0808-周报

DIY卡片质量检测方法

面临的问题：

1、每张卡片具有唯一性，无法获取标准正常样本，传统监督学习方法难以适用。

2、当通过DIY 预览图（如渲染图、设计图稿）与实际生产出的卡片的图片进行比对，会有背景/颜色差异、位置/视角变形等问题

两阶段检测策略：

- **视觉层面检测**：基于无监督算法（如 PatchCore / FastFlow）识别划痕、气泡、污点等图案异常。
- **结构要素检测**：基于预览图做结构模板，通过图像配准与区域对比判断 Logo、芯片、卡号、防伪图案的位置与尺寸合法性。

输入数据：

- 每张卡片的 DIY 预览图（设计图）
- 实拍图像（多个角度，如正视、斜视等 6~8 张）
- 紫光图（用于防伪图案检测）

输出结果：

- 每张图像的缺陷分数、热力图（heatmap）
- 结构偏移量（以毫米计）与位置合规判断
- 防伪图案是否存在判断结果
- 最终合格/不合格综合判定

Anomalib：工业异常检测的开源利器

由 Intel OpenVINO 团队开发，集成多种 SOTA 无监督算法

优势：

开源异常检测工具库

聚焦无监督视觉检测（图像/视频）

支持训练、推理、可视化、部署一体化

工具库中的部分算法

算法名	类型	特点
PatchCore	最近邻匹配	小样本表现强
PaDiM	高斯建模	推理快、部署友好
STFPM	模仿学习	多尺度、定位准
FastFlow	概率建模	实时检测、结构轻

算法名	类型	特点
Ganomaly	GAN重建	图像生成对比（需训练）

算法：PathCore-patch特征+最近邻

论文：Towards Total Recall in Industrial Anomaly Detection（CVPR2022）

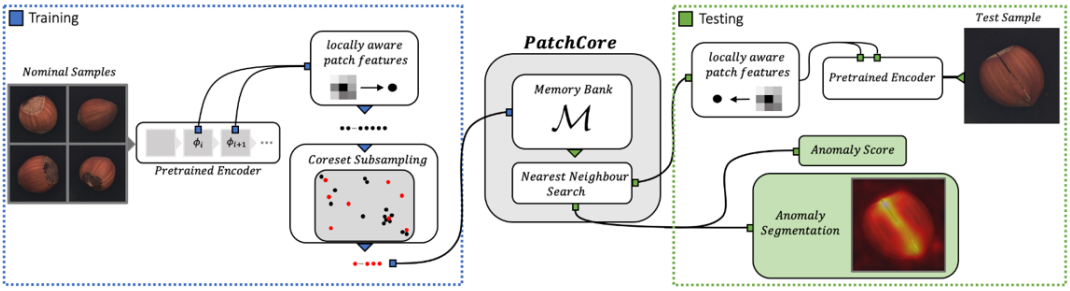


Figure 2. Overview of *PatchCore*. Nominal samples are broken down into a memory bank of neighbourhood-aware patch-level features. For reduced redundancy and inference time, this memory bank is downsampled via greedy coreset subsampling. At test time, images are classified as anomalies if at least one patch is anomalous, and pixel-level anomaly segmentation is generated by scoring each patch-feature.

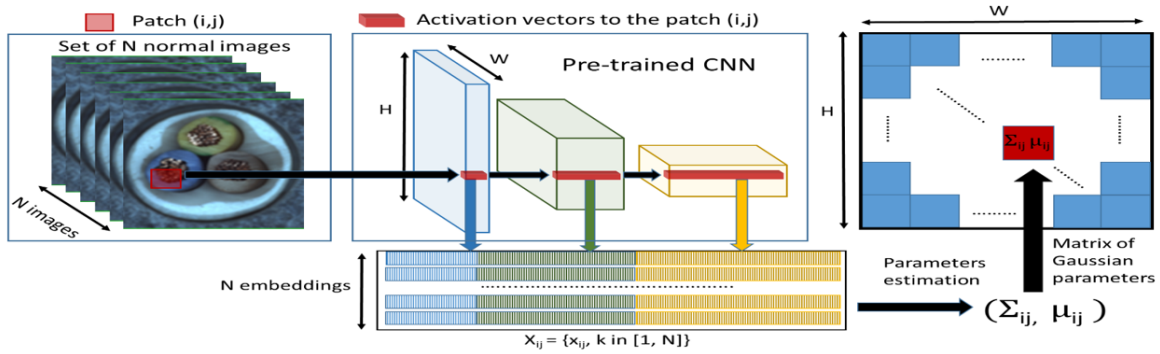
算法思路：1、只使用少量无瑕疵图进行训练；2、使用预训练模型ImageNet生成图向量；3、核心集子采样（Coreset Subsampling），从中挑选出最有代表性的一小部分特征；4、将特征信息存入Memory Bank中；5、将带检测的图片进行相同的操作，结合Memory Bank，使用KNN遍历每个特征，计算相似性；6、相似性低于阈值则检测不合格

卡片检测中：如一张卡片拍摄8张图片，7张来构建Memory Bank，1张来test

算法：PaDIM-pathch特征+马氏距离

论文：PaDiM: a Patch Distribution Modeling Framework for Anomaly Detection and Localization

Fig. 2. For each image patch corresponding to position (i, j) in the largest CNN feature map, PaDiM learns the Gaussian parameters (μ_{ij}, Σ_{ij}) from the set of N training embedding vectors $X_{ij} = \{x_{ij}^k, k \in [\![1, N]\!]\}$, computed from N different training images and three different pretrained CNN layers.



算法思路：1、为每个patch位置学习一个“正常特征的概率分布”（将CNN的几个中间层的向量表示拼接起来）2、用马氏距离判断测试图片是否在分布之外，从未判断定位和检测异常区域

算法：STFPM-学生教师模型

论文：Student-Teacher Feature Pyramid Matching for Anomaly Detection（BMVC 2021）

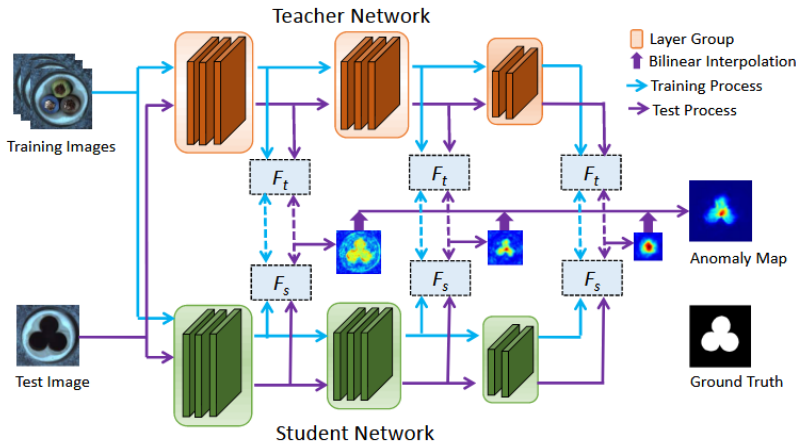


Figure 2: Schematic overview of our method. The feature pyramid of a student network is trained to match with the counterpart of a pre-trained teacher network. A test image (or pixel) has a high anomaly score if its features from the two models differ significantly. The feature pyramid matching enables our method to detect anomalies of various sizes with a single forward pass.

算法思路：让一个“学生网络”去模仿一个“老师网络”在正常图像上的特征输出，如果在测试图中，学生无法成功模仿老师，那这个位置就是异常。

论文-Accurate and interpretable drug-drug interaction prediction enabled by knowledge subgraph learning

问题及解决方法

问题	解决方法
1、DDI样本稀缺，模型难以泛化	将原始DDI图（DrugBank、TWOSIDES）与外部生物医学知识图（Hetionet）合并成一个大图，通过GNN学习丰富的药物表示（如蛋白质、疾病、通路等）
2、知识图信息噪声大，影响模型性能	构建“知识子图”，通过计算每条边的连接强度自动保留重要边、剔除无关边、添加“resemble”边
3、缺乏可解释性，预测结果难以理解	通过每条边的连接强度学习“解释路径”，提供明确的推理链条增强临床可信度

框架图

$$\mathbf{a}_v^{(l)} = \text{MEAN}\left(\{\text{ReLU}(\mathbf{W}_a^{(l)}\mathbf{e}_u^{(l)}) : (u, r, v) \in \mathcal{E}\}\right), \quad (1)$$

$$\mathbf{e}_v^{(l)} = \mathbf{W}_c^{(l)} \cdot \left[\mathbf{a}_v^{(l)} \parallel \mathbf{e}_v^{(l-1)}\right], \quad (2)$$

使用GraphSAGE在融合图上学习每个节点的初始向量表示

$$\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathcal{R}\} = \{\mathcal{V}_{\text{DDI}} \cup \mathcal{V}_{\text{KG}}, \mathcal{E}_{\text{DDI}} \cup \mathcal{E}_{\text{KG}}, \mathcal{R}_{\text{DDI}} \cup \mathcal{R}_{\text{KG}}\}.$$

注意：外部知识图 中移除了 DDI 边

从融合图中提取所有从H到 T的长度≤P 的路径，得到子图

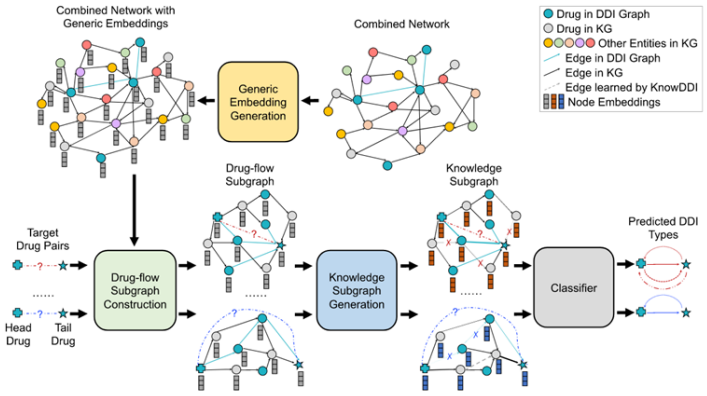
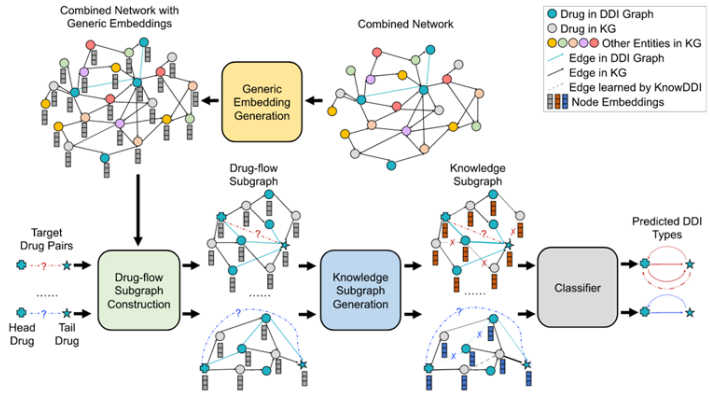


Fig. 1 | Overview of KnowDDI. On a combined network which merges the drug-drug interaction (DDI) graph with an external knowledge graph (KG), generic embeddings of all nodes are firstly learned to capture generic knowledge. Then for each target drug-pair, a drug-flow subgraph is extracted from the combined network, whose node embeddings are initialized as the generic embeddings. Via propagating drug resembling relationships, the generic embeddings are transformed to be more predictive of the DDI types between the drug-pair, and the drug-flow subgraph is adapted as knowledge subgraph which contains explaining paths to interpret the prediction result.



$$\mathbf{h}_{uv}^{\tau-1} = \exp(-|\mathbf{h}_u^{(\tau-1)} - \mathbf{h}_v^{(\tau-1)}|),$$

表示节点之间的相似性，约相似约接近1

$$\mathbf{C}_{h,t}^{(\tau)}(u, v, r) = \text{MLP}\left(\left[\mathbf{h}_{uv}^{\tau-1} \parallel \mathbf{h}_r\right]\right),$$

计算连接强度。
如果节点对之间相似但没有边，则添加新边类型“resemble”；如果边重要性低，则删除边。

$$\mathbf{h}_{\mathcal{S}_{h,t}} = \text{MEAN}\left(\{\mathbf{h}_v | v \in \bar{\mathcal{V}}_{h,t}\}\right).$$

获得整个子图的嵌入表示

$$\hat{\mathbf{y}}_{h,t} = \delta\left(\mathbf{W}_c \cdot \left[\mathbf{h}_{\mathcal{S}_{h,t}} \parallel \mathbf{h}_h \parallel \mathbf{h}_t\right]\right),$$

Fig. 1 | Overview of KnowDDI. On a combined network which merges the drug-drug interaction (DDI) graph with an external knowledge graph (KG), generic embeddings of all nodes are firstly learned to capture generic knowledge. Then for each target drug-pair, a drug-flow subgraph is extracted from the combined network, whose node embeddings are initialized as the generic embeddings. Via propagating drug resembling relationships, the generic embeddings are transformed to be more predictive of the DDI types between the drug-pair, and the drug-flow subgraph is adapted as knowledge subgraph which contains explaining paths to interpret the prediction result.

实验：性能对比

任务：多分类（DrugBank），多标签（TWOSIDES）

Table 1 | Performance (%) is evaluated on two benchmark DDI datasets DrugBank and TWOSIDES

	Dataset	DrugBank (multiclass)			TWOSIDES (multilabel)			Avg.
	Statistics	$\|\mathcal{V}\| = 1710, \|\mathcal{R}\| = 86, \|\mathcal{E}\| = 192284$			$\|\mathcal{V}\| = 604, \|\mathcal{R}\| = 200, \|\mathcal{E}\| = 41270$			
	Metric	F1	ACC	Cohen's κ	AUROC	AUPRC	AP@50	Rank
	TransE	18.32 ± 0.16	64.60 ± 0.11	57.19 ± 1.22	77.53 ± 0.02	70.16 ± 0.02	77.54 ± 0.03	15
Traditional	KG-DDI	37.21 ± 0.36	82.74 ± 0.10	78.71 ± 0.33	90.64 ± 0.09	87.99 ± 0.11	83.50 ± 0.06	10
Two-stage	MSTE	53.96 ± 0.07	77.76 ± 0.11	73.35 ± 0.05	89.40 ± 0.04	83.06 ± 0.06	79.38 ± 0.03	12
(w/o external	node2vec	50.00 ± 1.67	62.39 ± 0.99	56.27 ± 0.89	90.62 ± 0.43	89.42 ± 0.47	82.21 ± 0.54	12
KG)	DeepWalk	49.17 ± 1.38	62.90 ± 0.37	56.77 ± 0.44	91.77 ± 0.26	90.56 ± 0.23	84.13 ± 0.35	9
	LINE	48.89 ± 1.38	59.87 ± 0.92	52.15 ± 1.51	88.63 ± 0.20	87.02 ± 0.22	80.80 ± 0.20	14
GNN-based	GAT	35.05 ± 0.41	78.02 ± 0.14	74.68 ± 0.21	91.22 ± 0.13	89.79 ± 0.10	83.05 ± 0.18	11
(w/o external	Decagon	56.24 ± 0.27	86.97 ± 0.31	86.12 ± 0.09	91.83 ± 0.14	90.79 ± 0.18	82.49 ± 0.36	7
KG)	SkipGNN	62.36 ± 0.96	88.04 ± 0.66	85.71 ± 0.81	92.31 ± 0.15	90.84 ± 0.03	84.23 ± 0.19	6
	GraIL	75.92 ± 0.69	89.63 ± 0.39	87.63 ± 0.47	93.73 ± 0.10	92.26 ± 0.07	86.89 ± 0.11	3
GNN-based	KGNN	74.08 ± 0.92	88.30 ± 0.08	86.09 ± 0.10	92.93 ± 0.10	90.11 ± 0.14	87.43 ± 0.09	5
(w/ external	DDKG	75.84 ± 0.22	88.70 ± 0.39	87.53 ± 0.21	93.15 ± 0.18	91.09 ± 0.39	87.50 ± 0.43	4
KG)	SumGNN	86.88 ± 0.63	91.86 ± 0.23	90.34 ± 0.28	94.61 ± 0.06	93.13 ± 0.15	88.38 ± 0.07	2
	LaGAT	83.69 ± 0.74	88.86 ± 0.12	87.33 ± 0.14	88.72 ± 0.22	84.03 ± 0.43	82.46 ± 0.41	8
	KnowDDI	**91.53 ± 0.24**	**93.17 ± 0.09**	**91.89 ± 0.11**	**95.43 ± 0.02**	**94.14 ± 0.03**	**89.54 ± 0.03**	1

Average (Avg.) rank of each method is reported in the last column, which is averaged over the six columns of performance. The best and comparable results (according to the pairwise t-test with 95% confidence) are highlighted in bold, and the second-best results are underlined. |·| counts the number of elements in a set. $\mathcal{V}$ is the set of drug nodes, $\mathcal{E}$ is the set of fact triplets, and $\mathcal{R}$ is the set of relation types.

Cohen's κ（Kappa系数）： *考虑了随机猜中标签的概率。Accuracy 看的是表面对了多少，Kappa 看的是：你是真的对，还是“刚好猜对了”？*
AP@50： *模型返回的前50个预测中，正确预测的比例，衡量前列结果质量*

三类对比模型：传统方法（非GNN，不使用外部KG）、GNN方法（不使用外部KG）、GNN方法（使用外部KG）

结论：KnowDDI对比次优模型SumGNN性能各方面都有提升。

实验：数据稀疏度

图a、DrugBank或TWOSIDES数据库中DDI出现的次数

图b、外部KG（Hetionet）的稀疏度（占比）

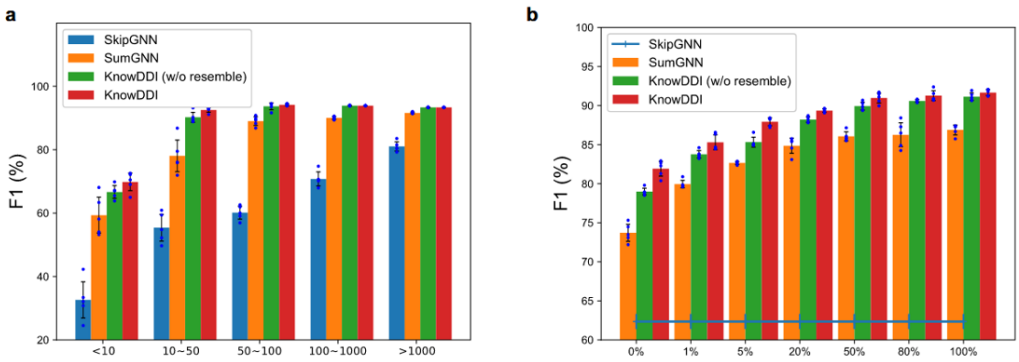


Fig. 2 | A closer examination and comparison of KnowDDI with SumGNN, SkipGNN and KnowDDI (w/o resemble). a F1 (%) obtained for relations with different number of DDI fact triplets on DrugBank. **b** F1 (%) obtained with different portion (%) of fact triplets sampled from the external KG on DrugBank. SkipGNN, which does not use external KG, is plotted just for reference. This bar plot illustrates the test performance (%), with each bar's height representing the mean result and the error bars indicating the standard deviation, both derived from five independent runs ($n = 5$).

结论：论文的模型性能都高于对比模型，随着DDI出现的次数/外部KG的占比增加，模型性能随之提高

实验：不同子图生成策略下的性能比较

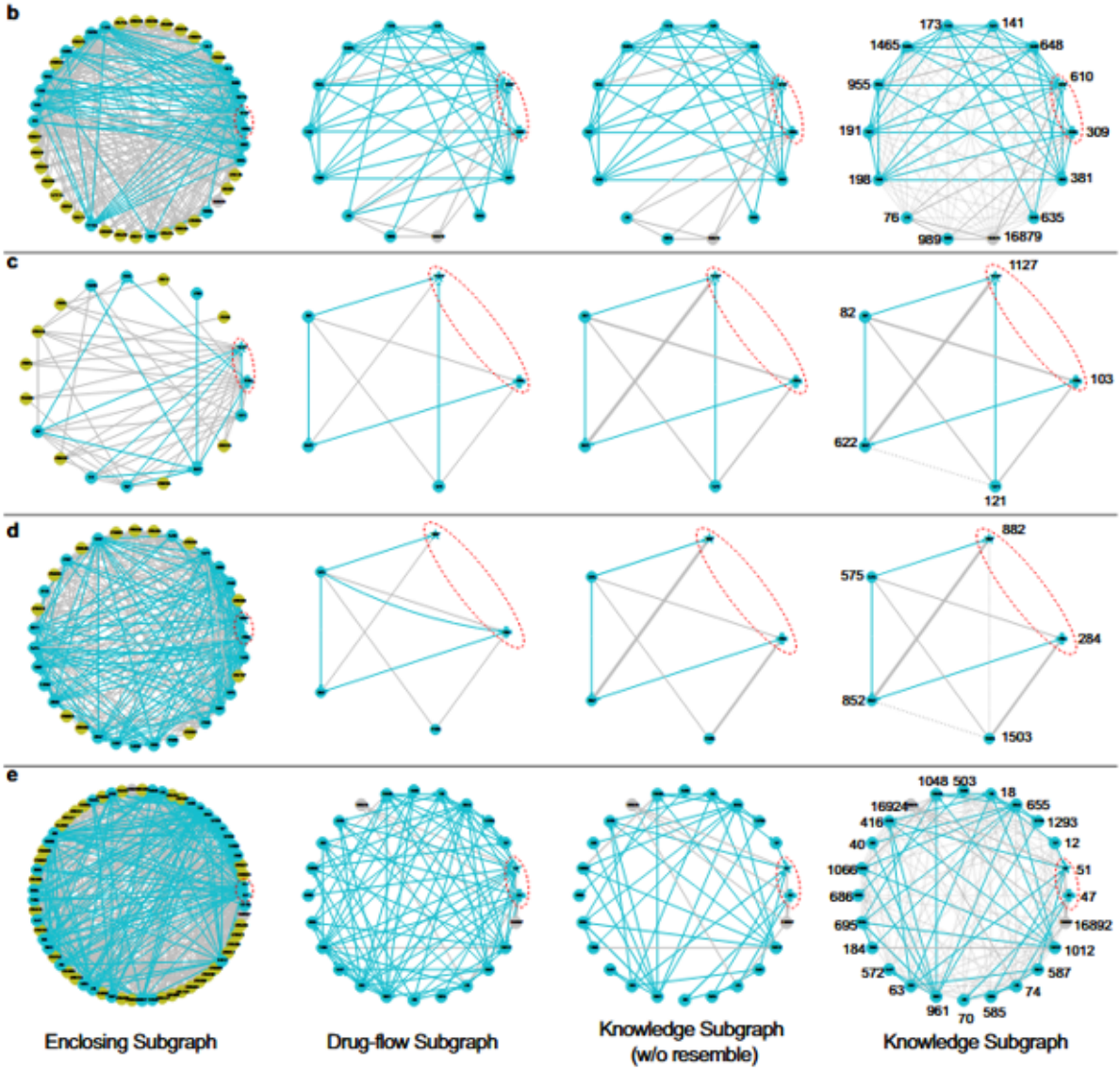
子图类型	描述
无子图	不使用任何局部结构，仅用通用节点表示
Random Subgraph	从邻居中随机采样固定数量节点
Enclosing Subgraph	提取药物对的K-hop邻居交集
Drug-flow Subgraph	从头药物到尾药物的有向路径

子图类型	描述
Knowledge Subgraph	动态学习边结构 + 加入 resemble 边

- 红色圆圈：表示目标药物对 (h,t)
- 蓝色实线：来自原始 DDI 图的边
- 灰色实线：来自外部知识图的原始边
- 灰色虚线：模型新加的 resemble 边
- 边的粗细：表示连接强度（由模型学习到）

a

F1	w/o Subgraph	Random Subgraph	Enclosing Subgraph	Drug-flow Subgraph	Knowledge Subgraph
100%	86.74 ± 0.48	89.49 ± 0.59	90.03 ± 0.28	90.63 ± 0.20	91.53 ± 0.24
5%	80.77 ± 1.19	84.82 ± 0.92	85.06 ± 0.50	85.32 ± 0.63	87.92 ± 0.50
0%	72.71 ± 0.92	75.88 ± 1.16	77.74 ± 0.25	78.99 ± 0.43	81.91 ± 0.94



b、c、d、e为四个例子

结论：1、文章的子图提取方法对模型模型性能提升最高。2、从图中可见，文章的子图提取方法中，边的信息更为丰富。

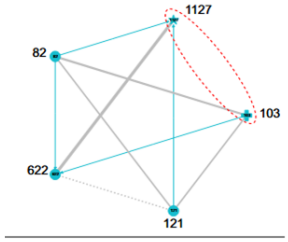
实验：可解释性

图中为c例

Table 2 | Explaining paths with the largest average connection strengths assigned by KnowDDI for four drug-pairs in DrugBank

Drug-Pair	(309,610)
DDI Type	The metabolism of Atomoxetine (610) can be decreased when combined with Reboxetine (309).
Explaining Path	$309 \xrightarrow{\text{resembles}} 16879 \xrightarrow{\text{resembles}} 610$
Explanation	Reboxetine (309) resembles Diphenylpyraline (16879), while Diphenylpyraline (16879) resembles Atomoxetine (610). We can deduce that Reboxetine (309) resembles Atomoxetine (610). When taking two similar drugs, the body may absorb less of the Atomoxetine (610).
Drug-Pair	(103,1127)
DDI Type	The serum concentration of Betamethasone (103) can be increased if combined with Estriol (1127).
Explaining Path	$103 \xrightarrow{\text{resembles}} 121 \xrightarrow{\text{resembles(knowledge)}} 622 \xrightarrow{\text{resembles}} 1127$
Explanation	Betamethasone (103) bears resemblance to Desonide (121). Although the interaction between Desonide (121) and Mestranol (622) is not provided, our search within DrugBank reveals that combining Mestranol (622) with Budesonide can elevate the serum concentration of Budesonide. Furthermore, Budesonide is similar to Desonide (121), and Mestranol (622) is similar to Estriol (1127). Given the tendency for similar drugs to exhibit akin properties, it is plausible that the serum concentration of Betamethasone (103) could rise when used alongside Estriol (1127).
Drug-Pair	(284,882)
DDI Type	The therapeutic efficacy of Sulfadiazine (284) can be increased when used in combination with Gatifloxacin (882).
Explaining Path	$284 \xrightarrow{\text{therapeuticefficacyincreased}} 852 \xrightarrow{\text{resembles}} 882$
Explanation	The combined use of Sulfadiazine (282) and Pefloxacin (852) can improve the efficacy. Meanwhile, Pefloxacin (852) resembles Gatifloxacin (882). It can be deduced that the therapeutic efficacy of Sulfadiazine (282) can be increased when used in combination with Gatifloxacin (882).
Drug-Pair	(47,51)
DDI Type	The risk or severity of adverse effects can be increased when Atropine (47) is combined with Scopolamine (51).
Explaining Path	$47 \xrightarrow{\text{resembles}} 16892 \xrightarrow{\text{resembles}} 51$
Explanation	Atropine (47) resembles Homatropine methylbromide (16892), while Homatropine methylbromide (16892) resembles Scopolamine (51). We can deduce that Atropine (47) resembles Scopolamine (51). The similarities between the two drugs can also be seen through the chemical structures of the drugs. As the two drugs are similar in structure, the effects of using both drugs at the same time should be similar to the side effects of overdose of either drug, which can cause serious side effects. Based on DrugBank, Scopolamine (51) overdose may manifest as lethargy, somnolence, coma, confusion, agitation, hallucinations, convulsion, visual disturbance, dry flushed skin, dry mouth, decreased bowel sounds, urinary retention, tachycardia, hypertension and supraventricular arrhythmias, while Atropine (47) overdose may cause palpitation, dilated pupils, difficulty swallowing, hot dry skin, thirst, dizziness, restlessness, tremor, fatigue and ataxia.

Possible explanations are discovered from Hetionet and DrugBank.



Budesonide

DDI 类型：1126与103合用时会提高血清浓度
解释：Betamethasone（103）与 Desonide（121）相似。虽然没有提供 Desonide（121）与 Mestranol（622）之间的直接相互作用信息，但我们在 DrugBank 中查阅发现，**Mestranol（622）与 Budesonide 联合使用可以提高 Budesonide 的血清浓度**。此外，Budesonide 与 Desonide（121）相似，而 Mestranol（622）也与 Estriol（1127）相似。鉴于**相似药物通常具有类似药理性质**，因此可以合理推测，当 Betamethasone（103）与 Estriol（1127）联合使用时，其血清浓度可能会上升。

103相似121
622相互作用Budesonide
Budesonide相似121
622相似1127
所以103相互作用1127

论文总结

创新点主要为：计算不同节点之间的连接强度，剔除连接强度低的边，添加相似（两个节点间没有边连接，但连接强度高）边。该方法简单有效，可借鉴。

下步计划

1、KnowDDI论文代码已复现，学习一下代码实现细节

2、卡片检测方法调研