

- Embedding-based models build embeddings for entities and relations to predict tuples.
- Simplest case: relations between two entities.
E.g., predicting the rating for a person on a movie (collaborative filtering).
- Knowledge graphs: predict subject-verb-object triples.

Learning a relation between two entities

A relation between users and items (movies). From MovieLens:

User	Item	Rating	Timestamp
196	242	3	881250949
186	302	3	891717742
22	377	1	878887116
244	51	2	880606923
...	

- Netflix: 500K users, 17k movies, 100M ratings (withdrawn).
- MovieLens: multiple datasets from 100K to 25M ratings, with links to IMDB, plus some user properties

\widehat{r}_{ui} = predicted rating of user u on item i

Es = set of (u, i, r) tuples in the training set (ignoring timestamp)

Minimize sum squares error:

$$\sum_{(u,i,r) \in Es} (\widehat{r}_{ui} - r)^2$$

Learning Relational Models with Latent Variables

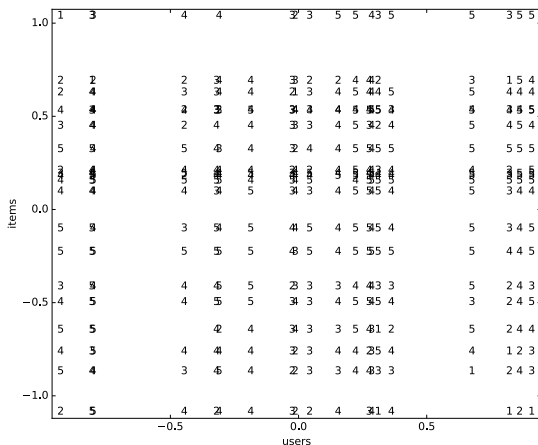
- Predict same for all ratings: $\widehat{r}_{ui} = \mu$
- Adjust for each user and item: $\widehat{r}_{ui} = \mu + b_1[u] + b_2[i]$
Question: $b_1[u]$ could be negative even though all ratings of u are higher than average. How?
- **Question:** How can this be used to personalize recommendations?
- One latent feature: f_i for each item and g_u for each user

$$\widehat{r}_{ui} = \mu + b_1[u] + b_2[i] + f_1[u] * f_2[i]$$

- ▶ Positive $f_1[u]$ forms a soft clustering of users.
- ▶ Positive $f_2[i]$ forms a soft clustering of items.
- ▶ How do these clusterings interact?
- ▶ What about negative values?

What is being learned? (Single latent feature)

for each (u, i, r) : r is plotted at point $(f_1[u], f_2[i])$.



aipython: relnCollFilt.py
What pattern would you expect?

- k latent features (Python notation):

$$\widehat{r}_{ui} = \mu + b_1[u] + b_2[i] + \sum_f E_1[u][f] * E_2[i][f]$$

$E_1[u]$ is the **user embedding**, a vector of numbers.

$E_2[i]$ is the **item embedding**, a vector of numbers.

- Regularize parameters except μ .

- $L2$ regularization, minimize:

$$\left(\sum_{(u,i,r) \in E_s} (\widehat{r}_{ui} - r)^2 \right) + \lambda \sum_{\text{parameter } p} p^2$$

L2 regularization

Minimize:

$$\left(\sum_{(u,i,r) \in E_s} (\mu + b_1[u] + b_2[i] + \sum_k E_1[u][f] * E_2[i][f] - r)^2 \right) + \lambda \left(\sum_i (b_1[u]^2 + \sum_f E_1[u][f]^2) + \sum_u (b_2[i]^2 + \sum_f E_2[i][f]^2) \right)$$

where λ is a regularization parameter.

To find minimizing parameters:

- Gradient descent
- Iterative least squares: fix one of E_1 and E_2 ; the problem is ridge regression in the other.

$\mu :=$ average rating

assign $E_1[u][f]$, $E_2[i][f]$ randomly and assign $b_1[i]$, $b_2[u]$ arbitrarily

repeat:

for each $(u, i, r) \in Es$:

$$e := \mu + b_1[i] + b_2[u] + \sum_k E_1[u][f] * E_2[i][f] - r$$

$$b_1[i] := b_1[i] - \eta * e$$

$$b_2[u] := b_2[u] - \eta * e$$

for each feature f :

$$E_1[u][f] := E_1[u][f] - \eta * e * E_2[i][f]$$

$$E_2[i][f] := E_2[i][f] - \eta * e * E_1[u][f]$$

for each item i :

$$b_1[i] := b_1[i] - \eta * \lambda * b_1[i]$$

for each feature f :

$$E_1[u][f] := E_1[u][f] - \eta * \lambda * E_1[u][f]$$

for each user u :

$$b_2[u] := b_2[u] - \eta * \lambda * b_2[u]$$

for each feature k :

$$E_2[i][f] := E_2[i][f] - \eta * \lambda * E_2[i][f]$$

- What is you want to predict Boolean $rating > 3$?
 - ▶ Use sigmoid.
 - ▶ What should we minimize?
 - ▶ How does the algorithm change?
- What if we want to predict $rated$, where $rated(u, i)$ is true if $(u, i, r) \in Es$ for some r ?
 - ▶ There are no negative examples!
 - ▶ Use k random examples for each positive example!
but the average probability is $1/k$, which is not derived from the data.

Knowledge Graphs and Triples

- A **knowledge graph** is defined in term of triples of the form (s, r, o) , with subject s , relation (verb) r , and object o
- The extension of matrix factorization to triples is **polyadic decomposition**:

$$\hat{p}((s, r, o)) = \text{sigmoid}(\mu + b_1[s] + b_2[r] + b_3[o] + \sum_f E_1[s][f] * E_2[r][f] * E_3[o][f])$$

- ▶ a global bias μ
- ▶ two biases for each entity e : $b_1[e]$ used when e is in the first position and $b_3[e]$, for when e in third position
- ▶ a bias for each relation r , namely $b_2[r]$
- ▶ matrixes E_1 and E_3
 - $E_1[e]$ is **subject embedding** for entity $e \rightarrow$ latent properties
 - $E_3[e]$, is **object embedding** entity e
- ▶ matrix E_2 , where $E_2[r]$ is **relation embedding** for relation r .

All embeddings $E_1[e]$, $E_2[r]$ and $E_3[e]$ are the same length.

- To optimize log loss with $L2$ regularization:
same as previous algorithm with a different predictor and more parameters to tune and regularize.
- Requires negative examples, but knowledge graphs don't have negative examples.
- Regularize μ or provide made-up negative examples.
- But, not all relations have same number of negative examples, eg. "*married-to*" vs "*has-streamed*".

Improving Polyadic Decomposition

- Suppose triples are of the form (u, \textit{likes}, m) and $(m, \textit{directed_by}, d)$.

How can we represent “Sam likes movies directed by Bong Joon-ho”?

The subject and object embeddings for movies are independent of each other, so this cannot be represented or learned.

- Solution: also represent $(m, \textit{likes}^{-1}, u)$ and $(d, \textit{directed_by}^{-1}, m)$.
- polyadic decomposition with inverses:

$$\widehat{p}(h, r, t) = \frac{1}{2}(\widehat{pd}(h, r, t) + \widehat{pd}(t, r^{-1}, h))$$

where \widehat{pd} is the prediction from the polyadic decomposition.

What does polyadic decomposition learn?

- The polyadic decomposition is **fully expressive**: it can represent (with error less than any ϵ), any relation.
- Initially assume subject and object embeddings are non-negative and bounded.
- Each embedding position in the subject/object embedding forms a soft clustering of entities.
- For each embedding position, a relation with a high value ($\gg 0$) in that position, the entities in the subject soft cluster are related to the entities in the object soft cluster. (The product is only high when all three are high).
- A relation with a value $\ll 0$ in a position forms exceptions.
- For possibly negative subject and object embeddings:
 - product of even number of negative values is positive
 - product of odd number of negative values is negative
- The addition lets these values be combined.

What does polyadic decomposition learn?

- The polyadic decomposition makes predictions by clustering entities in different ways.
- It learns about each entity; embeddings are used to predict interactions.
- It does not learn general knowledge that can be applied to other populations.