SVD Models I

STAT3009 Recommender Systems

by Ben Dai (CUHK)
on Department of Statistics and Data Science

» What You Should Know by Now

1. RS data and Python & Numpy Programming
   * Basic RS data structures
   * Array operations and vectorization
2. Machine Learning Basics
   * Linear regression, regularization (Ridge)
   * Cross-validation techniques, Grid search
3. Baseline Methods (global mean, user/item bias)
4. **scikit-learn Usage**
   * Implement a RS method using sklearn `BaseEstimator` framework
   * Automatically perform hyperparameter tuning with `GridSearchCV`
5. **Kaggle Platform Operations**

» Recall: RS

* Training dataset: [**userID**, **itemID**, **rating**]
* Testing dataset: [**userID**, **itemID**, **?**]
* Evaluation: Given a testing index set Ω^{te} (set of user-item pairs we want to predict),

$$RMSE = \left(\frac{1}{|\Omega^{\mathrm{te}}|} \sum_{(u,i) \in \Omega^{\mathrm{te}}} \left(\hat{r}_{ui} - r_{ui} \right)^2 \right)^{1/2}.$$

* Goal: Find predicted ratings $(\hat{r}_{ui})_{(u,i) \in \Omega^{\mathrm{te}}}$ such that **minimizes RMSE**
* Baseline methods: Global-average, user-average, item-average, user-item average

» Machine learning (ML): RS

Using ML methods to build RS:

Step 1. Introduce a model with some **parameters** and hyperparameters

Step 2. Estimate the **parameters** by minimizing (maximizing) the **Evaluation Loss** in **Training Set**

Step 3. Using Cross-Validation to determine the optimal hps

Step 4. Refit the best model, and make **prediction**

» Components in ML

- Data (feat, label) is a pair of input features and its outcome
- Model f_θ: a parameterized function to map features to label
- Loss $L(\cdot, \cdot)$: The measure of how good the predicted outcome compared with the true outcome
- hp hyperparameter to control the complexity of the model to prevent overfitting
- Opt The algorithm for solving the problem

» Rethink baseline methods: Opt

Step 1. Introduce a method with some **params**

method	MATH	**parameters**
Global pred	$\hat{r}_{ui} = \mu_0$	μ_0
User pred	$\hat{r}_{ui} = a_u$	$\boldsymbol{a} = (a_1, \cdots, a_n)^\intercal$
Item pred	$\hat{r}_{ui} = b_i$	$\boldsymbol{b} = (b_1, \cdots, b_m)^\intercal$

Step 2. Estimate the **parameters** by minimizing **RMSE**

Global $\widehat{f}_\theta(u,i) = \bar{r}$

User $\widehat{f}_\theta(u,i) = \bar{r}_u$

Item $\widehat{f}_\theta(u,i) = \bar{r}_i$

Step 3. CV to find the best model

Step 4. Refit the best model on the whole dataset, and make prediction

InClass demo: Recall Kaggle Quiz 1

» Discussion: Baseline Methods

"All models are wrong, but some are useful." — George E. P. Box

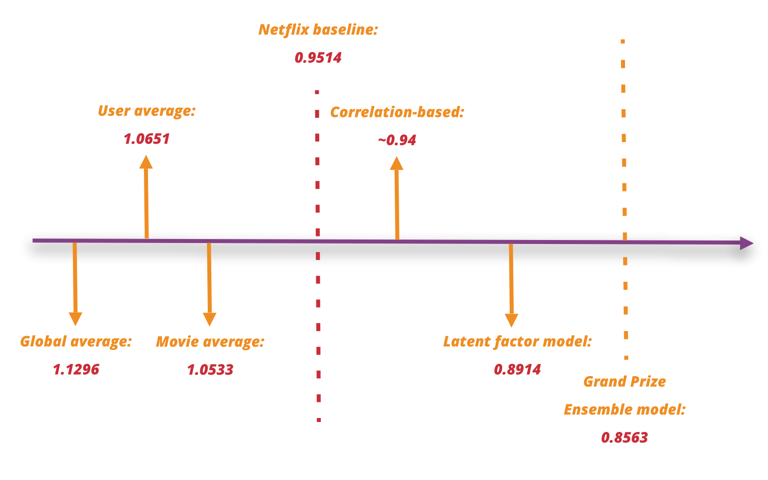
To evaluate each method, we need to understand the underlying **assumptions**.

* Global average assumes that all users and items are homogeneous.
* User average assumes that a user has uniform preference for all items.
* Item average assumes that all users prefer "good" items.
* User-item average assumes additive effects from users and items, with **no interaction**.

Example: Eric is a generous person, and this is indeed an excellent film, but he simply do not like it.

To improve upon these methods, we need to model the user-item **interaction**.

» Motivation: SVD Model



» Motivation: SVD Model

A new Python sklearn-type `Estimator` for RS...

Step 1. Introduce a method with **parameters** (latent factors):

- Associate each user u with a K-length latent factor vector
$$\boldsymbol{p}_u = (p_{u1}, \cdots, p_{uK})^\intercal.$$
- Associate each item i with a K-length latent factor vector
$$\boldsymbol{q}_i = (q_{i1}, \cdots, q_{iK})^\intercal.$$
- Model the user-item **interaction** as the **inner product** of these vectors:
$$\hat{r}_{ui} = \boldsymbol{p}_u^\intercal \boldsymbol{q}_i \to r_{ui}.$$

- The number of latent factors, K, is a pre-specified **hyperparameter**.

Intuition: Each user/item is represented by a k-dimensional vector capturing latent preferences/attributes.

Example with $k = 2$ latent factors:

User vectors $\mathbf{p}_u \in \mathbb{R}^2$:

$$\mathbf{p}_{\text{Alice}} = \begin{bmatrix} 0.9 \\ 0.2 \end{bmatrix}$$

$$\mathbf{p}_{\text{Bob}} = \begin{bmatrix} 0.3 \\ 0.8 \end{bmatrix}$$

Item vectors $\mathbf{q}_i \in \mathbb{R}^2$:

$$\mathbf{q}_{\text{Avengers}} = \begin{bmatrix} 1.0 \\ 0.1 \end{bmatrix}$$

$$\mathbf{q}_{\text{Notebook}} = \begin{bmatrix} 0.2 \\ 0.9 \end{bmatrix}$$

Predicted Ratings:

Alice watches Avengers:

$$r_{\text{Alice,Avengers}} = 0.9 \times 1.0 + 0.2 \times 0.1 = \boxed{0.92}$$

Bob watches Avengers:

$$r_{\text{Bob,Avengers}} = 0.3 \times 1.0 + 0.8 \times 0.1 = \boxed{0.38}$$

Alice watches Notebook:

$$r_{\text{Alice,Notebook}} = 0.9 \times 0.2 + 0.2 \times 0.9 = \boxed{0.36}$$

...

» Geometric Interpretation of $r_{ui} = \mathbf{p}_u^T \mathbf{q}_i$

Dot Product as Similarity:

$$\mathbf{p}_u^T \mathbf{q}_i = \|\mathbf{p}_u\| \|\mathbf{q}_i\| \cos(\theta)$$

* $\theta \approx 0$: vectors aligned $\Rightarrow$ high rating
* $\theta \approx 90$: orthogonal $\Rightarrow$ neutral rating
* Large $\|\mathbf{p}_u\|$: user with strong preferences
* Large $\|\mathbf{q}_i\|$: item with distinct features

» Loss: SVD Model

Step 2. Estimate the **parameters** by minimizing **RMSE**

$$\min_{\boldsymbol{P}\in\mathbb{R}^{n\times K},\boldsymbol{Q}\in\mathbb{R}^{m\times K}} \frac{1}{|\Omega|} \sum_{(u,i)\in\Omega} (r_{ui} - \boldsymbol{p}_u^\intercal \boldsymbol{q}_i)^2 \tag{1}$$

Question: What are the parameters and hyperparameters of this model?

» SVD Model

Param $\boldsymbol{p}_u (u = 1, \cdots, n)$ and $\boldsymbol{q}_i (i = 1, \cdots, m)$ are the parameters we want to learn from data.

hp K is a pre-specified #Latent Factor, can **NOT** be solved from data.

* K increases $\Longrightarrow$ more **parameters** $\Longrightarrow$ lower **training loss**

How many params?

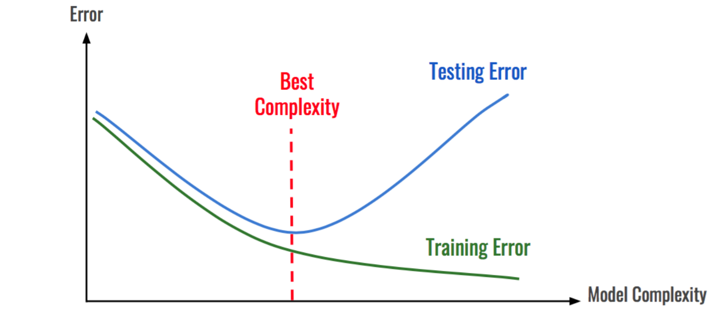
» Overfitting in ML: SVD Model

Source[1]

- **Overfitting**: fit the noise
- Too many **parameters** (**model complexity**) leads to **overfitting**

[1] https://hackernoon.com/memorizing-is-not-learning-6-tricks-to-prevent-overfitting-in-machine-learning-820b091dc42

» Overfitting in ML: SVD Model



Source[2]

* **Complexity** too large $\implies$ Low Training loss but high Testing loss

[2] https://hackernoon.com/memorizing-is-not-learning-6-tricks-to-prevent-overfitting-in-machine-learning-820b091dc42

» Overfitting in ML: SVD Model

	Low *Training* Error	High *Training* Error
Low *Testing* Error	The model is learning!	Probably some error in your code. Or you've created a *psychic* AI.
High *Testing* Error	OVERFITTING	The model is not learning.

Source[3]

3 https://hackernoon.com/memorizing-is-not-learning-6-tricks-to-prevent-overfitting-in-machine-learning-820b091dc42

» Tuning: SVD Model

- **Q1:** How to **quantify** the Model **Complexity**:
  - **#Parameters**: $(n+m)K$
  - **Magnitude** of Parameters: $\sum_{u=1}^{n} \|\boldsymbol{p}_u\|_2^2, \sum_{i=1}^{m} \|\boldsymbol{q}_i\|_2^2$
- **A1:** Control (#Parameters by K, **Magnitude** by l_2-norm).
- **Regularized** SVD Model:

$$\min_{\boldsymbol{P},\boldsymbol{Q}} \underbrace{\frac{1}{|\Omega|} \sum_{(u,i)\in\Omega} (r_{ui} - \boldsymbol{p}_u^\intercal \boldsymbol{q}_i)^2}_{\text{Training loss}} + \lambda \underbrace{\Big(\sum_{u=1}^{n} \|\boldsymbol{p}_u\|_2^2 + \sum_{i=1}^{m} \|\boldsymbol{q}_i\|_2^2 \Big)}_{\text{Params magnitude}} \qquad (2)$$

  where K and $\lambda > 0$ are **tuning** parameters to **balance** the model complexity and training loss.
- Why the later term can control the magnitude?

InClass demo: Implement `Estimator.__init__` and a method `obj` to compute the objective function in (2).

» Tuning: SVD Model

Step 3. Using **GridSearch** + **CV** to find the optimal (K, λ).

* (holdout or K-Fold CV)

Step 4. Refit the model with the optimal (K, λ) and make prediction.

» Summary: SVD Model

Step 1. Introduce a method with some **params** + hps

- Model the user-item **interaction** as **inner production**

$$\hat{r}_{ui} = \boldsymbol{p}_u^\intercal \boldsymbol{q}_i \to r_{ui}$$

Step 2. Estimate the **parameters** by minimizing **RMSE**

$$\min_{\boldsymbol{P},\boldsymbol{Q}} \frac{1}{|\Omega|} \sum_{(u,i)\in\Omega} (r_{ui} - \boldsymbol{p}_u^\intercal \boldsymbol{q}_i)^2 + \lambda \Big(\sum_{u=1}^{n} \|\boldsymbol{p}_u\|_2^2 + \sum_{i=1}^{m} \|\boldsymbol{q}_i\|_2^2 \Big) \quad (3)$$

Step 3. Using **Cross-Validation** to determine the optimal **tuning parameters** (K, λ), denote as K^* and λ^*

Step 4. **Refit** the model based on **full training data** with K^* and λ^* and make prediction.

» Big Picture: MF RS

Algorithm 1 Fitting+Tuning+Prediction MF

```
Input: Training set $(u, i, r_{ui})_{(u,i)\in\Omega}$
Return: Predicted ratings for Testing set: $(u, i) \in \Omega^{\text{te}}$
for $(K, \lambda) \in$ Grid Set do
    (Tuning: compute CV score)
    Estimate the model with $(K, \lambda)$ by solving (3)
    Compute CV Score
end for
Find the best hps $(K^*, \lambda^*)$ with smallest RMSE on valid set
(Refitting) Estimate the best tuned model by solving (3)
(Predict) test ratings by the estimated best tuned model
```

Question: What's the Python workflow?

» Python Estimator

`SVD(BaseEstimator)`

* `__init__`
* `fit(X, y)`: Solving optimization problem in (3)
* `predict(X)`

Then, GridSearch + CV can automatically implemented by `GridSearchCV`

Thus, the **key** is to implement the **fit** method to solve (3)?

InClass demo: Implement predict method.

» Optimization I: Matrix Factorization (Optional)

Recall the regularized Matrix Factorization (MF) problem:

$$\min_{\boldsymbol{P},\boldsymbol{Q}} \frac{1}{|\Omega|} \sum_{(u,i)\in\Omega} (r_{ui} - \boldsymbol{p}_u^\top \boldsymbol{q}_i)^2 + \lambda \left(\sum_{u=1}^{n} \|\boldsymbol{p}_u\|_2^2 + \sum_{i=1}^{m} \|\boldsymbol{q}_i\|_2^2 \right)$$

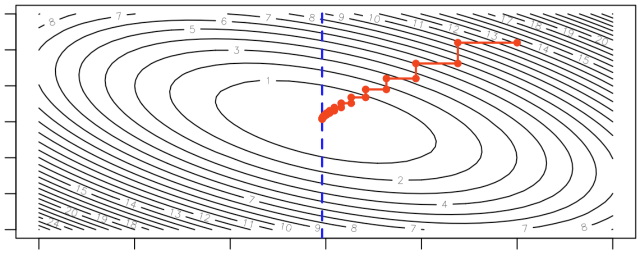
We make the following key observations:

Obs 1 The optimization problem is **nonconvex** due to the **bilinear** term $\boldsymbol{p}_u^\top \boldsymbol{q}_i$.

Obs 2 However, when either $\boldsymbol{P}$ or $\boldsymbol{Q}$ is fixed, the problem becomes **convex** and can be solved as a standard Quadratic Program (QP), which is essentially a *ridge regression* problem.

These observations motivate us to consider using *coordinate descent* to solve this problem.

CD **Coordinate Descent**



Idea At the $(l+1)$th iteration, minimize the objective w.r.t. one coordinate, while keeping all others fixed:

$$\theta_j^{(l+1)} = \text{argmin}_x \; \text{Obj}\left(\theta_1^{(l+1)}, \cdots, \theta_{j-1}^{(l+1)}, x, \theta_{j+1}^{(l+1)}, \cdots, \theta_{|\theta|}^{(l)}\right)$$

* Repeat until a termination condition is met.
* This approach is useful when the **joint** optimization problem is difficult to solve, but the **sub-problems** (minimizing w.r.t. one coordinate) are easy to solve.

Image Source: https://egallic.fr/Enseignement/ML/ECB/book/gradient-descent.html

BCD Blockwise Coordinate Descent

Idea At the $(l+1)$th iteration, minimize the objective function with respect to a block of coordinates:
$\boldsymbol{\theta}_j^{(l+1)} = \operatorname{argmin}_{\boldsymbol{x}} \operatorname{Obj}\big(\boldsymbol{\theta}_1^{(l+1)}, \cdots, \boldsymbol{\theta}_{j-1}^{(l+1)}, \boldsymbol{x}, \boldsymbol{\theta}_{j+1}^{(l+1)}, \cdots, \boldsymbol{\theta}_{|\boldsymbol{\theta}|}^{(l)}\big)$,
where each $\boldsymbol{\theta}_j$ is a *vector*.

* This approach is useful when the **joint** optimization problem is difficult to solve, but the **sub-problems** (minimizing with respect to a block of coordinates) are easy to solve.

Blockwise Coordinate Descent perfectly fits with our Matrix Factorization formulation...

» Example: BCD for Matrix Factorization ($k = 1$) - Part 1

Setup: 2 users, 2 items, $k = 1$ latent factor, $\lambda = 0$
Observed ratings: $r_{12} = 5$, $r_{21} = 4$
Objective: $\min_{p_1,p_2,q_1,q_2} (5 - p_1 q_2)^2 + (4 - p_2 q_1)^2$

Iteration 0 (Initialize):

$$p_1 = 1, \quad p_2 = 1, \quad q_1 = 1, \quad q_2 = 1$$

Current obj: $(5-1)^2 + (4-1)^2 = 16 + 9 = \boxed{25}$

BCD Strategy: Alternate between two blocks:

* Block 1: Update all p's (user factors) while fixing all q's (item factors)
* Block 2: Update all q's (item factors) while fixing all p's (user factors)

» Example: BCD for Matrix Factorization ($k = 1$) - Part 2

Iteration 1, Step 1: Fix $q_1 = 1, q_2 = 1$, update $\mathbf{p}$

- Update p_1: $\min_{p_1}(5 - p_1 \cdot 1)^2 = (5 - p_1)^2$
  Derivative: $\frac{d}{dp_1}(5 - p_1)^2 = -2(5 - p_1) = 0 \Rightarrow \boxed{p_1 = 5}$
- Update p_2: $\min_{p_2}(4 - p_2 \cdot 1)^2 = (4 - p_2)^2$
  Derivative: $\frac{d}{dp_2}(4 - p_2)^2 = -2(4 - p_2) = 0 \Rightarrow \boxed{p_2 = 4}$

Iteration 1, Step 2: Fix $p_1 = 5, p_2 = 4$, update $\mathbf{q}$

- Update q_1: $\min_{q_1}(4 - 4 \cdot q_1)^2 = 16(1 - q_1)^2$
  Derivative: $32(1 - q_1)(-1) = 0 \Rightarrow \boxed{q_1 = 1}$
- Update q_2: $\min_{q_2}(5 - 5 \cdot q_2)^2 = 25(1 - q_2)^2$
  Derivative: $50(1 - q_2)(-1) = 0 \Rightarrow \boxed{q_2 = 1}$

After Iteration 1: $p_1 = 5, p_2 = 4, q_1 = 1, q_2 = 1$
New predictions: $\hat{r}_{12} = 5 \times 1 = 5$ ✓, $\hat{r}_{21} = 4 \times 1 = 4$ ✓
New obj: $(5 - 5)^2 + (4 - 4)^2 = \boxed{0}$ Obj is decreasing!

» Optimization II: Matrix Factorization (Optional)

Let's take a closer look...

Update $\boldsymbol{Q}$ When $(\boldsymbol{p}_u)_{u=1}^n$ are fixed, (3) is a quadratic program (QP) with respect to $(\boldsymbol{q}_i)_{i=1,\cdots,m}$

$$\begin{aligned}
&\min_{\boldsymbol{Q}} \frac{1}{|\Omega|} \sum_{(u,i)\in\Omega} (r_{ui} - \boldsymbol{p}_u^\intercal \boldsymbol{q}_i)^2 + \lambda \Big(\sum_{u=1}^n \|\boldsymbol{p}_u\|_2^2 + \sum_{i=1}^m \|\boldsymbol{q}_i\|_2^2 \Big) \\
\iff &\min_{\boldsymbol{Q}} \frac{1}{|\Omega|} \sum_{(u,i)\in\Omega} (r_{ui} - \boldsymbol{p}_u^\intercal \boldsymbol{q}_i)^2 + \lambda \sum_{i=1}^m \|\boldsymbol{q}_i\|_2^2 \\
\iff &\min_{\boldsymbol{Q}} \sum_{i=1}^m \Big(\frac{1}{|\Omega|} \sum_{u\in\mathcal{U}_i} (r_{ui} - \boldsymbol{p}_u^\intercal \boldsymbol{q}_i)^2 + \lambda \|\boldsymbol{q}_i\|_2^2 \Big). \qquad (4)
\end{aligned}$$

* Note that the objective function in (4) is *separable* with respect to $\boldsymbol{q}_i$ for $i = 1, \cdots, m$.

Decompose

Thus, solving the objective function in (4) is equivalent to separately solving m **small quadratic programs (QPs)**:

$$\begin{aligned} &\min_{\boldsymbol{Q}} \sum_{i=1}^{m} \Big(\frac{1}{|\Omega|} \sum_{u \in \mathcal{U}_i} (r_{ui} - \boldsymbol{p}_u^\top \boldsymbol{q}_i)^2 + \lambda \|\boldsymbol{q}_i\|_2^2 \Big) \\ \Longleftrightarrow\ &\min_{\boldsymbol{q}_i} \frac{1}{|\Omega|} \sum_{u \in \mathcal{U}_i} (r_{ui} - \boldsymbol{q}_i^\top \boldsymbol{p}_u)^2 + \lambda \|\boldsymbol{q}_i\|_2^2, \text{ for } i = 1, \cdots, m \end{aligned}$$

» Optimization III: Matrix Factorization (Optional)

Decompose Thus, solving the objective function in (4) is equivalent to separately solving m **small quadratic programs (QPs)**:

$$
\min_{\boldsymbol{Q}} \sum_{i=1}^{m} \Big(\frac{1}{|\Omega|} \sum_{u \in \mathcal{U}_i} (r_{ui} - \boldsymbol{p}_u^\intercal \boldsymbol{q}_i)^2 + \lambda \|\boldsymbol{q}_i\|_2^2 \Big)
$$

$$
\iff \min_{\boldsymbol{q}_i} \frac{1}{|\Omega|} \sum_{u \in \mathcal{U}_i} (r_{ui} - \boldsymbol{q}_i^\intercal \boldsymbol{p}_u)^2 + \lambda \|\boldsymbol{q}_i\|_2^2, \text{ for } i = 1, \cdots, m
$$

Interestingly, each sub-QP is essentially a *Ridge Regression* problem:

$$
\min_{\boldsymbol{q}_i} \frac{1}{|\Omega|} \sum_{u \in \mathcal{U}_i} (r_{ui} - \underbrace{\boldsymbol{q}_i^\intercal \boldsymbol{p}_u}_{\beta^\intercal \boldsymbol{x}_i \text{ in Linear Regression}})^2 + \lambda \underbrace{\|\boldsymbol{q}_i\|_2^2}_{\|\beta\|_2^2}.
$$

InClass demo: Solve the sub-problem by `sklearn.linear_model.Ridge` for `i = 1`.

» Optimization SUM: MF

BCD perfectly fits our model (alternative least squares (ALS))

Steps solve $\mathbf{Q}$ (fixed $\mathbf{P}$) $\rightarrow$ solve $\mathbf{P}$ (fixed $\mathbf{Q}$) $\rightarrow$ ...

- When $\mathbf{P}$ is fixed, the objective function for $\mathbf{Q}$ is *a* standard QP, and each $\mathbf{q}_i$ can be solved **parallelly** with an *analytic solution*.
- When $\mathbf{Q}$ is fixed, the objective function for $\mathbf{P}$ is *a* standard QP, and each $\mathbf{p}_i$ can be solved **parallelly** with an *analytic solution*.

» ALS: MF

Algorithm 2 ALS for solving MF

Input: *Training* set $(u, i, r_{ui})_{(u,i)\in\Omega}$, *hps:* K, λ
Return: Est params: $(\widehat{\boldsymbol{P}}, \widehat{\boldsymbol{Q}})$
(**Initialization**) Initialize $\boldsymbol{P}^{(0)}$
for $l = 0, \cdots, Max\_Iter$ **do**
    (**Item-Update**)
    for $i = 1, \cdots, m$ **do**
        $\boldsymbol{q}_i^{(l+1)}$ updated by Ridge regression
    end for

» ALS: MF

Algorithm 3 ALS for solving MF

Input: *Training* set $(u, i, r_{ui})_{(u,i)\in\Omega}$, *hps:* K, λ
Return: Est params: $(\widehat{\boldsymbol{P}}, \widehat{\boldsymbol{Q}})$
(**Initialization**) Initialize $\boldsymbol{P}^{(0)}$
for $l = 0, \cdots, Max\_Iter$ **do**
  (**Item-Update**)
  for $i = 1, \cdots, m$ **do**
    $\boldsymbol{q}_i^{(l+1)}$ updated by Ridge regression
  end for
  (**User-Update**)
  for $u = 1, \cdots, n$ **do**
    $\boldsymbol{p}_u^{(l+1)}$ updated by Ridge regression
  end for
  Break the loop if *termination condition*.
end for
Return $(\boldsymbol{P}^{(l+1)}, \boldsymbol{Q}^{l+1})$

» ALS: Latent Factor Model

Termination condition:

* Diff in params:

$$\frac{1}{n}\sum_{u=1}^{n}\|\boldsymbol{p}_u^{(l+1)}-\boldsymbol{p}_u^{(l)}\|_2^2+\frac{1}{m}\sum_{i=1}^{m}\|\boldsymbol{q}_i^{(l+1)}-\boldsymbol{q}_i^{(l)}\|_2^2\leq\varepsilon,$$

* Diff in objective function:

$$\mathrm{MSE}^{(l)}+\lambda\mathrm{Reg}^{(l)}-(\mathrm{MSE}^{(l+1)}+\lambda\mathrm{Reg}^{(l+1)})\leq\varepsilon.$$

InClass demo: Implementation of Algorithm 3.

» Theory of Algorithms

- An iterative algorithm is said to **converge** when, as the iterations proceed, the output gets closer and closer to a specific value.
- **Conditions** for convergence

Lemma (Monotone Convergence Lemma)

If a sequence of real numbers is decreasing and bounded below, then it will converge to its infimum.

» Theory of Algorithms

* An iterative algorithm is said to **converge** when, as the iterations proceed, the output gets closer and closer to a specific value.
* **Conditions** for convergence

Lemma (Monotone Convergence Lemma)

If a sequence of real numbers is decreasing and bounded below, then it will converge to its infimum.

* Most algorithms use this lemma to show convergence

C1 The objective function is **bounded below**

  e.g. Most objective functions are bounded below by their definition: Root Mean Squared Error (RMSE) + Regularization (Reg)

C2 Each step should result in a **decreasing** objective function

  e.g. Block Coordinate Descent (BCD) and Alternating Least Squares (ALS)

» Tips for Debugging Block Coordinate Descent (BCD)

Identifying a bug in the algorithm with multiple blocks in one iteration

* Handling multiple blocks in a single iteration
* Monitor the **objective function** after each block update
* Identify the blocks for which the **objective function** is not decreasing
* Pinpoint the location of the bug