}^{(t)}, 0 \right\}$

# Take-home messages

- Motivation
- Gradient Descent
  - Convex Functions
  - Gradient Descent
- Matrix Factorization
  - Gradient Descent algorithm
  - Regularization
  - Collaboration Filtering
- Non-negative Matrix Factorization