Self introduction and future plans

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Basic information

- I'm from Suzhou, Jiangsu.
- I got my bachelor's degree at Nanjing University of Information Science & Technology and currently a master degree candidate of science in Zhejiang Gongshang University.
- My github page is `https://github.com/LEOXC1571` and my personal blog is `https://leoxc1571.github.io/`

A fairness-aware graph contrastive learning recommender framework for social tagging systems

- The proposed method integrates contrastive learning into tag-aware recommender systems. By perturbing features with normalized noises, different perspectives on features are generated. They help the model learn high quality features via contrastive learning tasks.
- In order to promote fairness of recommendations, we introduce fairness-aware learning, which jointly optimizes TAGCL through negative tag loss and TransT regularization. Negative tag loss leverages the distribution difference between items and tags in the training data.
- TransT regularization is also propsosed to promote consistency between two bipartite graphs. The differences between tag embeddings in separate graphs are regarded as relations between users and items.

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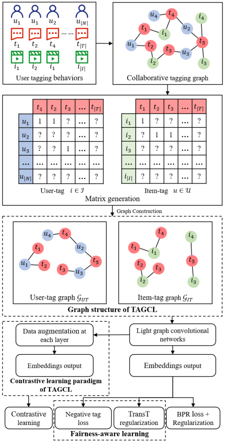

图 1: Overall structure of TAGCL

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Table 3
Performance Comparison.

Dataset	Metric	General		Tag-aware			TAGCL	imp. SOTA	imp. TRS
		LGCN	SimGCL	BPR-T	TGCN	LFGCF			
ML	Rec.	0.2788	0.2857	0.2826	0.2774	<u>0.2929</u>	**0.3180**	8.57%	8.57%
	Pre.	0.0349	<u>0.0385</u>	0.0365	0.0351	0.0365	**0.0405**	5.19%	10.96%
	NDCG	0.2015	<u>0.2279</u>	0.2209	0.2147	0.2140	**0.2338**	2.59%	5.84%
	MRR	0.2101	**0.2372**	0.2273	0.2202	0.2183	<u>0.2356</u>	-0.67%	3.65%
	ARP	26.78	<u>17.87</u>	22.76	19.87	18.10	**14.96**	16.26%	17.29%
LFM	Rec.	0.4742	0.5055	0.4759	0.4663	<u>0.5057</u>	**0.5199**	2.81%	2.81%
	Pre.	0.1350	<u>0.1534</u>	0.1374	0.1313	0.1465	**0.1611**	5.02%	9.97%
	NDCG	0.4015	<u>0.4680</u>	0.4358	0.4149	0.4482	**0.4949**	5.75%	10.42%
	MRR	0.4598	<u>0.5263</u>	0.5132	0.4727	0.5033	**0.5541**	5.28%	7.97%
	ARP	114.46	<u>51.67</u>	102.84	80.76	80.65	**42.99**	16.79%	46.70%
DE	Rec.	0.3337	<u>0.3351</u>	0.3150	0.3158	0.3300	**0.3432**	2.42%	4.00%
	Pre.	0.3525	<u>0.3554</u>	0.3409	0.3407	0.3498	**0.3705**	4.25%	5.92%
	NDCG	<u>0.4213</u>	0.4177	0.3984	0.4044	0.4080	**0.4385**	4.08%	7.48%
	MRR	<u>0.5786</u>	0.5529	0.5373	0.5577	0.5395	**0.5828**	0.73%	4.45%
	ARP	**3.11**	<u>4.67</u>	6.32	7.25	4.69	5.61	-79.99%	-19.62%

Pursuit and Evasion Strategy of a Differential Game Based on Deep Reinforcement Learning

- For the kinematic solve of dog sheep game, by finding the equilibrium point in the game, this study successfully establishes the kinematic pursuit and evasion policies.
- Leverage DQN and DDPG models to train the escaping strategy for intelligent agent.
- Propose a refined reward mechanism and an attenuation mechanism to minimize the defect of DQN.

Internship at Zhejiang Lab

- 生成模型近年来在作画、视频创作、空间建模、文本生成等多方面都有了成功的应用。早期的生成模型研究主要集中在变分自编码器（VAE）、生成对抗网络（GAN）、流型模型（Flow-based models）、自回归模型（Auto-regressive models）及深度强化学习领域。近两年来，基于扩散模型的生成模型（Diffusion-based models）以其优异的性能、计算资源消耗相对较少在学术圈与工业界爆火。
- 相关 Diffusion 模型的研究包括对干扰、去噪过程的改进（DDPMs，SGMs，Score SDEs），采样策略的改进，损失函数，各类型数据应用（计算机视觉、自然语言处理、时序建模、信号传递、多模态学习、图建模、医学影像）等。

计算医药

- 生成模型的发展也带动了其在智能计算领域的应用。5 年前，药物分子、蛋白质配体分子等分子学习任务主要聚焦于 2D 分子结构，但实际上，分子结构信息远不止原子间的拓扑结构信息这么简单，因此某一分子在自然界中可能存在种类繁多的同分异构体，故近来对分子的研究拓展到了结合 3D 信息对不同分子构型的相关研究。因此在 3D 分子生成任务上，目标不再是生成简单的可能有效的分子，更要生成具备理想属性和性质稳定的分子 3D 构型。
- 3D 分子生成任务又可分为 3D 构型生成与全新分子生成。3D 构型生成的目标是根据给定的分子式，生成理想的三维构型。全新分子生成的目标则是凭空生成全新的、有效的分子。
- 3D 构型生成的研究有基于 VAE 的 CVGAE，GraphDG，ConfVAE，基于扩散模型的 ConfGF，EVFN，GeoDiff 等。

前期准备

- 本文意在利用生成模型，提出创新的算法，生成全新且有效的分子。
- 本文首先选取 GEOM-QM9 和 GEOM-Drugs 作为研究数据集。GEOM-QM9 包含 130831 个分子，平均每个分子由 19 个分子构成。
- GEOM-Drugs 包含超过 600W 个分子构型，将每个分子的不同构型经过筛选后，处理得到 29W 个稳定的分子构型，平均每个分子由 44 个原子构成。

生成模型构建

- 本文基于 DDPMs 构建分子生成模型框架，包括扩散过程与去噪过程。
- 扩散过程本质是通过给初始数据有规律地增加噪声，使其经过 T 时间步后收敛至高斯噪声。
- 去噪过程的本质是通过设计的去噪神经网络内核，将高斯噪声还原至初始状态，使其与初始数据相似。

- 2023.01-2023.03：前期调研与相关文献阅读
- 2023.03-2023.04：模型搭建
- 2023.04-2023.05：模型训练，性能调优与对比试验
- 2023.05-2023.07：文章撰写
- 2023.07-2023.09：文章修改

Thanks!