SVD Models I

STAT3009 Recommender Systems

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» 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),

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

* Goal: Find predicted ratings $(\hat{r}_{ui})_{(u,i) \in \Omega^{\text{te}}}$ 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

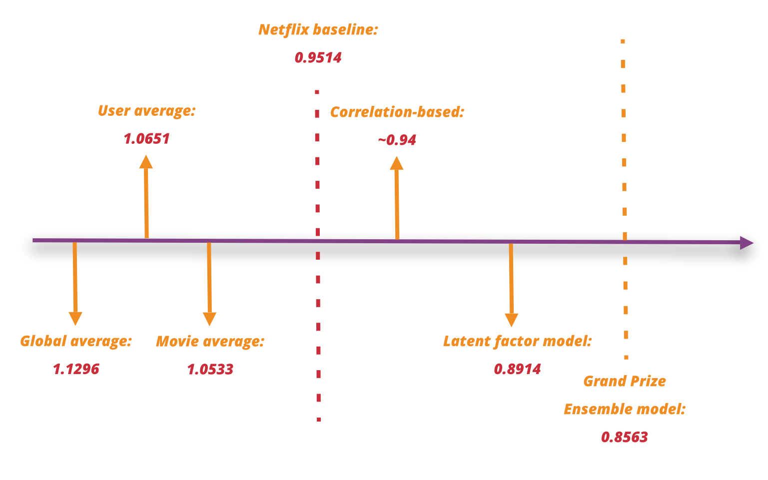
To evaluate each method, we need to understand the underlying **assumptions**.

* 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**.

» 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 $\implies$ more **parameters** $\implies$ 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**

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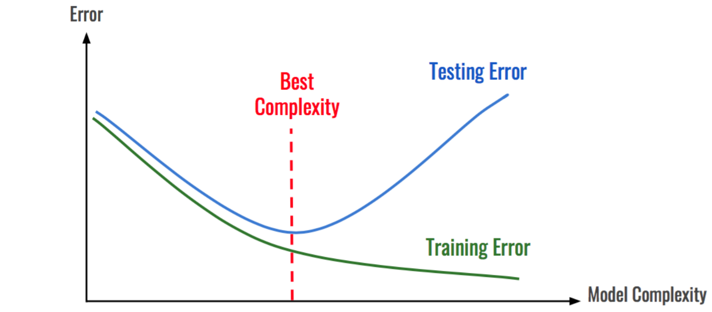
1 https://hackernoon.com/memorizing-is-not-learning-6-tricks-to-prevent-overfitting-in-machine-learning-820b091dc42

» 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__`

» 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: $(u, i) \in \Omega^{\mathrm{te}}$
for $(K, \lambda) \in$ Grid Set **do**
    (*Tuning*: compute CV score)
    Estimate the model with (K, λ) by solving (3)
    Compute *CV Score*
end for
Find the **best** hps (K^*, λ^*) 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:

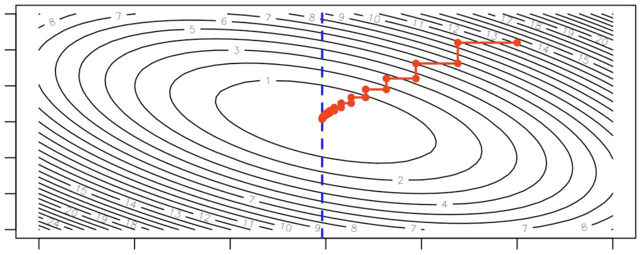
Obs 1 The optimization problem is **nonconvex** due to the **bilinear** term $\boldsymbol{p}_u^\top \boldsymbol{q}_i$.

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.

» Optimization I: Matrix Factorization (Optional)

CD Coordinate Descent



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

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

* 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:
$\boldsymbol{\theta}_j^{(l+1)} = \mathrm{argmin}_{\boldsymbol{x}} \, \mathrm{Obj}\big(\boldsymbol{\theta}_1^{(l+1)}, \cdots, \boldsymbol{\theta}_{j-1}^{(l+1)}, \boldsymbol{x}, \boldsymbol{\theta}_{j+1}^{(l+1)}, \cdots, \boldsymbol{\theta}_{|\boldsymbol{\theta}|}^{(l)}\big)$,
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...

» 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 $(\boldsymbol{q}_i)_{i=1,\cdots,m}$

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

* 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)**:

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

» Optimization III: Matrix Factorization (Optional)

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

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

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

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)∈Ω}, hps: K, λ
Return: Est params: (P̂, Q̂)
(Initialization) Initialize P^(0)
for l = 0, ···, Max_Iter do
    (Item-Update)
    for i = 1, ···, m do
        q_i^(l+1) updated by Ridge regression
    end for
```

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 $(\boldsymbol{P}^{(l+1)}, \boldsymbol{Q}^{l+1})$

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