

# DGL on Real World Applications

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# Various GNN Business Applications

- Recommender Systems: find the most relevant items for a given user.
- Product Search: find the most relevant items given a set of keywords.
- Fraud Detection: detect anomaly of entities in a supervised/unsupervised manner.
- Community Detection: cluster entities in a supervised/unsupervised manner.

# Recommender System: Problem Statement



Image source: Wikipedia

# Collaborative Filtering



# Collaborative Filtering



# Collaborative Filtering




































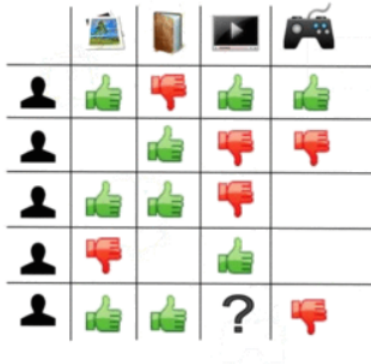
Image source: Wikipedia

# Collaborative Filtering with Machine Learning

We were "representing" users and items with the items/users that had interactions with them.

# Collaborative Filtering with Machine Learning



	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

X

	Item 1	Item 2	Item 3	Item 4	Item 5
Feature 1	?	?	?	?	?
Feature 2	?	?	?	?	?

=

	Item 1	Item 2	Item 3	Item 4	Item 5
User 1	0?	3	0?	3	0?
User 2	4	0?	0?	2	0?
User 3	0?	0?	3	0?	0?
User 4	3	0?	4	0?	3
User 5	4	3	0?	4	0?

We were "representing" users and items with the items/users that had interactions with them.

Source: [Kat Bailey](#)

Can we represent users and items as a set of features?



# Latent User/Item Representations

- An item can be described with a set of features (e.g. how sweet some food is).

	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

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	Item 1	Item 2	Item 3	Item 4	Item 5
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	Item 1	Item 2	Item 3	Item 4	Item 5
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Source: [Kat Bailey](#)

# Latent User/Item Representations

- An item can be described with a set of features (e.g. how sweet some food is).
- A user can be described with preferences of the same set of features (e.g. how much a user likes sweet food).

	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

X

	Item 1	Item 2	Item 3	Item 4	Item 5
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Source: [Kat Bailey](#)

# Latent User/Item Representations

- An item can be described with a set of features (e.g. how sweet some food is).
- A user can be described with preferences of the same set of features (e.g. how much a user likes sweet food).
- The interaction is defined by how well the item features match the user preferences.

	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

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	Item 1	Item 2	Item 3	Item 4	Item 5
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Source: [Kat Bailey](#)

# Latent User/Item Representations

- An item can be described with a **vector**  $v_j$  (sweet, organic, etc.).
- A user can be described with preferences of the same set of features (e.g. how much a user likes sweet food).
- The interaction is defined by how well the item features match the user preferences.

	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

X

	Item 1	Item 2	Item 3	Item 4	Item 5
Feature 1	?	?	?	?	?
Feature 2	?	?	?	?	?

	Item 1	Item 2	Item 3	Item 4	Item 5
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# Latent User/Item Representations

- An item can be described with a vector  $v_j$  (sweet, organic, etc.).
- A user can be described with **another vector  $u_i$**  (likes sweet, likes organic, etc.)
- The interaction is defined by how well the item features match the user preferences.

	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

X

	Item 1	Item 2	Item 3	Item 4	Item 5
Feature 1	?	?	?	?	?
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## Latent User/Item Representations

- An item can be described with a vector  $v_j$  (sweet, organic, etc.).
- A user can be described with another vector  $u_i$  (likes sweet, likes organic, etc.)
- The rating on item  $j$  by user  $i$ . is defined by  $u_i^\top v_j$ .

The diagram illustrates the process of matrix factorization. It shows a user-item rating matrix being decomposed into two lower-rank matrices,  $U$  and  $V$ , which are then multiplied back together to approximate the original matrix.

**Original Matrix (User-Item Ratings):**

	Item 1	Item 2	Item 3	Item 4	Item 5
Feature 1	?	?	?	?	?
Feature 2	?	?	?	?	?
Feature 3	?	?	?	?	?
Feature 4	?	?	?	?	?
Feature 5	?	?	?	?	?

**Decomposition:**

The matrix is decomposed into two lower-rank matrices,  $U$  and  $V$ , which are then multiplied back together to approximate the original matrix.

**Matrix  $U$  (User Latent Factors):**

	Item 1	Item 2	Item 3	Item 4	Item 5
User 1	0.?	3	0.?	3	0.?
User 2	4	0.?	0.?	2	0.?
User 3	0.?	0.?	3	0.?	0.?
User 4	3	0.?	4	0.?	3
User 5	4	3	0.?	4	0.?

**Matrix  $V$  (Item Latent Factors):**

	Item 1	Item 2	Item 3	Item 4	Item 5
User 1	0.?	3	0.?	3	0.?
User 2	4	0.?	0.?	2	0.?
User 3	0.?	0.?	3	0.?	0.?
User 4	3	0.?	4	0.?	3
User 5	4	3	0.?	4	0.?

**Approximation:**

The matrices  $U$  and  $V$  are multiplied back together to approximate the original matrix.

Source: [Kat Bailey](#)

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- The rating on item  $j$  by user  $i$ . is defined by  $u_i^\top v_j$ .
- We minimize

$$\sum_{i,j} \left( r_{i,j} - \left( u_i^\top v_j \right) \right)^2$$

	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

X

	Item 1	Item 2	Item 3	Item 4	Item 5
Feature 1	?	?	?	?	?
Feature 2	?	?	?	?	?

	Item 1	Item 2	Item 3	Item 4	Item 5
User 1	0.?	3	0.?	3	0.?
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$$\sum_{i,j} \left( r_{i,j} - \left( u_i^\top v_j + b_{u_i} + b_{v_j} \right) \right)^2$$

	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

X

	Item 1	Item 2	Item 3	Item 4	Item 5
Feature 1	?	?	?	?	?
Feature 2	?	?	?	?	?

	Item 1	Item 2	Item 3	Item 4	Item 5
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$$\sum_{i,j} \left( r_{i,j} - \left( u_i^\top v_j + b_{u_i} + b_{v_j} \right) \right)^2$$

$+\alpha \mathcal{R}(U, V)$

	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

X

	Item 1	Item 2	Item 3	Item 4	Item 5
Feature 1	?	?	?	?	?
Feature 2	?	?	?	?	?

  
=

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- The rating on item  $j$  by user  $i$ . is defined by  $u_i^\top v_j$ .
- We minimize

$$\sum_{(i,j) \in \mathcal{B}} \left( r_{i,j} - \left( u_i^\top v_j + b_{u_i} + b_{v_j} \right) \right)^2 + \alpha \mathcal{R}(U, V)$$

	Feature 1	Feature 2
User 1	?	?
User 2	?	?
User 3	?	?
User 4	?	?
User 5	?	?

X

	Item 1	Item 2	Item 3	Item 4	Item 5
Feature 1	?	?	?	?	?
Feature 2	?	?	?	?	?

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Source: [Kat Bailey](#)

## What if we don't have ratings?



	Item 1	Item 2	Item 3	Item 4	Item 5
User 1		3	0		0
User 2	4			2	0
User 3	0			0	0
User 4		0	4		3
User 5	4	3	0	4	0

	$i_1$	$i_2$	$i_3$	$i_4$	
$u_1$	?	+	+	?	user
$u_2$	+	?	?	+	
$u_3$	+	+	?	?	
$u_4$	?	?	+	+	
$u_5$	?	?	+	?	
	item				

Source: BPR: Bayesian Personalized Ranking from

*Implicit Feedback*, Rendle et al. 2012

# Implicit Feedback

- For a given user  $i$ , an item being interacted  $j$  should have a higher score than another item  $k$  which was never being interacted.

	$i_1$	$i_2$	$i_3$	$i_4$	
$u_1$	?	+	+	?	user ↑ ↓
$u_2$	+	?	?	+	
$u_3$	+	+	?	?	
$u_4$	?	?	+	+	
$u_5$	?	?	+	?	
	← item →				

Source: *BPR: Bayesian Personalized Ranking*  
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# Implicit Feedback

- For a given user  $i$ , an item being interacted  $j$  should have a higher score than another item  $k$  which was never being interacted.
- We maximize

$$\sum_{i,j,k \in I \setminus I_{u_i}} \log \text{sigmoid}((u_i^\top v_j - u_i^\top v_k))$$

	$i_1$	$i_2$	$i_3$	$i_4$	
$u_1$	?	+	+	?	user ↑ ↓
$u_2$	+	?	?	+	
$u_3$	+	+	?	?	
$u_4$	?	?	+	+	
$u_5$	?	?	+	?	
	← item →				

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# Implicit Feedback

- For a given user  $i$ , an item being interacted  $j$  should have a higher score than another item  $k$  which was never being interacted.
- We maximize


























$$\sum_{i,j,k \in I \setminus I_{u_i}} \log \text{sigmoid}((u_i^\top v_j - u_i^\top v_k))$$

- We usually *sample* one or multiple  $k$  when computing gradients (**negative sampling**).
  - Commonly uniformly, but adaptive sampling often helps.

	$i_1$	$i_2$	$i_3$	$i_4$	
$u_1$	?	+	+	?	user ↑ ↓
$u_2$	+	?	?	+	
$u_3$	+	+	?	?	
$u_4$	?	?	+	+	
$u_5$	?	?	+	?	
	← item →				


























Source: *BPR: Bayesian Personalized Ranking*  
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# Formulating Recommender Systems as Graph Learning

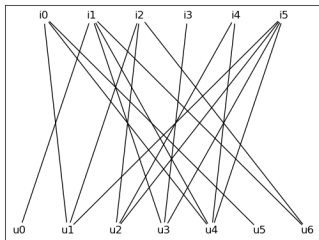
				
				
				
				
				
				

- Explicit Feedback
- Implicit Feedback

# Formulating Recommender Systems as Graph Learning

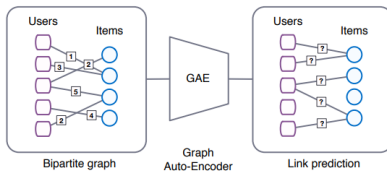
- Explicit Feedback
- Implicit Feedback



- Edge Classification/Regression
- Link Prediction



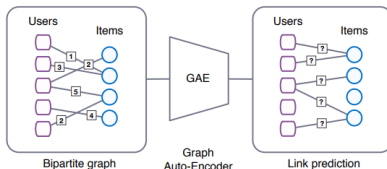
# GCMC: Learning $u_i$ and $v_j$ from User-Item Graph



Source: *Graph Convolutional Matrix Completion*, van den Berg et al. 2017

$$1. \mu_{v_j \rightarrow u_i, r} = \frac{1}{c_{u_i v_j}} W_r x_{v_j}$$

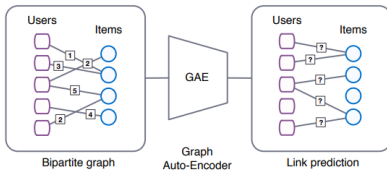
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1.  $\mu_{v_j \rightarrow u_i, r} = \frac{1}{c_{u_i v_j}} W_r x_{v_j}$
2.  $h_{u_i} = \sigma \left[ \text{agg} \left( \sum_{v_j \in \mathcal{N}_{u_i, 1}} \mu_{v_j \rightarrow u_i, 1}, \dots, \sum_{v_j \in \mathcal{N}_{u_i, R}} \mu_{v_j \rightarrow u_i, R} \right) \right]$

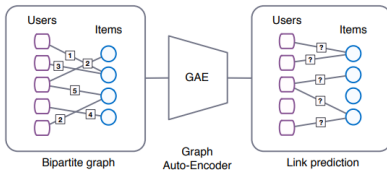
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3.  $u_i = \sigma(W_u h_{u_i})$  and similarly we compute  $v_j$

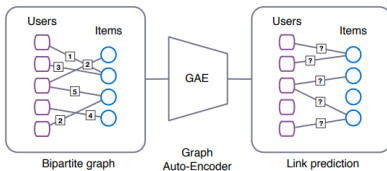
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3.  $u_i = \sigma(W_u h_{u_i})$  and similarly we compute  $v_j$
4.  $p(\hat{M}_{ij} = r) = \text{softmax}(u_i^\top Q_r v_j)$

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3.  $u_i = \sigma(W_u h_{u_i})$  and similarly we compute  $v_j$
4.  $p(\hat{M}_{ij} = r) = \text{softmax}(u_i^\top Q_r v_j)$
5. If users and items have no features, we make  $x_{v_j}$  and  $x_{u_i}$  themselves learnable parameters.

## Other Meaningful Aspects to Consider

- **Cold-start:** What if we have *new* users and items coming in, with few to no historical interactions and features?

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## Other Meaningful Aspects to Consider

- **Cold-start:** What if we have *new* users and items coming in, with few to no historical interactions and features?
- **Bias correction:** The training dataset usually comes from the result of a *previous recommender system*. How to mitigate the bias?
- **Diversity:** Always recommending the same items (or even the same kind of item) to a user would make him/her feel *bored*.
- **Fraud:** How to detect and deal with fabricated explicit feedbacks (e.g. fake ratings and reviews)?

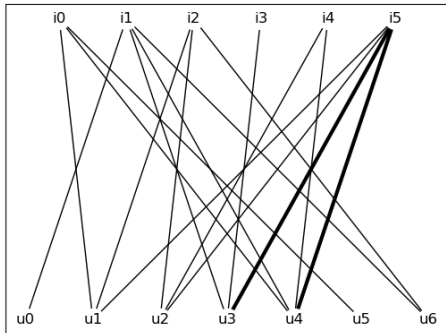
# Non-exhaustive List of Recommender System Models

- PinSAGE
- STAR-GCN
- Knowledge Graph Attention Networks
- Knowledge Graph Convolutional Networks
- Inductive Matrix Completion (IGMC)
- ...

# Hands-on Session

Miniature GCMC on bipartite user-item graph with  
DGL.

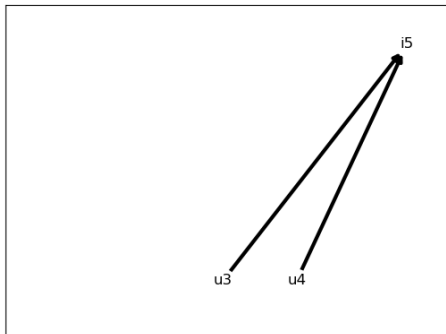
## How to Train GCMC Stochastically?



- Given the graph above, we wish to predict the rating of the selected edge minibatch with a 1-layer GCMC.

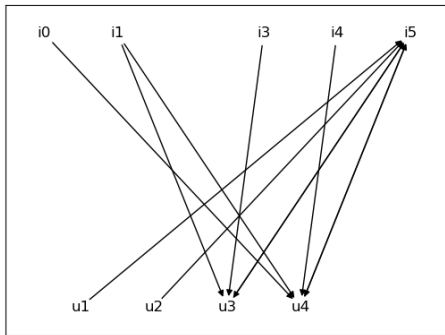
## Constructing a "Pair Graph"

- DGL provides an `apply_edges` method that computes edge features in parallel based on source, destination, and other edge features.
- Construct a pair graph that consists of the edges to be trained only.



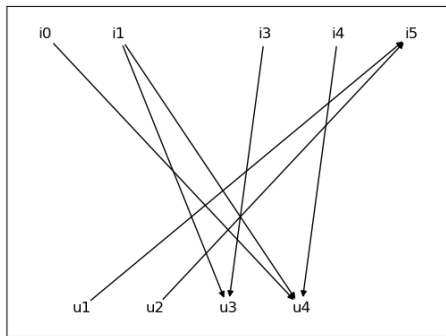
## Find Necessary Neighbors

- The computation dependency can be used in message passing by transforming the dependency graph by `dg1.to_block` into a bipartite-structured graph as explained in the previous tutorial.



## Removing Information Leakage

- Since we are training to predict the rating of  $(u_3, i_5)$  and  $(u_4, i_5)$ , we don't want to tell the model that these edges exist. Therefore we need to remove these edges.



## The Computation Procedure (Reference to Notebook)

- Sample a minibatch of edges.
- Construct a pair graph from those edges.
- Construct the computation dependency graph.
- Transform the dependency graph with `dgl.to_block` for message passing.
- Copy features from the original graph to the blocks.
- Compute the outputs from the GNN layers on the blocks.
- Copy the output of the GNN layers to the pair graph.
- Compute the score on the edges of the pair graph with `dgl.apply_edges`.