<AAAI2020>Generative Adversarial Zero-Shot Relational Learning for Knowledge Graphs

Pengda Qin, Xin Wang, Wenhu Chen, Chunyun Zhang, Weiran Xu, William Yang Wang.Generative Adversarial Zero-Shot Relational Learning for Knowledge Graphs. AAAI 2020.

Qiang Liu
July 24

Outline

- Reading
  - Motivation
  - Method
  - Experiment
  - Conclusion
- Reproduce

Pengda Qin, Xin Wang, Wenhu Chen, Chunyun Zhang, Weiran Xu, William Yang Wang.Generative Adversarial Zero-Shot Relational Learning for Knowledge Graphs. AAAI 2020.

Reading

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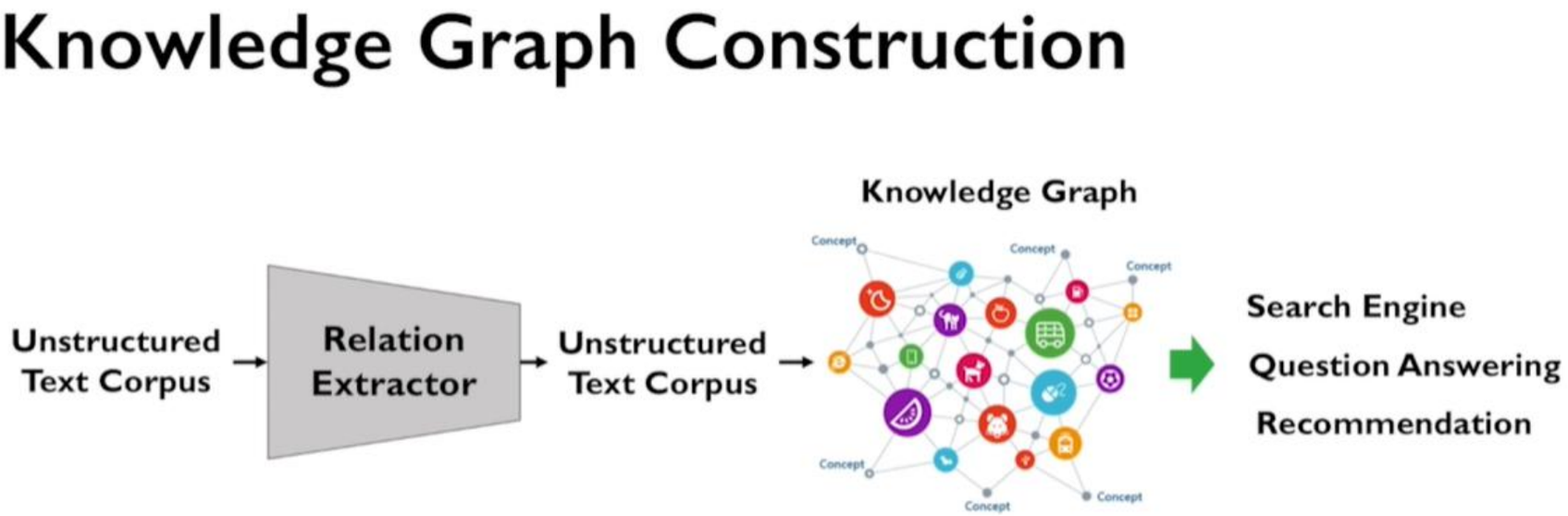
Motivation

- Knowledge Graph

知识图谱使用图的形式存储实体键关系的结构化数据，大量的关系三元组通过共同的关系和实体建立联系，形成图的形式，提升机器的理解、处理能力，服务于问答系统、推荐引擎、搜索引擎



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Motivation

- Problem
  - 当有新的关系（unseen relation）时如何扩充知识图谱。扩充即为这些unseen relations涉及到的head entity预测对应的tail entity
  - 本文只考虑新的关系，不考虑新的实体
  - 本篇文章的问题设定集中在处理zero-shot relations，未考虑会出现一些新的实体，即KG中的实体在训练集和测试集中都出现过。换句话说，在测试时，对于KG中已经存在的实体添加了一些zero-shot relations，预测它们是否构成一个完整的三元组。

- Supervised Learning

  需要标注训练数据，问题是数据成本高和标注数据的时间长，不适应互联网大规模的数据情况。同时可能存在数据集不均衡问题

- Zero-Shot Learning

  考虑利用大量已知关系类别三元组的基础上，不借助标注的数据，就对未知关系的关系三元组识别，也就是零样本学习

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Method

- Attribute-based Model
  - 人工归纳重要的特征属性，通过学习属性和实体间转换矩阵，建立转换媒介
  - 问题是需要人工标注属性，且效果对属性选取敏感
- Text-based Model
  - 通过非结构化的文本描述，生成媒介与表征，完成零样本学习。
  - 本文采用此种方法

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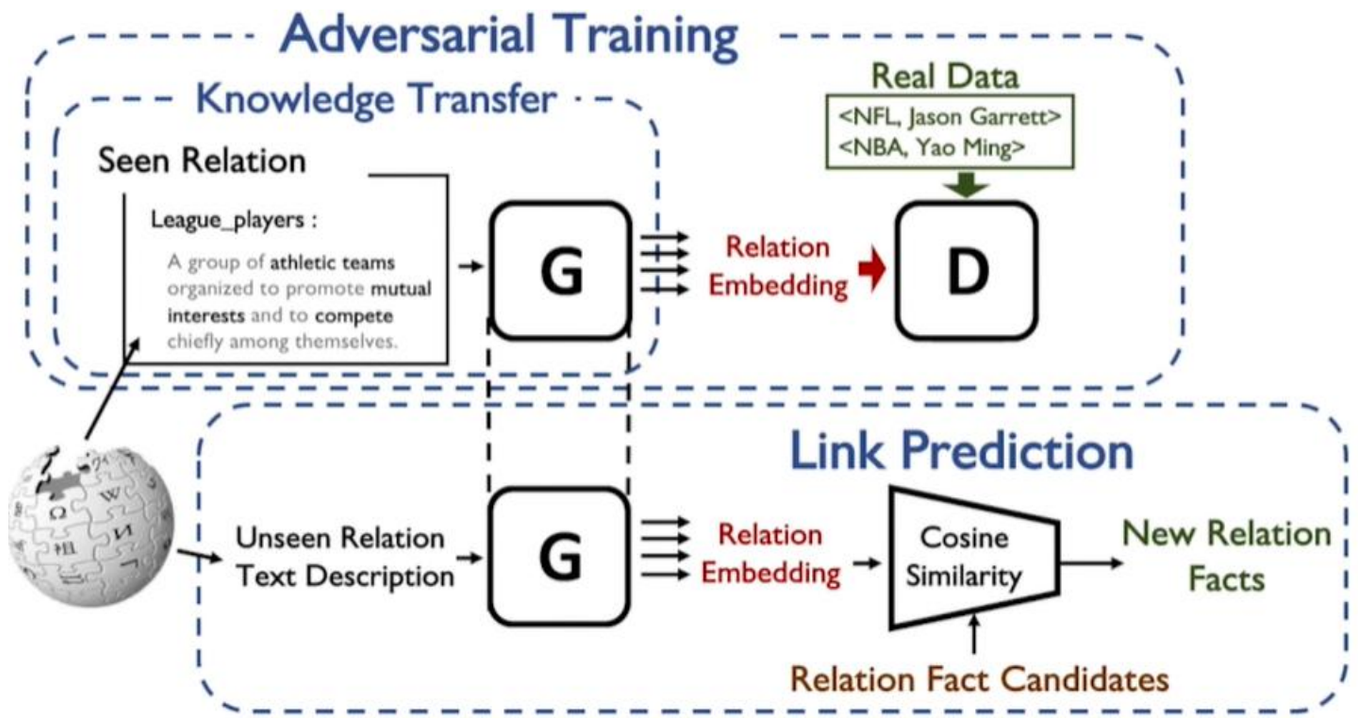
Method

- Overview
  - 采用基于条件的生成对抗网络，通过设置合理的对抗学习目标，让生成器具备通过文本描述生成文本类别表征的能力。
  - 通过上述的对抗学习，建立了生成器。对于新的关系类型，如果已知文本描述定义，就可以生成关系类别向量
  - 新的类型的识别就可以通过计算余弦相似度完成



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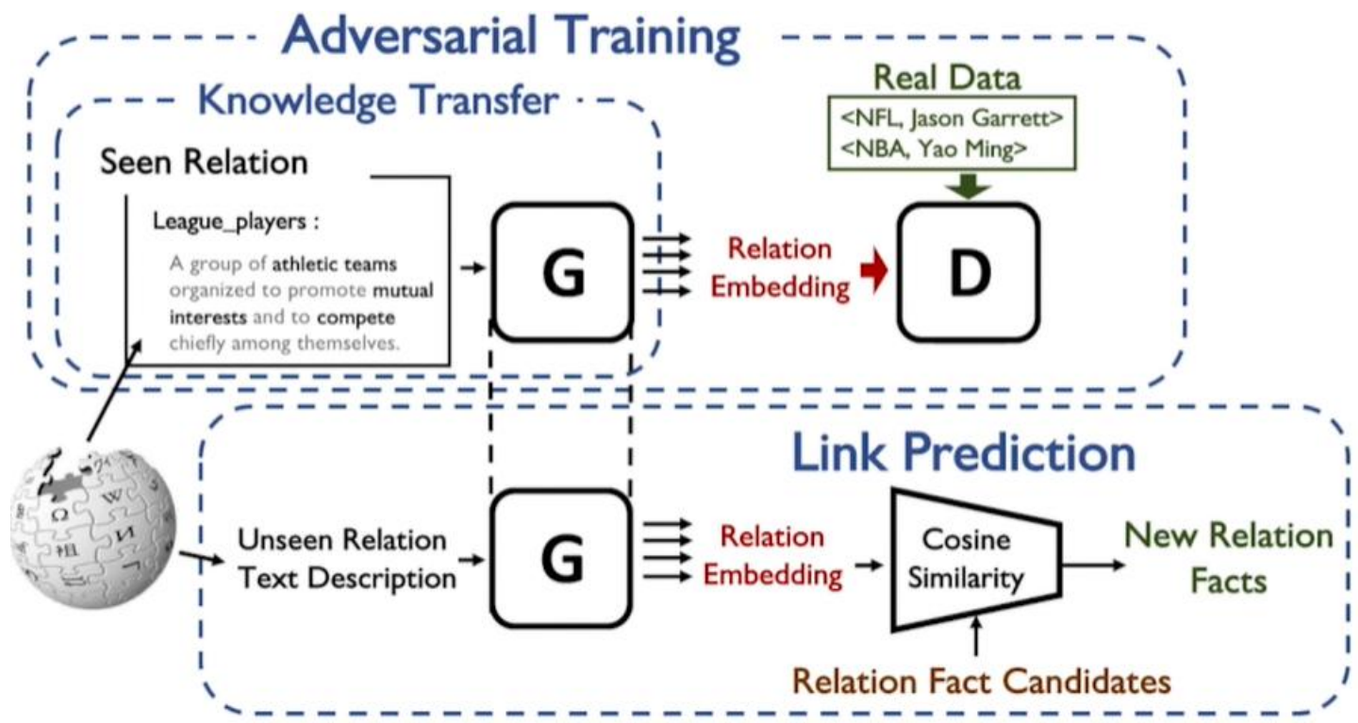
Method

- Overview
  - 首先类别的文本描述中可以提取出类别的表征向量，这是一个知识转移的问题
  - 第二unseen和seen的relations具备相同的知识背景
  - 因此，如果可以利用seen的relations，很好的学习从文本描述提取表征的能力，就可以对任意的关系建立关系向量表征



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Method

- Definition
  - Rs，Ru
    - 两个不同的关系集合：Rs（seen classes），Ru（unseen classes）
    - 不重叠。Rs ∩ Ru = φ
  - E
    - 实体集合。闭集。（这里只考虑新加入的关系，不考虑新加入实体）
  - Background Knowledge Graph G，
    - G包含大量的已知三元组，且所含关系类型均属于已知关系集合Rs
    - 只用于训练集

$$\mathcal{G} = \{(e_1, r_s, e_2) | e_1 \in E, e_2 \in E\}$$

- Ds，Du
  - 训练集和测试集。

$$\boldsymbol{D_s = \{(e_1, r_s, e_2, C_{(e_1,r_s)}) | e_1 \in E, e_2 \in E\}}$$

$$\boldsymbol{D_u = \{(e_1, r_u, e_2, C_{(e_1,r_u)}) | e_1 \in E, e_2 \in E\}}$$

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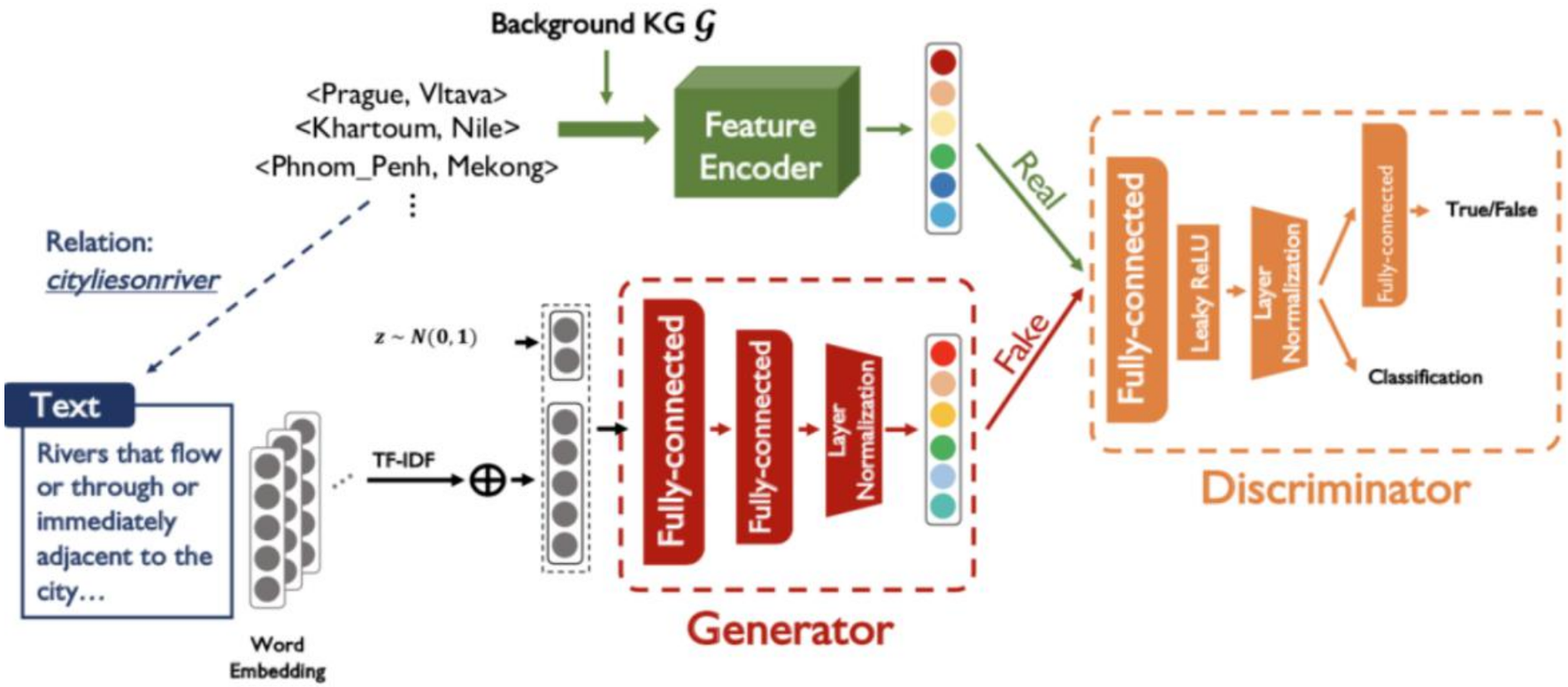
Method

- Framework 对抗学习的结构
  - Text 关系类别的文本描述
  - 通过generator生成表征，认为是虚假的。而相应的标注数据是为real数据
  - 鉴别器区分fake和real的数据



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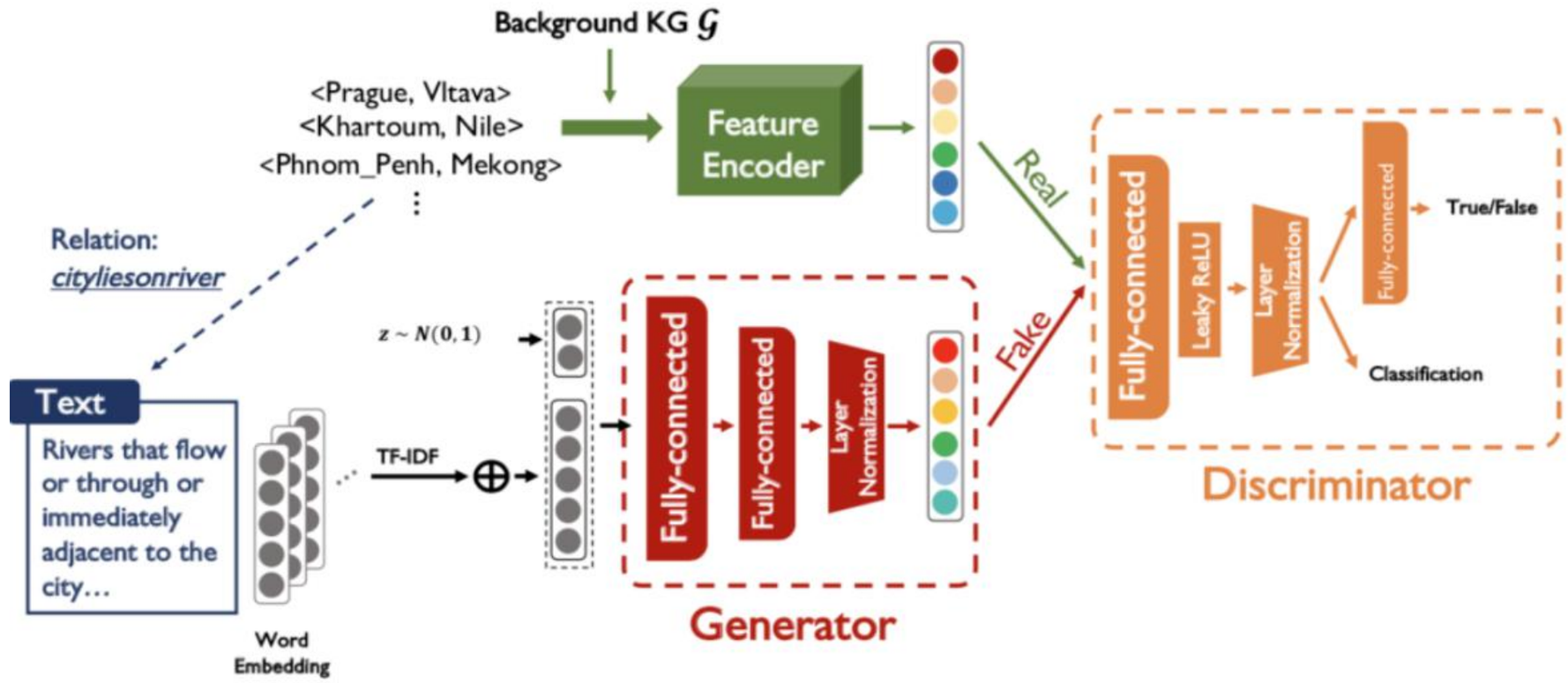
Method

- Text 编码
  - Word embedding 基于词向量的词袋模型，利用文本中每个词的Word embedding
  - TF-IDF 然后采用TF-IDF进行加权
  - 得到文本描述的向量表示
  - Generator输入还引入随机向量z，0~1高斯分布
  - 然后二者作为生成器输入



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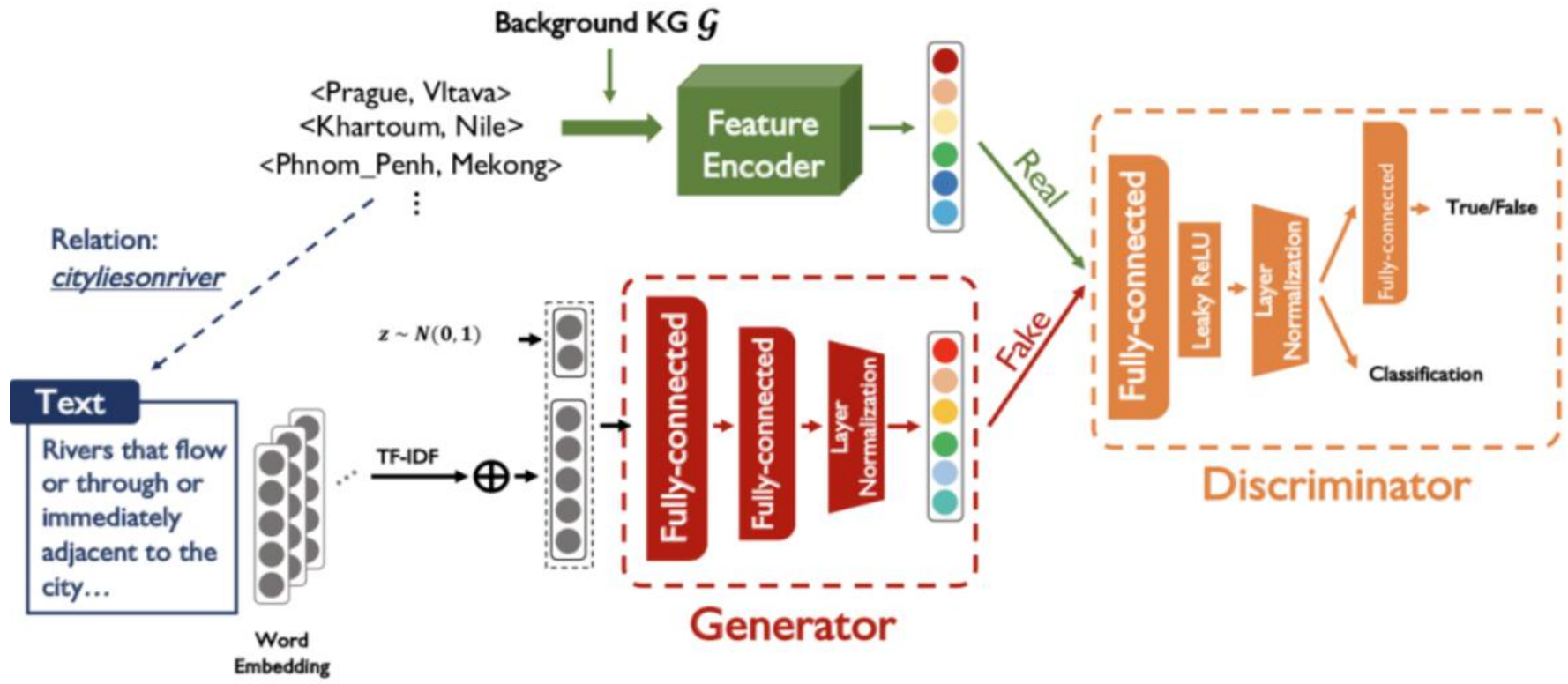
Method

- Generator
  - 两层全连接层和一层激活层函数（layer normalization）
  - Generator生成关系的特征表示



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Method

- Generator
  - Generator的目标（损失）函数

$$L_{G_\theta} = \underbrace{-\mathbb{E}_{z\sim p_z}\left[D_\phi\left(G_\theta(T_r, z)\right)\right]}_{\text{Adversarial}} + \underbrace{L_{cls}\left(G_\theta(T_r, z)\right)}_{\text{Classification}} + \underbrace{L_p}_{\text{Visual Pivot Regularization}}$$

WGAN

(Zhu et al., CVPR 2018)

- 其中 $G_\theta(T_r, z)$ 为生成样本。
- 第一部分GAN的Wasserstein loss，防止模型崩塌（生成样本多样性不足），
  第二部分为针对类别分类的训练目标，第三部分为 visual pivot 正则化项，
  提供足够的类间区分度（CVPR 2018）

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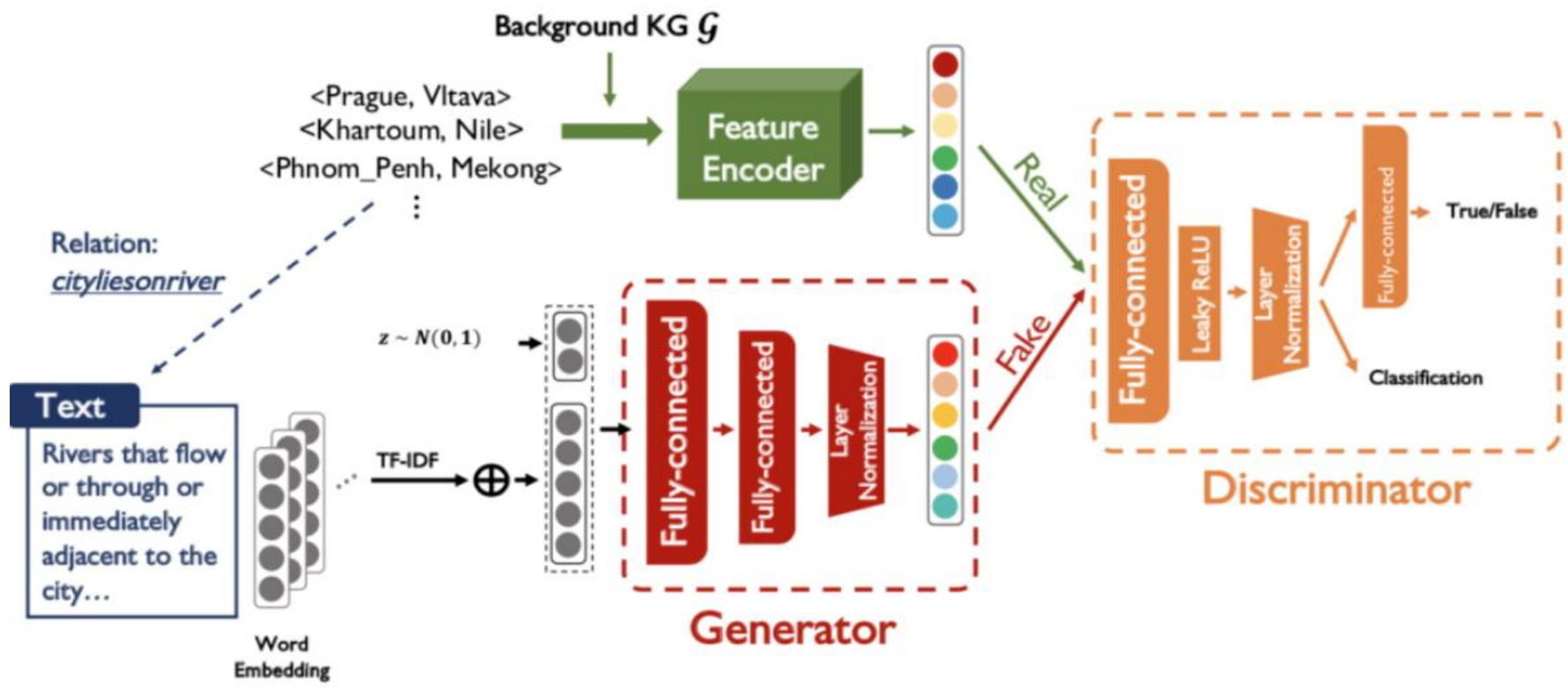
Method

- Feature Encoder
  - Feature Encoder对真实数据编码
  - 这里Feature Encoder的训练在对抗学习前完成，参数在对抗学习中不变，也就是真实数据不变



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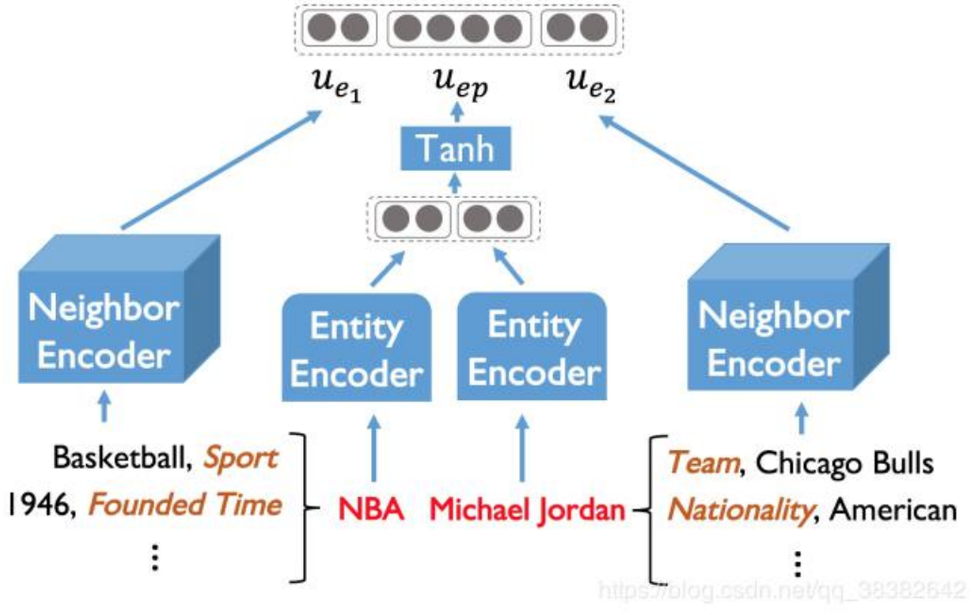
Method

- Feature Encoder
  - 对三元组中的实体对的关系进行建模，其通过已知和未知的标注类别的数据(seen/unseen classes)进行训练。要求不仅给出已知类别的实体对合理的特征表征，也需要给出未知unseen类别实体对的特征标准。传统有监督方法会造成对已知关系类型的过拟合，因此采用基于matching的方法进行训练。



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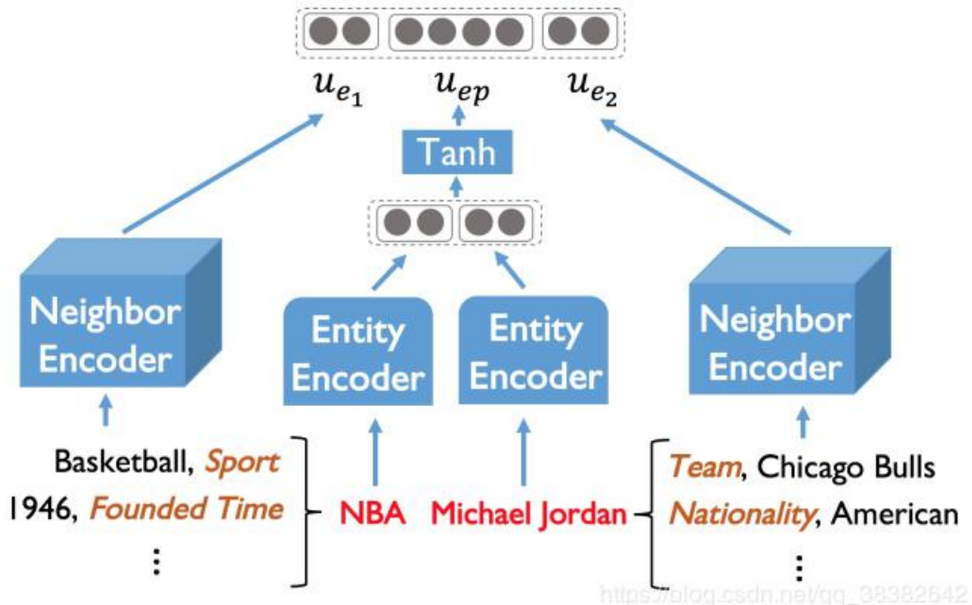
Method

- Feature Encoder
  - 对于某关系r，存在一系列的实体对集合，这些实体对描述了该关系的样本特征分布。对于其中的一对实体(e1,e2)，特征编码器首先通过一个entity encoder和一个neighbor encoder捕获这个实体对的蕴含的特征 $x_{(e_1,e_2)}$
  - 随后，对关系r所有的实体对的表示进行聚类可得到关系r的特征表示
  - 包含两个子编码器 Entity 和Neghbor Encoder



$$x_c^r = \frac{1}{N_r} \sum_{i=1}^{N_r} x_{(e_1,e_2)}^i$$

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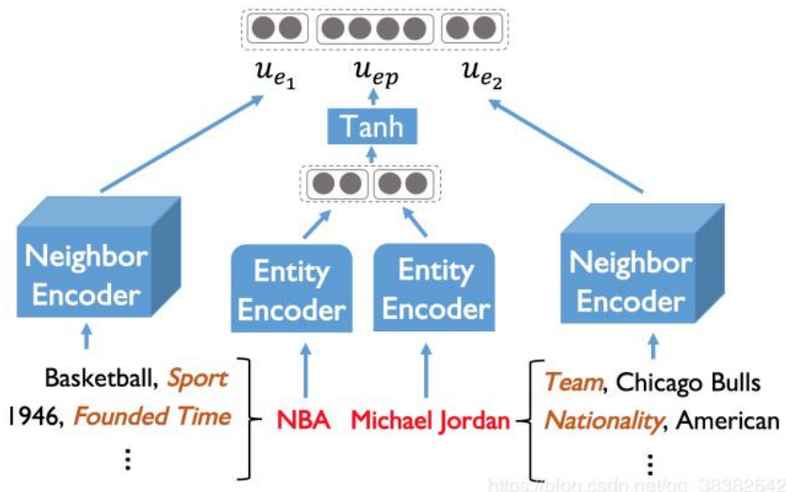
Method

- Feature Encoder
  - Entity Encoder 包含实体对本身的信息。经过线性变换、链接、非线性激活函数（Tanh）得到u_{ep}的表征
  - Neighbor Encoder 找到实体对应的周围一跳（one-hop）实体，将这些实体和关系表示为Ne，将一个实体e所有的one-hop三元组拼接，经过全连接层，计算均值，得到u_e。这样两个Neighbor Encoder得到两个u_{e1}， u_{e2}
  - 然后实体对对应的表征就由上述三个表征链接得到
  - 对于所涉及实体和关系的初始化表示可由TransE等经典的KG embedding模型得到

$$x_{(e_1,e_2)} = u_{e_1} \oplus u_{ep} \oplus u_{e_2}$$



- **Entity Encoder**

$$\begin{cases} f_2(v_e) = W_2(v_e) + b_2 \\ u_{ep} = \sigma(f_2(v_{e_1}) \oplus f_2(v_{e_2})) \end{cases}$$

- **Neighbor Encoder**

$$\mathcal{N}_e = \{(r^n, e^n) | (e, r^n, e^n) \in \mathcal{G}\}$$

$$\begin{cases} f_1(v_{r^n}, v_{e^n}) = W_1(v_{r^n} \oplus v_{e^n}) + b_1 \\ u_e = \sigma\left(\frac{1}{|\mathcal{N}_e|} \sum_{(r^n,e^n)\in\mathcal{N}_e} f_1(v_{r^n}, v_{e^n})\right) \end{cases}$$

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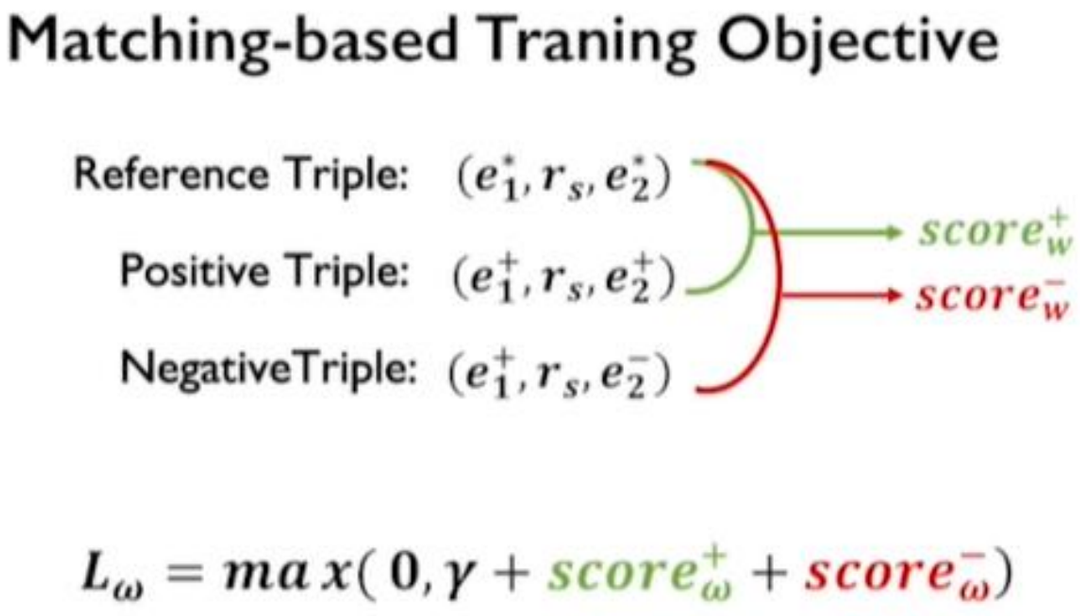
Method

- Feature Encoder
  - Matching
  - 对于某关系rs，从训练集rs随机选取k个Reference Triple，再从训练集剩余部分抽取一个batch的positive triple。Negative Triple是随机替换positive triple的尾实体得到的。
  - 采用margin loss的损失函数，用于训练Feature Encoder
  - 训练refrerence triple的embedding，计算positive triple的embedding与refrerence triple的embedding的余弦相似度为 $score_{\omega}^{+}$



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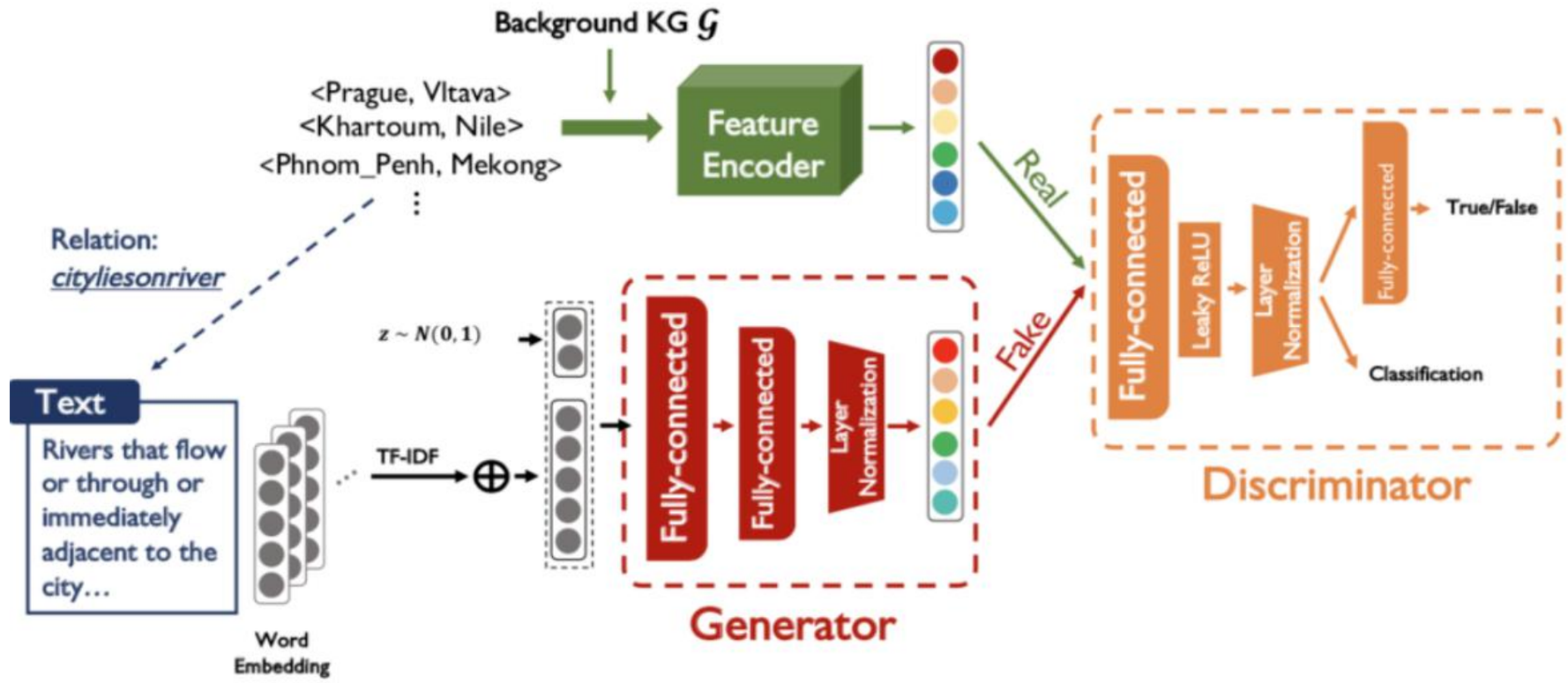
Method

- Discriminator
  - 对Real、Fake data鉴别并给出分类。这样提升Generator生成数据的多样性
  - 首先通过全连接成和非线性激活函数提取特征。
  - 然后两个分支，分别判断时Real/Fake，以及具体的关系类别



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Method

- Discriminator
  - Discriminator的目标（损失）函数

$$L_{D_\phi} = \underbrace{\mathbb{E}_{z\sim p_z}\left[D_\phi\left(G_\theta(T_r, z)\right)\right] - \mathbb{E}_{x\sim p_{data}}\left[D_\phi(x)\right]}_{\text{Adversarial}} + \underbrace{\frac{1}{2}L_{cls}\left(G_\theta(T_r, z)\right) + \frac{1}{2}L_{cls}(x)}_{\text{Classification}} + \underbrace{L_{GP}}_{\text{Gradient Penalty}}$$

WGAN

- 第一部分的两项为计算真实样本和生成样本的Wasserstein距离，希望将生成器的表征判为fake，将真实样本表征判为real
- 第二部分两项为分类真实样本和生成样本的分类损失函数
- 第三部分也是用于防止模型崩溃

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Method

- Spectral Normalization
- 作者通过实验发现Spectral Normalization方法用于G和D可以进一步提高GAN的可靠性

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Method

- Predicting Unseen Relations
  - 通过之前的GAN，得到G。输入unseen relation的text，就可以生成对应表征（embedding）

$$\tilde{x}_{r_u} \leftarrow G_\theta(T_{r_u}, z)$$

  - 对于query triple (e1,ru)，计算候选尾实体组成的三元组(e1,ru,e2)对应的生成表征x(e1,e2)的score.公式为cosine(xru,x(e1,e2))
  - 为了实现更好的泛化能力，采用对关系r生成一组(Ntest个)特征向量，然后计算score取均值的方法

$$score_{(e_1,r_u,e_2)} = \frac{1}{N_{test}} \sum_{i=1}^{N_{test}} score^i_{(e_1,r_u,e_2)}$$

备注：删掉。。。。。余弦值的范围在[-1,1]之间，值越趋近于1，代表两个向量的方向越接近；越趋近于-1，他们的方向越相反；接近于0，表示两个向量近乎于正交。
每个测试relation都有一个candidate list，里面有一系列尾实体。0号对应正确的尾实体每个实体计算score，最终根据0号判定的rank（排第几）计算hit10等

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Experiment

- Dataset
  - 没有现成的，利用大规模且有官方定义的关系类别表述的数据集构建。
  - 基于NELL和Wikidata构建了NELL-ZS、Wiki-ZS

Dataset	# Ent.	# Triples	# Train/Dev/Test
NELL-ZS	65,567	188,392	139/10/32
Wiki-ZS	605,812	724,967	469/20/48

- Baseline
  - 基于现有的TransE, DistMult 和ComplEx算法。
  - 这三种算法原本采用随机初始化关系向量。改进为通过类似于本文Generator结构的前馈网络，也是利用文本embedding等得到relation向量。
  - 这样这三种算法可以对unseen的关系表示预测，同时可以利用各自原有的score function优化
  - 改进和命名为ZS-TransE, ZS-DistMult and ZS-ComplEx

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Experiment

- Result

Model	NELL-ZS				Wiki-ZS			
	MRR	Hits@10	Hits@5	Hits@1	MRR	Hits@10	Hits@5	Hits@1
ZS-TransE	0.097	20.3	14.7	4.3	0.053	11.9	8.1	1.8
ZS-DistMult	0.235	32.6	28.4	18.5	0.189	23.6	21.0	16.1
ZS-ComplEx	0.216	31.6	26.7	16.0	0.118	18.0	14.4	8.3
ZSGAN$_{KG}$ (TransE)	0.240	**37.6**	**31.6**	17.1	0.185	26.1	21.3	14.1
ZSGAN$_{KG}$ (DistMult)	**0.253**	37.1	30.5	**19.4**	**0.208**	**29.4**	**24.1**	**16.5**
ZSGAN$_{KG}$ (ComplEx-re)	0.231	36.1	29.3	16.1	0.186	25.7	21.5	14.5
ZSGAN$_{KG}$ (ComplEx-im)	0.228	32.1	27.0	17.4	0.185	24.8	20.9	14.7

- 尽管NELL和Wiki有不同的规模和实体关系三维组，论文提出的ZSGAN方法都表现出优势。 括号内为Feature encoder初始化实体和关系的方法
- 说明生成器通过文本描述生成的关系向量表征效果不错
- 三种改进的方法对于KG embedding method很敏感，比如ZS-DistMult yeilds respectively 0.138 and 12.3% higher performance than ZS-TransE on NELL-ZS dataset.
- 但是ZSGAN表现的相对稳定

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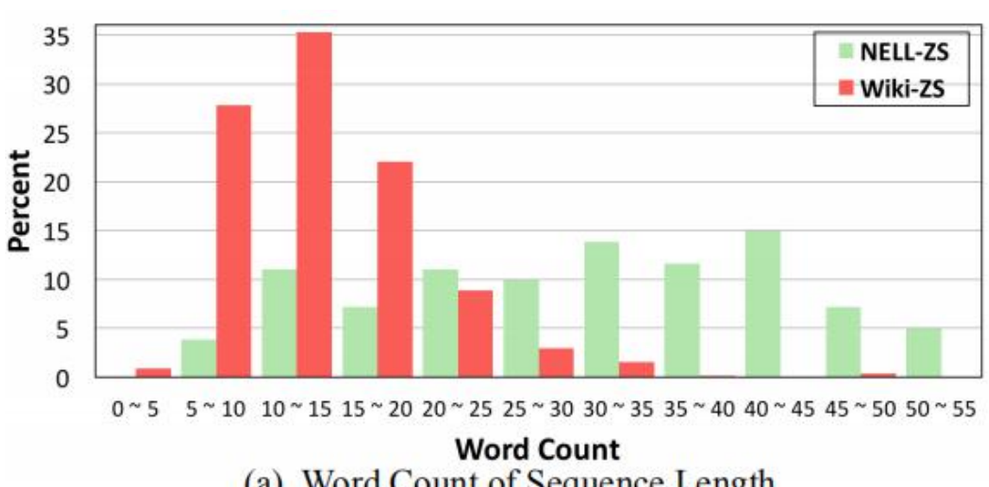
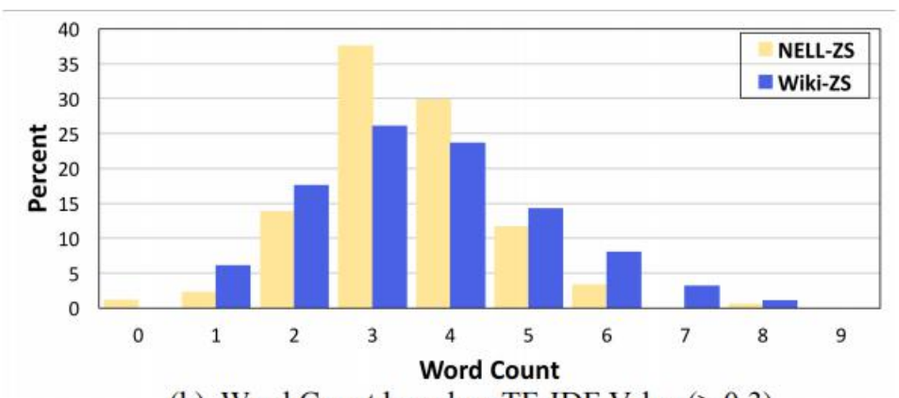
Experiment

- Result
  - 分析过滤噪声的效果
    - a图可以看出NELL-ZS的文本描述比Wiki-ZS长。
    - b图可以看出两个Dataset的文本描述中权重大的词数量范围都在2-5.
    - 因此可以证明通过简单的TF-IDF策略可以过滤文本描述的噪声



(a) Word Count of Sequence Length



(b) Word Count based on TF-IDF Value (> 0.3)

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Experiment

- Result
  - 文章还分析了生成样本的质量。部分关系生成的relation embedding和真实样本的embedding的距离如下

			MRR		Hits@10	
Relations	# Can. Num.	# Cos. Sim.	ZSGAN$_{KG}$	ZS-DistMult	ZSGAN$_{KG}$	ZS-DistMult
animalThatFeedOnInsect	293	0.8580	**0.347**	0.302	**63.4**	61.8
automobileMakerDealersInState	600	0.1714	**0.066**	0.039	**15.4**	5.1
animalSuchAsInvertebrate	786	0.7716	**0.419**	0.401	**59.8**	57.6
sportFansInCountry	2100	0.1931	**0.066**	0.007	**15.4**	1.3
produceBy	3174	0.6992	**0.467**	0.375	**65.3**	51.2
politicalGroupOfPoliticianus	6006	0.2211	0.018	**0.039**	**5.3**	3.9
parentOfPerson	9506	0.5836	0.343	**0.381**	56.2	**60.4**
teamCoach	10569	0.6764	**0.393**	0.258	**53.7**	39.9

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Conclusion

- summary：
  - 利用GAN从文本描述中生成合理的关系embedding。 将零样本学习转换为传统的监督分类问题

- Characteristics：
  - 首次在知识图片扩充中采用ZSL方法

  - model-agnostic 与模型无关。框架不依赖于特定的embedding方法
  - 相比baseline的三种方法，取得了更好的效果

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Conclusion

- Need to be Improved：
  - 对于unseen entity的扩展
  - 改进文本描述的编码方式
  - 利用文本描述之外的信息，如实体属性

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Reproduce

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Reproduce

- Environment
  - Pytorch 1.5.0, tqdm, nltk
  - Python 3.8
  - NVIDIA GeForce RTX 2080 Ti
  - Intel (R) Xeon (R) CPU E5-2678 v3 @ 2.50GHz

- Dataset
  - NELL-ZS

- code
  - github.com/Panda0406/Zero-shot-knowledge-graph-relational-learning

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- stages
  - stage 1 pretrain
    train feature encoder. obtain reasonable real data embeddings
  - stage 2 GAN training
    train Generator and Discriminator
  - stage 3 evaluation

- parameters
  - embed_model 'DistMult', 'TransE', 'ComplEx', 'RESCAL'
  - embedding dimension
    - 'dimension of triple embedding',default=100, type=int
    - 'dimension of word embedding [50, 300]',type=int, default=50
    - 'dimension of entity pair embedding',default=200, type=int
    - 'dimension of noise',default=15, type=int

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- parameters
  - feature extractor pretraining related
    - "pretrain_batch_size",default=64, type=int
    - "--pretrain_subepoch", default=20, type=int
    - "pretrain_margin",default=10.0, type=float,'pretraining margin loss'
    - "pretrain_times", default=16000, type=int,'total training steps for pretraining'
    - ...View more in arg.py
  - adversarial training related
    - batch size default 256 256 2
    - learning rate
      - "--lr_G", default=0.0001, type=float
      - "--lr_D", default=0.0001, type=float
      - "--lr_E", default=0.0005, type=float
    - training times
      - "--train_times", default=3000, type=int
      - "--D_epoch", default=5, type=int
      - "--G_epoch", default=1, type=int
  - ...View more in arg.py

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Reproduce

- Reproduction method
  - 由于GAN和feature encoder的优化过程都是随机的，考虑到时间有限，采用每种embedding method 训练三次的结果，取均值来做最后的结果

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Reproduce

- Screenshots

```
Step: 8500, Feature Extractor Pretraining loss: 0.07
Step: 9000, Feature Extractor Pretraining loss: 0.07
Step: 9500, Feature Extractor Pretraining loss: 0.07
Step: 10000, Feature Extractor Pretraining loss: 0.08
Step: 10500, Feature Extractor Pretraining loss: 0.07
Step: 11000, Feature Extractor Pretraining loss: 0.06
Step: 11500, Feature Extractor Pretraining loss: 0.07
Step: 12000, Feature Extractor Pretraining loss: 0.06
Step: 12500, Feature Extractor Pretraining loss: 0.07
Step: 13000, Feature Extractor Pretraining loss: 0.07
Step: 13500, Feature Extractor Pretraining loss: 0.07
Step: 14000, Feature Extractor Pretraining loss: 0.07
Step: 14500, Feature Extractor Pretraining loss: 0.06
Step: 15000, Feature Extractor Pretraining loss: 0.06
Step: 15500, Feature Extractor Pretraining loss: 0.07
Step: 16000, Feature Extractor Pretraining loss: 0.06
SAVE FEATURE EXTRACTOR PRETRAINING MODEL!!!
Finish Pretraining!
```

```
############   test    ############
HITS10: 0.347
HITS5: 0.287
HITS1: 0.170
MAP: 0.232
####################################
```

```
Epoch: 2450, D_loss: -8.19 [12.02, 0.13, -21.31, 0.00], G_loss: 31.61 [21.29, 0.00, 0.15, 3.44]
Epoch: 2500, D_loss: -8.19 [12.17, 0.14, -21.48, 0.00], G_loss: 31.37 [21.54, 0.00, 0.12, 3.28]
Epoch: 2550, D_loss: -8.20 [12.30, 0.14, -21.63, 0.00], G_loss: 31.30 [21.60, 0.00, 0.12, 3.23]
Epoch: 2600, D_loss: -8.13 [12.43, 0.14, -21.69, 0.00], G_loss: 31.45 [21.80, 0.00, 0.13, 3.22]
Epoch: 2650, D_loss: -8.16 [12.50, 0.14, -21.80, 0.00], G_loss: 31.65 [21.76, 0.00, 0.12, 3.30]
Epoch: 2700, D_loss: -8.14 [12.67, 0.14, -21.93, 0.00], G_loss: 31.49 [22.00, 0.00, 0.12, 3.16]
Epoch: 2750, D_loss: -8.20 [12.76, 0.15, -22.11, 0.00], G_loss: 31.56 [22.27, 0.00, 0.14, 3.10]
Epoch: 2800, D_loss: -8.18 [12.97, 0.13, -22.32, 0.00], G_loss: 31.70 [22.24, 0.00, 0.15, 3.16]
Epoch: 2850, D_loss: -8.15 [13.02, 0.13, -22.32, 0.00], G_loss: 31.97 [22.30, 0.00, 0.15, 3.22]
Epoch: 2900, D_loss: -8.16 [13.13, 0.14, -22.49, 0.00], G_loss: 32.12 [22.48, 0.00, 0.11, 3.21]
Epoch: 2950, D_loss: -8.28 [13.15, 0.13, -22.66, 0.00], G_loss: 31.69 [22.52, 0.00, 0.15, 3.06]
##EVALUATING ON TEST DATA
testconcept:leaguecoaches Hits10:0.056, Hits5:0.028, Hits1:0.000 MRR:0.020
testconcept:airportincity Hits10:0.805, Hits5:0.776, Hits1:0.557 MRR:0.656
testconcept:countryoforganizationheadquarters Hits10:0.000, Hits5:0.000, Hits1:0.000 MRR:0.002
testconcept:inverseofarthropodcalledarthropod Hits10:0.472, Hits5:0.327, Hits1:0.141 MRR:0.246
testconcept:agriculturalproductcomingfromvertebrate Hits10:0.048, Hits5:0.024, Hits1:0.000 MRR:0.024
testconcept:cityradiostation Hits10:0.828, Hits5:0.758, Hits1:0.475 MRR:0.609
```

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Reproduce

- Results and Comparison
  - results in the paper

Model	NELL-ZS			
	MRR	Hits@10	Hits@5	Hits@1
ZS-TransE	0.097	20.3	14.7	4.3
ZS-DistMult	0.235	32.6	28.4	18.5
ZS-ComplEx	0.216	31.6	26.7	16.0
ZSGAN$_{KG}$ (TransE)	0.240	**37.6**	**31.6**	17.1
ZSGAN$_{KG}$ (DistMult)	**0.253**	37.1	30.5	**19.4**
ZSGAN$_{KG}$ (ComplEx-re)	0.231	36.1	29.3	16.1
ZSGAN$_{KG}$ (ComplEx-im)	0.228	32.1	27.0	17.4

  - results of my tests

	MRR	HITS10	HITS5	HITS1
ZSGAN(TransE)	0.216	0.353	0.280	0.148
ZSGAN(DistMult)	**0.245**	**0.363**	**0.305**	**0.184**
ZSGAN(ComplEx-e	0.232	0.347	0.287	0.170
ZSGAN(ComplE	0.231	0.352	0.295	0.168

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Thank you!