RS Basics and Classic Algorithms

密言

2025年5月30日

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What is RS?

- 推荐问题的建模
 - 基于"信息过载"的问题,联系用户和信息,帮助用户获取有价值的信息,将信息展现给对应感兴趣的用户。
 - 本质: "评分预测"问题。预测评分 → Top-K 推荐
- 推荐方法分类
 - Traditional RS
 - Collaborative Filtering (User-based, Item-based, Model-based, Hybrid) / (explicit, implicit(e.g. browsing history))
 - Content-based Recommendation
 - Deep Learning based RS
- RS 面临的问题
 - 数据稀疏问题
 - Cold start 问题
 - 安全性问题
 - Others: 隐私问题、可解释问题、etc.

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RS Basics: RS 的技术流程

- ① 数据收集与存储 (Data Collection & Storage)
 - User and Item data
 - Interaction data
 - Explicit: rating, Review, like or unlike
 - Implicit: click, View
 - Contextual Data
- ② 特征工程 (Feature Engineering)
 - 将原始数据转换为能够被推荐模型有效利用的特征(Features)。决定推荐系统性能上限的关键步骤。
- ③ 候选集生成 (Candidate Generation / Retrieval)
 - "召回", 筛选出与用户相关的候选物品集合
- A Ranking / Scoring
 - 预测用户对物品的打分,排序并推荐
- **⑤** 后处理 (Post-processing)
 - 多样性,解释性问题
- 6 Evaluation

Traditional RS: Collaborative Filtering

User-based CF

- 基本思想:相似偏好的用户在物品的打分上是相似的("用户会喜欢相似用户所喜欢的物品)
- Method:
 - 确定目标用户
 - 根据相似度确定与目标用户最相似的 N 个用户
 - 根据相似用户预测评分
 - 根据评分对用户进行物品推荐

	item 1	item 2	item 3	item 4	item 5
user 1	5	2	1	3	?
user 2	4	1	1	2	5
user 3	1	3	4	5	2
user 4	3	2	1	2	3

Traditional RS: Collaborative Filtering

相似度的计算方式:

- Jaccard 相似度: 集合交并比
- 余弦相似度: $Sim(u_1, u_2) = \frac{\vec{u_1} \cdot \vec{u_2}}{|\vec{u_1}| \cdot |\vec{u_2}|}$
- Pearson 相关系数: 减去打分均值后, 计算余弦相似度(归一化的余弦相似度)
- 欧式距离: 适合度量包含相似度和强度(e.g. 访问频率)的场景

评分预测方式:

- 加权预测: $R_{u_1,item_5} = \frac{\sum_{i=1}^N \omega_i R_{i,item_5}}{\sum_{i=1}^N \omega_i}$, 其中 ω 是相似度
- 基于用户评分均值增量: $R_{u_1,item_5} = \overline{R_{u_1}} + \frac{\sum_{i=1}^N \omega_i(R_{i,item_5} \overline{R_i})}{\sum_{i=1}^N \omega_i}$,能够缓解不同用户不同打分习惯带来的影响

Traditional RS: Collaborative Filtering

Item-based CF

- 思想: 用户可能喜欢与曾经喜欢物品相似的物品
- Method:
 - 确定需要预测的目标物品
 - 根据相似度确定与目标物品相似的 N 个物品
 - 根据相似物品预测评分
 - 根据预测评分推荐相关物品
- 评分计算:

• 基于物品均分增量:
$$R_{u_1,item_5} = \overline{R_{item_5}} + \frac{\sum_{j=1}^N \omega_j (R_{u_1,j} - \overline{R_j})}{\sum_{j=1}^N \omega_j}$$

	item 1	item 2	item 3	item 4	item 5
user 1	5	2	1	3	?
user 2	4	1	1	2	5
user 3	1	3	4	5	2
user 4	3	2	1	2	3

User-based vs Item-based

- 计算复杂性:对于用户数》物品数且物品更新频率低,计算物品间相似度 计算量低且不必实时更新, Item-based 更优;对于 item 时效性高且数 量多时, User-based 更优。
- 场景: 非社交网络中, Item 间的联系是很重要的推荐原则, 选用 Item-based; 在社交网络中, User 间的联系是重要信息, 选用 User-based

• 推荐多样性:

- 从单个用户看,Item-based 推荐用户历史相似物品,多样性较差
- 从系统层面看, Item-based 推荐覆盖率远远优于 User-based,
 User-based 倾向于推荐热门物品, Item-based 对长尾物品推荐表现好(只要某用户同时购买两个冷门物品,即可建立起联系)

• 用户对推荐算法的适应程度:

密言

- 有共同喜好的用户: User-based 效果好
- 喜爱物品自相似: Item-based 效果好

Model-based CF and Hybrid-based CF

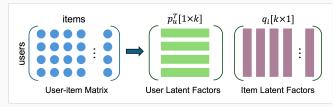
- Model-basd CF
 - 先用历史数据训练得到一个模型,再用此模型进行预测
 - e.g. Latent Factor Model (LFM)
- Hybrid-based CF
 - 将多种推荐技术进行混合以此弥补相互间的缺点
 - Hybrid Method:
 - Weighted
 - Switch
 - 特征组合(Feature Combination)
 - 级联型 (Cascade)
 - 特征递增 (Feature Augmentation)
 - 元层次混合 (Meta-level hybrid)

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Matrix Factorization: Key Technique for Model-based CF

Funk-SVD (Latent Factor Model)

- 对于每个评分,有 $R_{u,i} = p_u^\top \cdot q_i = \sum_{k=1}^K p_{u,k}^\top \cdot q_{i,k}$
- 使用 SGD 优化目标: $min \sum_{R \in R_{train}} (\|R_{u,i} \hat{-} R_{u,i}\|_F^2 + \lambda(\|p_u^\top\|_F^2 + \|q_i\|_F^2))$
- BiasSVD: 加入偏移项
- 本质: 单层的图神经网络



NGCF: Intro

Motivation: Embedding function 缺乏对协同信号的明确编码

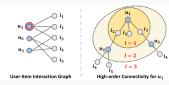
协同信号 (Collaborative Signal)

协同信号 (Collaborative Signal) 指的是隐藏在用户与项目交互数据中的潜在信息,这些信息能够揭示用户之间的行为相似性或项目之间的关联性。

Two key components in learnable CF models:

- 1) Embedding: 将 User 和 Item 转化成 vectorized representations
- 2) Interact Modeling (e.g. inner product, non-linear NN, etc.)

Method of Distill collaborative Signal: high-order connectivity (高阶连通性) from user-item interactions



NGCF: Intro2

Contributions:

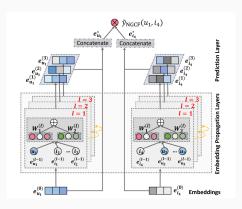
- * Highlight the critical importance of **explicitly** exploiting the **collaborative signal** in the embedding function
- * propose NGCF, a new recommendation framework based on graph neural network, which explicitly encodes the collaborative signal in the form of high-order connectivities by performing embedding propagation
- * Conduct empirical studies on three million-size datasets

NGCF: Methodology

3 components:

- (1) embedding layer
- (2) multiple embedding propagation layers
- (3) predict layer

Architecture:



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Embedding layer and Embedding Propagation Layers (1)

Embedding layer:

describe each user u (or item i) with a embedding vector $e \in \mathbb{R}^d$, d is embedding size.

$$\mathbf{E} = \left[\begin{array}{c} \mathbf{e}_{u_1}, \cdots, \mathbf{e}_{u_N} \\ \\ \text{users embeddings} \end{array}\right], \quad \underbrace{\mathbf{e}_{i_1}, \cdots, \mathbf{e}_{i_M}}_{\text{limiting embeddings}} \right].$$

Embedding Propagation Layers

- First-order Propagation
 - Message Construction
 - Message Aggregation
- High-order Propagation

Message Construction

W₁: item 信息, W₂: user-item 交互信息

$$\mathbf{m}_{u \leftarrow i} = \frac{1}{\sqrt{|\mathcal{N}_u||\mathcal{N}_i|}} \Big(\mathbf{W}_1 \mathbf{e}_i + \mathbf{W}_2 (\mathbf{e}_i \odot \mathbf{e}_u) \Big),$$

Message Aggregation

$$\mathbf{e}_{u}^{(1)} = \text{LeakyReLU}\Big(\mathbf{m}_{u \leftarrow u} + \sum_{i \in \mathcal{N}_{u}} \mathbf{m}_{u \leftarrow i}\Big),$$

Embedding Propagation Layers (2)

High-order Propagation

stack more embedding propagation layers to connect high-order collaborative signal.

$$\mathbf{e}_{u}^{(l)} = \text{LeakyReLU}\left(\mathbf{m}_{u \leftarrow u}^{(l)} + \sum_{i \in \mathcal{N}_{u}} \mathbf{m}_{u \leftarrow i}^{(l)}\right),$$

$$\mathbf{e}_{u}^{(l)} = \text{LeakyReLU}\left(\mathbf{m}_{u \leftarrow u}^{(l)} + \sum_{i \in \mathcal{N}_{u}} \mathbf{m}_{u \leftarrow i}^{(l)}\right), \\ \begin{cases} \mathbf{m}_{u \leftarrow i}^{(l)} = p_{ui}\left(\mathbf{W}_{1}^{(l)} \mathbf{e}_{i}^{(l-1)} + \mathbf{W}_{2}^{(l)}(\mathbf{e}_{i}^{(l-1)} \odot \mathbf{e}_{u}^{(l-1)})\right), \\ \mathbf{m}_{u \leftarrow u}^{(l)} = \mathbf{W}_{1}^{(l)} \mathbf{e}_{u}^{(l-1)}, \end{cases}$$

Propagation Rule in Matrix Form

$$\mathbf{E}^{(l)} = \mathsf{LeakyReLU}\Big((\mathcal{L} + \mathbf{I})\mathbf{E}^{(l-1)}\mathbf{W}_1^{(l)} + \mathcal{L}\mathbf{E}^{(l-1)}\odot\mathbf{E}^{(l-1)}\mathbf{W}_2^{(l)}\Big),$$

$$\mathcal{L} = D^{-\frac{1}{2}}AD^{-\frac{1}{2}} \text{ and } A = \begin{bmatrix} 0 & R \\ R^{\top} & 0 \end{bmatrix},$$

- R: user-item 交互矩阵
- D: 度矩阵(对角线元素是节点度数)
- \mathcal{L} : 拉普拉斯矩阵,非对角线元素是 $\frac{1}{\sqrt{|\mathcal{N}_{i}||\mathcal{N}_{i}|}}$
- ℓ + I: 为每个节点加入一个自环

Model Predict, Optimization

Model Predict

Concatenating the representations learned by different layers.

$$\mathbf{e}_{u}^{*} = \mathbf{e}_{u}^{(0)} \| \cdots \| \mathbf{e}_{u}^{(L)}, \quad \mathbf{e}_{i}^{*} = \mathbf{e}_{i}^{(0)} \| \cdots \| \mathbf{e}_{i}^{(L)},$$

Estimate the user's preference towards the target item:

$$\hat{y}_{NGCF}(u,i) = e_u^{*\top} \cdot e_i^*$$

Optimization

$$Loss = \sum_{(u,i,j) \in O} -\ln \sigma(\hat{y}_{ui} - \hat{y}_{uj}) + \lambda \|\Theta\|_2^2, \tag{11}$$

where $O=\{(u,i,j)|(u,i)\in\mathcal{R}^+,(u,j)\in\mathcal{R}^-\}$ denotes the pairwise training data, \mathcal{R}^+ indicates the observed interactions, and \mathcal{R}^- is the unobserved interactions; $\sigma(\cdot)$ is the sigmoid function; $\Theta=\{\mathbb{E},\{\mathbf{W}_i^{(l)},\mathbf{W}_i^{(l)}\}_{l=1}^L\}$ denotes all trainable model parameters, and λ controls the L_2 regularization strength to prevent overfitting. We

Evaluation

Evaluation 流程

- 在训练集中未出现、但在原始数据中实际交互过的物品作为正例 (positive items);与用户未交互过的物品为负例(negative items)
- 对每个用户,对潜在推荐物品生成评分并排序
- 截取 Top-K 个物品
- 计算相关指标. RecallaK and NDCGaK

Recall aK

 Recall@K = Top-K 列表中属于测试集 positive items 的数量

 测试集中该用户所有 positive item 的数量

NDCGaK

CG 累积增益: Top-K 列表中的相关性总和(出现测试集 positive item 为 1, 否 则为 0)

DCG 折损累积增益: $DCG@K = \sum \frac{rel_i}{loa_2(i+1)}$

NDCG 归一化折损累积增益: NDCG@K = DCG@K ,IDCG 是理想状态下的 DCG

LightGCN: Intro

Motivation: 直接基于 GCN 的 NGCF 设计复杂, 其中的特征变换和非线性激活反 而给模型训练带来困难。

Contributions:

- 证明了 GCN 中的 feature transformation 和 non-linear activation 对 collaborative filter 没有积极影响
- LightGCN 大大简化模型设计
- 对比 NGCF 产生显著的改进

LightGCN: Method

Light Graph Convolution (LGC)

$$\begin{split} \mathbf{e}_{u}^{(k+1)} &= \sum_{i \in \mathcal{N}_{u}} \frac{1}{\sqrt{|\mathcal{N}_{u}|} \sqrt{|\mathcal{N}_{i}|}} \mathbf{e}_{i}^{(k)}, \\ \mathbf{e}_{i}^{(k+1)} &= \sum_{u \in \mathcal{N}_{i}} \frac{1}{\sqrt{|\mathcal{N}_{i}|} \sqrt{|\mathcal{N}_{u}|}} \mathbf{e}_{u}^{(k)}. \end{split}$$

$$\begin{split} \mathbf{e}_{u}^{(k+1)} &= \sigma \Big(\mathbf{W}_{1} \mathbf{e}_{u}^{(k)} + \sum_{i \in \mathcal{N}_{u}} \frac{1}{\sqrt{|\mathcal{N}_{u}||\mathcal{N}_{i}|}} (\mathbf{W}_{1} \mathbf{e}_{i}^{(k)} + \mathbf{W}_{2} (\mathbf{e}_{i}^{(k)} \odot \mathbf{e}_{u}^{(k)})) \Big), \\ \mathbf{e}_{i}^{(k+1)} &= \sigma \Big(\mathbf{W}_{1} \mathbf{e}_{i}^{(k)} + \sum_{u \in \mathcal{N}_{i}} \frac{1}{\sqrt{|\mathcal{N}_{u}||\mathcal{N}_{i}|}} (\mathbf{W}_{1} \mathbf{e}_{u}^{(k)} + \mathbf{W}_{2} (\mathbf{e}_{u}^{(k)} \odot \mathbf{e}_{i}^{(k)})) \Big), \end{split}$$

propagation rule in LightGCN

propagation rule in NGCF

Layer Combination

$$\mathbf{e}_u = \sum_{k=0}^K \alpha_k \mathbf{e}_u^{(k)}; \quad \mathbf{e}_i = \sum_{k=0}^K \alpha_k \mathbf{e}_i^{(k)},$$

$$\begin{cases} \mathbf{m}_{u \leftarrow i}^{(l)} = p_{ui} \Big(\mathbf{W}_{1}^{(l)} \mathbf{e}_{i}^{(l-1)} + \mathbf{W}_{2}^{(l)} (\mathbf{e}_{i}^{(l-1)} \odot \mathbf{e}_{u}^{(l-1)}) \Big), \\ \mathbf{m}_{u \leftarrow u}^{(l)} = \mathbf{W}_{1}^{(l)} \mathbf{e}_{u}^{(l-1)}, \end{cases}$$

Why weighted sum?

- 1) 随层数增加, embedding 会过度平滑
- 2) 相加有利于捕获不同层次的语义
- 3) 加权相加实际上包含了自连接的效果

Method: Matrix Form

3.1.3 Matrix Form. We provide the matrix form of LightGCN to facilitate implementation and discussion with existing models. Let the user-item interaction matrix be $\mathbf{R} \in \mathbb{R}^{M \times N}$ where M and N denote the number of users and items, respectively, and each entry R_{ui} is 1 if u has interacted with item i otherwise 0. We then obtain the adjacency matrix of the user-item graph as

$$\mathbf{A} = \begin{pmatrix} \mathbf{0} & \mathbf{R} \\ \mathbf{R}^T & \mathbf{0} \end{pmatrix},\tag{6}$$

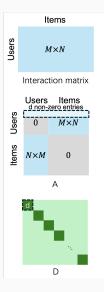
Let the 0-th layer embedding matrix be $\mathbf{E}^{(0)} \in \mathbb{R}^{(M+N) \times T}$, where T is the embedding size. Then we can obtain the matrix equivalent form of LGC as:

$$\mathbf{E}^{(k+1)} = (\mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}) \mathbf{E}^{(k)}, \tag{7}$$

where \mathbf{D} is a $(M+N) \times (M+N)$ diagonal matrix, in which each entry D_{ii} denotes the number of nonzero entries in the *i*-th row vector of the adjacency matrix \mathbf{A} (also named as degree matrix). Lastly, we get the final embedding matrix used for model prediction as:

$$\begin{split} \mathbf{E} &= \alpha_0 \mathbf{E}^{(0)} + \alpha_1 \mathbf{E}^{(1)} + \alpha_2 \mathbf{E}^{(2)} + \dots + \alpha_K \mathbf{E}^{(K)} \\ &= \alpha_0 \mathbf{E}^{(0)} + \alpha_1 \tilde{\mathbf{A}} \mathbf{E}^{(0)} + \alpha_2 \tilde{\mathbf{A}}^2 \mathbf{E}^{(0)} + \dots + \alpha_K \tilde{\mathbf{A}}^K \mathbf{E}^{(0)}, \end{split} \tag{8}$$

where $\tilde{\mathbf{A}} = \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}$ is the symmetrically normalized matrix.



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Model Analysis

通过修改 Weighted sum, LightGCN 与 SGCN、APPNP 是等价的。

SGCN 考虑了用户自连接,即度矩阵 D 加上单位矩阵

$$\mathbf{E}^{(k+1)} = (\mathbf{D} + \mathbf{I})^{-\frac{1}{2}} (\mathbf{A} + \mathbf{I}) (\mathbf{D} + \mathbf{I})^{-\frac{1}{2}} \mathbf{E}^{(k)}, \tag{9}$$

where $\mathbf{I} \in \mathbb{R}^{(M+N)\times(M+N)}$ is an identity matrix, which is added on \mathbf{A} to include self-connections. In the following analysis, we omit the $(\mathbf{D}+\mathbf{I})^{-\frac{1}{2}}$ terms for simplicity, since they only re-scale embeddings. In SGCN, the embeddings obtained at the last layer are used for downstream prediction task, which can be expressed as:

$$\begin{split} \mathbf{E}^{(K)} &= (\mathbf{A} + \mathbf{I})\mathbf{E}^{(K-1)} = (\mathbf{A} + \mathbf{I})^K \mathbf{E}^{(0)} \\ &= \binom{K}{0} \mathbf{E}^{(0)} + \binom{K}{1} \mathbf{A} \mathbf{E}^{(0)} + \binom{K}{2} \mathbf{A}^2 \mathbf{E}^{(0)} + \ldots + \binom{K}{K} \mathbf{A}^K \mathbf{E}^{(0)}. \end{split}$$
(10)

APPNP 通过在每层补充 $E^{(0)}$ 初始特征,避免过于平滑

$$\mathbf{E}^{(k+1)} = \beta \mathbf{E}^{(0)} + (1 - \beta)\tilde{\mathbf{A}}\mathbf{E}^{(k)}, \tag{11}$$

where β is the teleport probability to control the retaining of starting features in the propagation, and $\tilde{\mathbf{A}}$ denotes the normalized adjacency matrix. In APPNP, the last layer is used for final prediction, i.e.,

$$\begin{split} \mathbf{E}^{(K)} &= \beta \mathbf{E}^{(0)} + (1 - \beta) \tilde{\mathbf{A}} \mathbf{E}^{(K-1)}, \\ &= \beta \mathbf{E}^{(0)} + \beta (1 - \beta) \tilde{\mathbf{A}} \mathbf{E}^{(0)} + (1 - \beta)^2 \tilde{\mathbf{A}}^2 \mathbf{E}^{(K-2)} \\ &= \beta \mathbf{E}^{(0)} + \beta (1 - \beta) \tilde{\mathbf{A}} \tilde{\mathbf{E}}^{(0)} + \beta (1 - \beta)^2 \tilde{\mathbf{A}}^2 \mathbf{E}^{(0)} + \dots + (1 - \beta)^K \tilde{\mathbf{A}}^K \mathbf{E}^{(0)}. \end{split}$$
(12)

Model Training

Employ the Bayesian Personalized Ranking (BPR) loss

$$L_{BPR} = -\sum_{u=1}^{M} \sum_{i \in \mathcal{N}_{u}} \sum_{j \notin \mathcal{N}_{u}} \ln \sigma(\hat{y}_{ui} - \hat{y}_{uj}) + \lambda ||\mathbf{E}^{(0)}||^{2}$$

- 可学习的参数只有 E⁽⁰⁾
- 不需要 dropout 机制, L2 正则化足够防止过拟合

SASRec: Intro

Motivation:

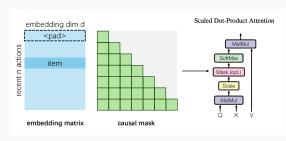
The goal of our work is to balance these two goals, by proposing a self-attention based sequential model (SASRec) that allows us to capture long-term semantics (like an RNN), but, using an attention mechanism, makes its predictions based on relatively few actions (like an MC).

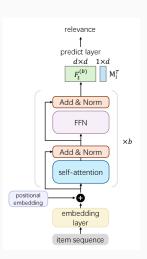
Contribution:

将注意力机制引入 Sequential Recommendation

SASRec: Method

- A. Embedding layer
- B. Self-attention Block
- C. Stacking SA Block
- D. Predict layer





Training & Complexity analysis

Training 训练使用交叉熵损失

Complexity analysis

- Space Complexity
 - $O(|\mathcal{I}|d + nd + d^2)$
- Time Complexity
 - computing: $O(n^2d + nd^2)$
 - testing: O(n)