Algorithm Foundations of Data Science and Engineering

Lecture 6: Matrix Factorization

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Outline

1. Motivation
2. Gradient Descent
   - Convex Functions
   - Gradient Descent
3. Matrix Factorization
   - Gradient Descent Algorithm
   - Regularization
   - Collaborative Filtering
4. Non-negative Matrix Factorization

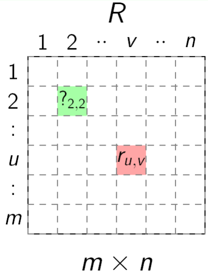
Motivation

Motivation

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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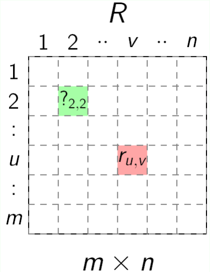

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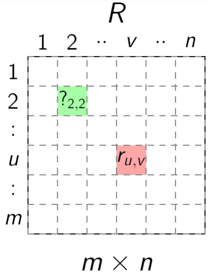

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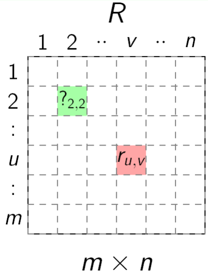

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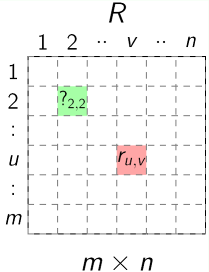

There are many missing values in the matrix, and many applications that can be modeled as the given matrix

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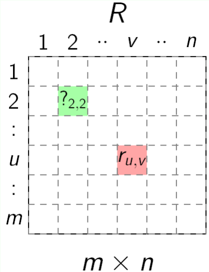

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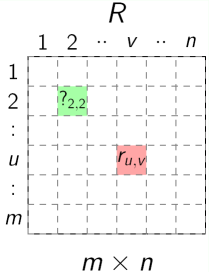

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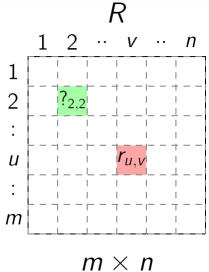

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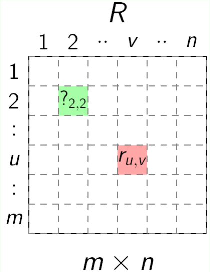

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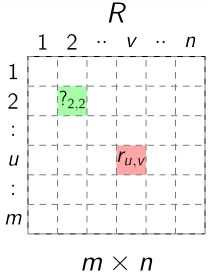

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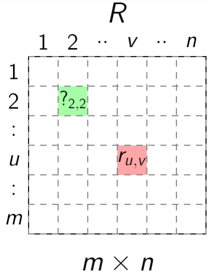

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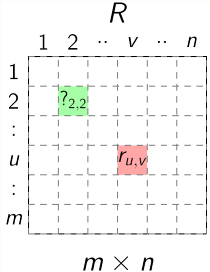

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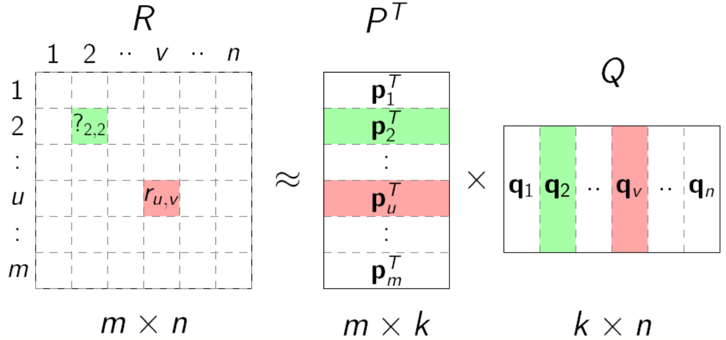
The given matrix can be used to model the online user behaviors.

Predicting the missing values



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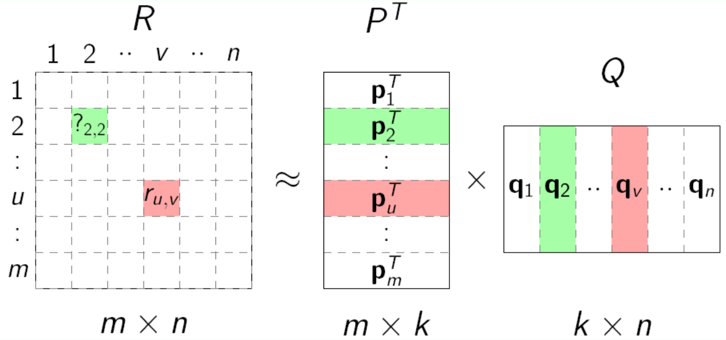

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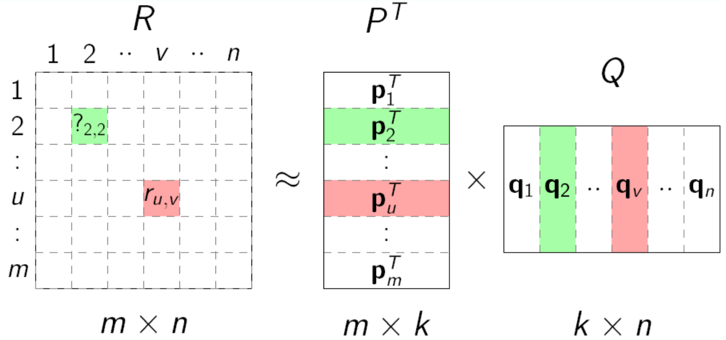

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- $r_{u,v} = \mathbf{p}_u^T \mathbf{q}_v$.

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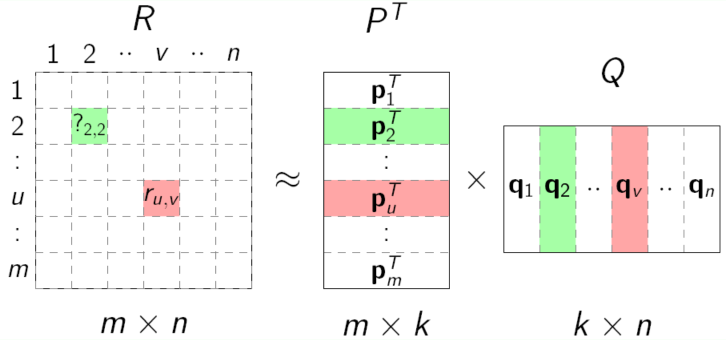

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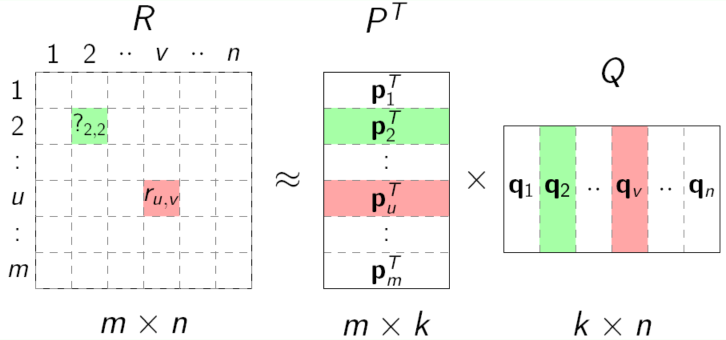

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The approach is called matrix factorization, i.e., $R_{n\times m} \approx P_{n\times k} \cdot Q_{k\times m}$

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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  - Non-convex optimization: NP-hard in general, includes deep learning.

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Convex functions

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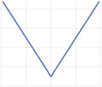

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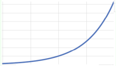

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Examples of convex functions

- $$f(x) = x^2;$$

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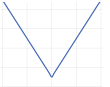

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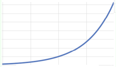

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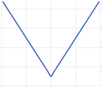

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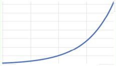

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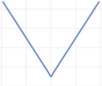

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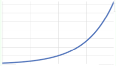

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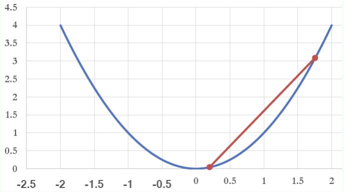

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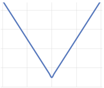

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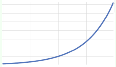

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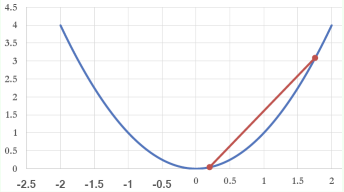

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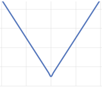

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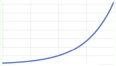

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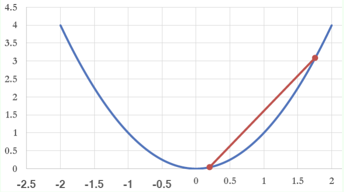

Any line segment we draw between two points lies above the curve.
Every local minimum is a global minimum.

Properties of convex functions

- Non-negative combinations of convex functions are convex

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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.

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Gradient descent

Problem formulation

Consider unconstrained, smooth convex optimization

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

i.e., f is convex and differentiable with $dom(f) = \mathbb{R}^n$.

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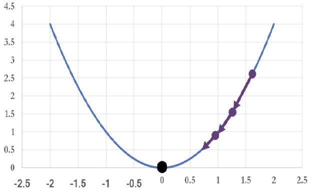
Gradient descent algorithm

1: Pick a starting point $\mathbf{x}^{(0)} \in \mathbb{R}^n$;

2: For $k = 1, 2, \cdots$;

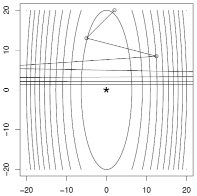
3: $\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} - \lambda \cdot \nabla f(\mathbf{x}^{(k-1)})$;

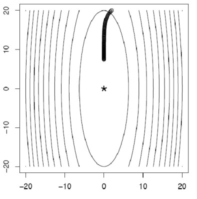
where λ is the step size.



 Gradient Descent

How to choose step size





How to choose step size

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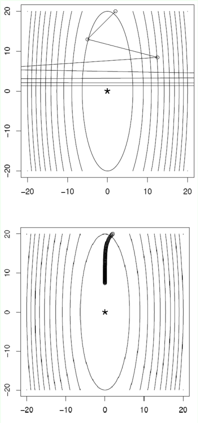

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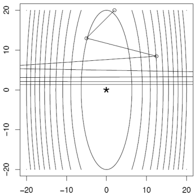

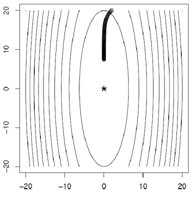

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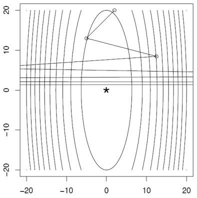

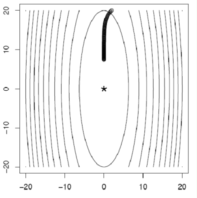

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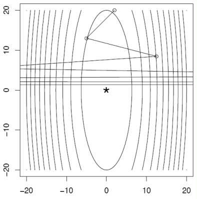
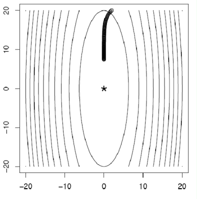
- It can also be slow if λ is to small (after 100 iterations).

How to choose step size





(Refer to [a])

Consider function $f(\mathbf{x}) = (10x_1^2 + x_2^2)/2$,

- Simply take a large value of λ, it will slowly converge (after 8 iterations).
- It can also be slow if λ 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

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

where f is the loss function, y_i is a training example.

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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

Stochastic Gradient Descent

Idea: rather than using the full gradient, just use one training example.

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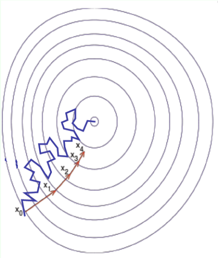
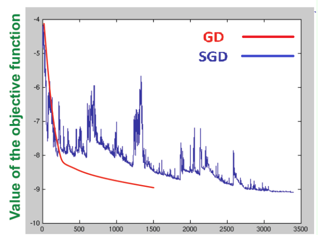
- Can SGD converge using just one example to estimate the gradient?

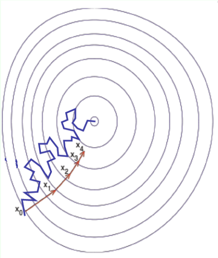
SGD VS. GD

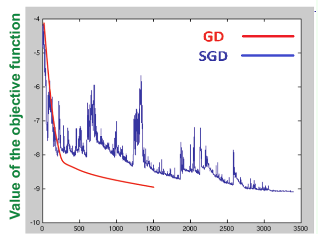




- GD improves the value of the objective function at every step.

SGD VS. GD





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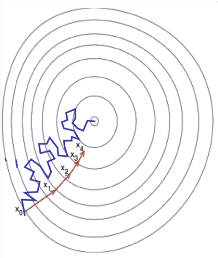

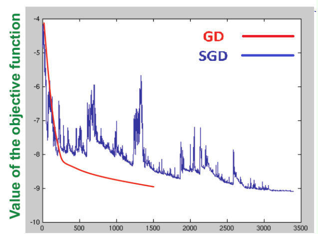

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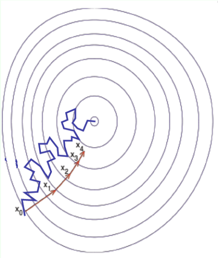

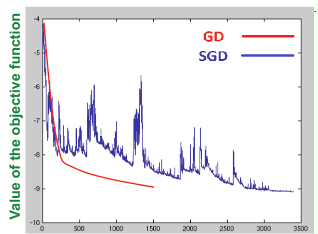

- GD improves the value of the objective function at every step.
- SGD improves the value but in a "noisy" way.
- GD takes fewer steps to converge but each step takes much longer to compute.
- In practice, SGD is much faster!

Matrix factorization

Motivation

How can one determine the factor matrices P and Q, so that the fully specified matrix R matches PQ^T as closely as possible?

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Formulate an optimization problem as:

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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.

Matrix factorization

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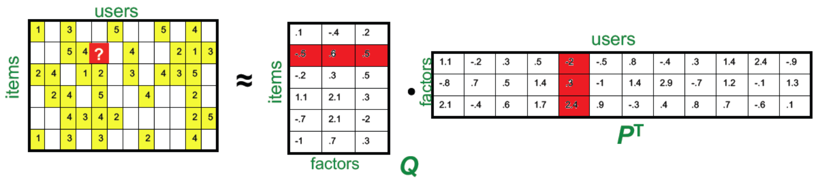
- Each row of Q would represent the strength of the associations between an item and the features.
- Now, we have to find a way to obtain P and Q.

Matrix factorization Cont'd

Example



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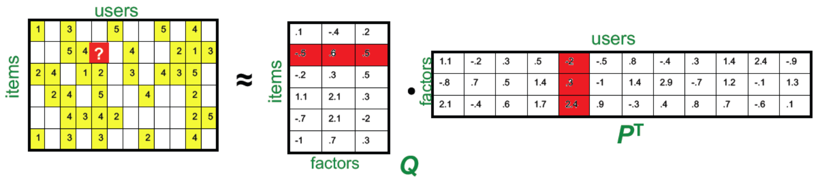

Using P and Q, how to estimate the missing rating of user u for item i?

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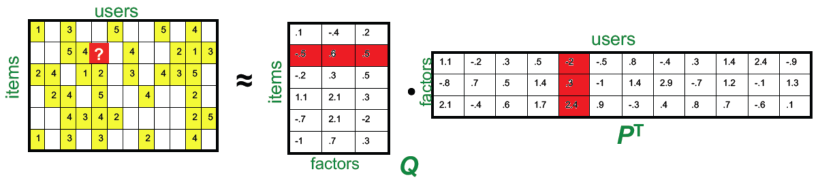

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$$\widehat{r}_{ui} = \mathbf{q}_i^T \mathbf{P}_u = \sum_{j=1}^{k} p_{uj} q_{ji}.$$

Matrix factorization Cont'd

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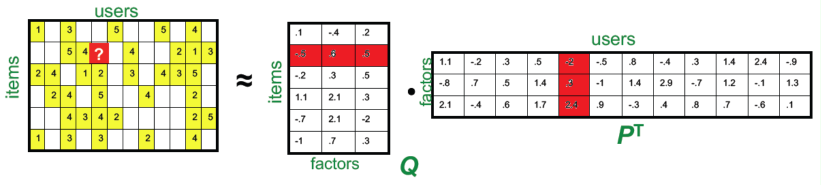

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The estimating error can be

$$e_{ui} = r_{ui} - \widehat{r}_{ui} = r_{ui} - \sum_{j=1}^{k} p_{uj} q_{ji}.$$

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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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1. Motivation
2. Gradient Descent
   - Convex Functions
   - Gradient Descent
3. Matrix Factorization
   - Gradient Descent Algorithm
   - Regularization
   - Collaborative Filtering
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Let's start at $P^{(0)}$ and $Q^{(0)}$.

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- Subsequently, the updates can be computed as follows:
  - $P^{(t+1)} \leftarrow P^{(t)} + \alpha E^{(t)} Q^{(t)}$.
  - $Q^{(t+1)} \leftarrow Q^{(t)} + \alpha {E^{(t)}}^T P^{(t)}$.

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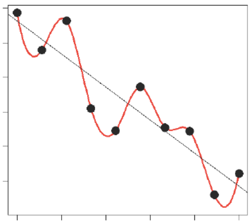
Matrix factorization: regularization



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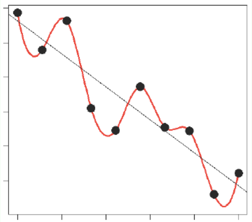

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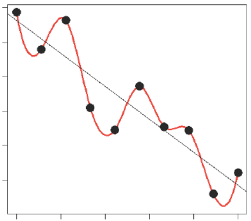

- The observed set $\mathcal{K}$ of ratings is small, which can cause overfitting (also common in classification problem).
- Regularization is a common approach to address the problem.

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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Gradient descent algorithm for regularization

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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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- Instead of having separate bias variables b_u and b_i for users and items, we can increase the size of the factor matrices to incorporate these bias variables.

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

  $$s.t. (k+2)\text{th column of } \widetilde{P} \text{ contains only 1s}$$

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

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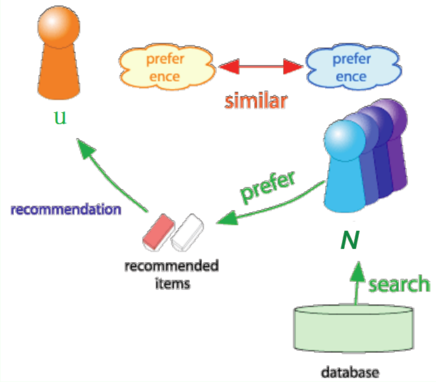
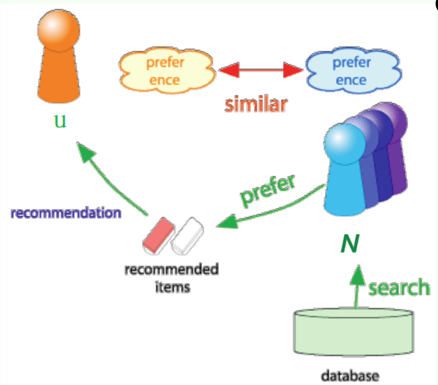
Motivation of collaborative filtering



Motivation of collaborative filtering



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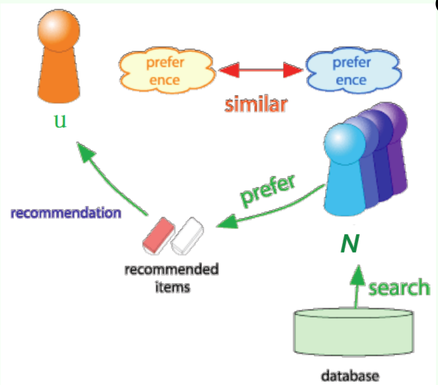

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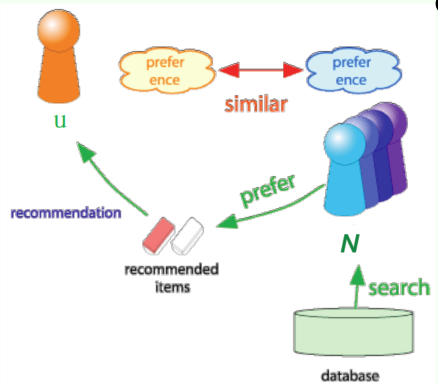

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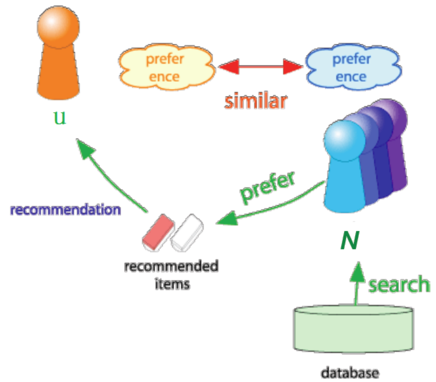

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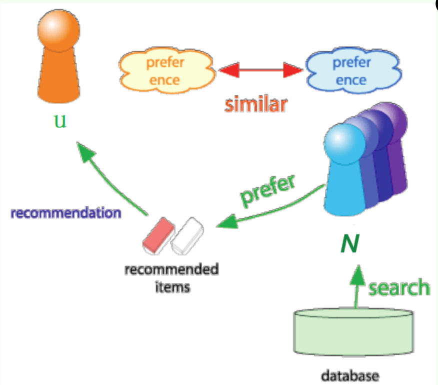

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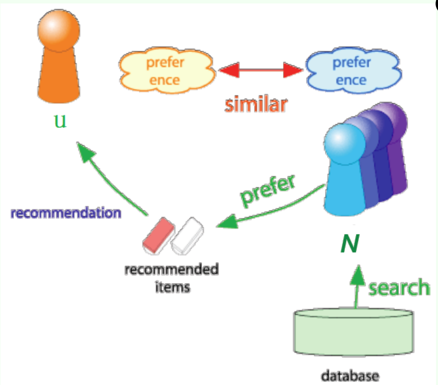

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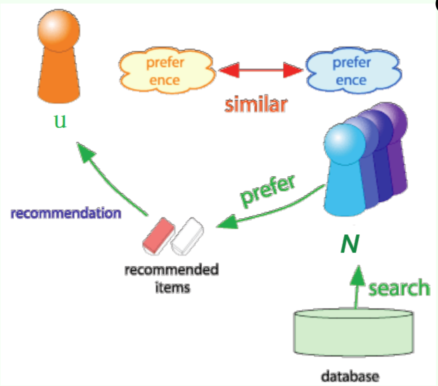

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MF for collaborative filtering

Problem formulation

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

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

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

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Non-negative matrix factorization

Formulation

Define an optimization problem as:

$$\text{Minimize } J = \frac{1}{2}\|R - UV^T\|_F^2$$
$$s.t. U \geq 0$$
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Non-negative matrix factorization

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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 ϵ 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 basic idea is to add the penalties $\frac{\lambda_1 \|U\|^2}{2} + \frac{\lambda_2 \|V\|^2}{2}$ to the objective function.
- 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