Knowledge Embedding-OpenKE

- **◆Conda安装及配置**
- **♦**Pytorch安装
- **◆OpenKE介绍及使用**

◈前置实验环境

♦ Linux操作系统

- ◈推荐稳定版本的Ubuntu
 - **◈如:** Ubuntu 20.04.3 LTS
 - ◆下载链接: https://ubuntu.com/download/desktop



◈VMWare:下载地址:

创建虚拟机时选择Minimal install

ubuntu®

https://www.vmware.com/products/workstation-pro/workstation-pro-evaluation.html

◈VMWare激活码(选择任意一个使用即可):

4A4RR-813DK-M81A9-4U35H-06KND

NZ4RR-FTK5H-H81C1-Q30QH-1V2LA

4C21U-2KK9Q-M8130-4V2QH-CF810

4Y09U-AJK97-089Z0-A3054-83KLA



◆Conda简介

Conda是包及其依赖项和环境的管理工具

- ◆ 适用语言: Python, R, Ruby, Lua, Scala, Java, JavaScript, C/C++, FORTRAN
- ◆ 适用平台: Windows, macOS, Linux

用途:

- ♦ 快速安装、运行和升级包及其依赖项。
- ◆ 在计算机中便捷地创建、保存、加载和切换环境。



◆Anaconda下载安装

1.**下载**: \$ wget

https://mirrors.tuna.tsinghua.edu.cn/anaconda/archive/Anaconda3-2022.10-Linux-x86_64.sh

或 \$ wget https://repo.anaconda.com/archive/Anaconda3-2022.10-Linux-x86_64.sh

2.修改安装包权限: chmod 777 Anaconda3-2022.10-Linux-x86_64.sh

3.安装: \$./Anaconda3-2022.10-Linux-x86_64.sh

◆conda环境变量

安装结束会提示以下内容:

Do you wish the installer to initialize Anaconda3 by running conda init?[yes|no]

1.输入yes,自动配置环境变量

◆Conda添加源

- 1. 添加源、删除源 conda config –add/remove channels xxxxx
- 2. 显示源 conda config --show channels

◈添加国内镜像源

1. 清华源

#添加镜像源

conda config --add channels https://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/main conda config --add channels https://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/free conda config --add channels https://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud/conda-forge/conda config --add channels https://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/r conda config --add channels https://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/pro conda config --add channels https://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/msys2

#显示检索路径 conda config --set show_channel_urls yes #显示镜像通道

conda config --show channels

◆利用conda创建 python环境

- 1. 创建python3.8环境: \$ conda create -n kg python=3.8
- 2. 激活环境: \$ conda activate kg 3.安装需要的tqdm和sklearn包 conda install tqdm

pip install –U scikit-learn

【或 pip3 install -U scikit-learn】

有问题重启试试

```
(base) zjt@test-Super-Server:~$ conda create -n kg python=3.7
Collecting package metadata (current repodata.json): done
Solving environment: done
## Package Plan ##
 environment location: /data/zjt/anaconda3/envs/kg
 added / updated specs:
    - python=3.7
The following packages will be downloaded:
   package
                                         build
   ca-certificates-2020.10.14
                                                      121 KB
   certifi-2020.6.20
                                  pyhd3eb1b0 3
                                                      155 KB
   pip-20.2.4
                                py37h06a4308 0
                                                      1.7 MB
    setuptools-50.3.1
                                                      711 KB
                                                      2.7 MB
                                        Total:
The following NEW packages will be INSTALLED:
  libgcc mutex
                   pkgs/main/linux-64:: libgcc mutex-0.1-main
  ca-certificates
                   pkgs/main/linux-64::ca-certificates-2020.10.14-0
  certifi
                   pkgs/main/noarch::certifi-2020.6.20-pyhd3eb1b0 3
                   pkgs/main/linux-64::ld_impl_linux-64-2.33.1-h53a641e_7
pkgs/main/linux-64::libedit-3.1.20191231-h14c3975_1
  ld impl linux-64
  libedit
  libffi
                   pkgs/main/linux-64::libffi-3.3-he6710b0_2
                   pkgs/main/linux-64::libgcc-ng-9.1.0-hdf63c60 0
  libgcc-ng
 libstdcxx-ng
                   pkgs/main/linux-64::libstdcxx-ng-9.1.0-hdf63c60_0
 ncurses
                   pkgs/main/linux-64::ncurses-6.2-he6710b0 1
                   pkgs/main/linux-64::openssl-1.1.1h-h7b6447c 0
 openssl
                   pkgs/main/linux-64::pip-20.2.4-py37h06a4308 0
 pip
 python
                   pkgs/main/linux-64::python-3.7.9-h7579374_0
 readline
                   pkgs/main/linux-64::readline-8.0-h7b6447c 0
 setuptools
                   pkgs/main/linux-64::setuptools-50.3.1-py37h06a4308 1
  sqlite
                   pkgs/main/linux-64::sglite-3.33.0-h62c20be 0
                   pkgs/main/linux-64::tk-8.6.10-hbc83047 0
 tk
 wheel
                   pkgs/main/noarch::wheel-0.35.1-py 0
                   pkgs/main/linux-64::xz-5.2.5-h7b6447c 0
 zlib
                   pkgs/main/linux-64::zlib-1.2.11-h7b6447c 3
Proceed ([y]/n)? y
Downloading and Extracting Packages
                     1.7 MB
pip-20.2.4
                                ca-certificates-2020
                     121 KB
                                setuptools-50.3.1
                     711 KB
                     155 KB
certifi-2020.6.20
                                Preparing transaction: done
Verifying transaction: done
Executing transaction: done
```

◈Pytorch简介

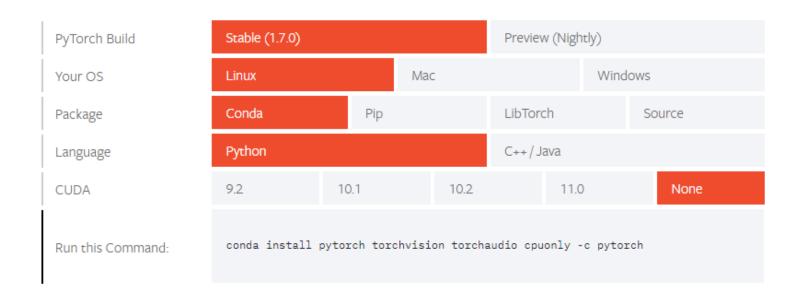
- ◆ PyTorch是一个基于Torch的Python开源机器学习库,用于自然 语言处理等应用程序。它主要由Facebookd的人工智能小组开发, 不仅能够实现强大的GPU加速,同时还支持动态神经网络,这一 点是现在很多主流框架如TensorFlow都不支持的。 PyTorch提 供了两个高级功能:
 - ◆ 具有强大的GPU加速的张量计算 (如Numpy)
 - ◆ 包含自动求导系统的深度神经网络



◆Pytorch安装

◆ **岡址**: https://pytorch.org/get-started/locally/

◈根据本机情况选择下载选项



♦Pytorch安装

◇输入生成的安装指令:

\$ conda install pytorch torchvision torchaudio cpuonly -c pytorch

```
(kg) zhangjiatao@DESKTOP-JC4BTTO:/mnt/c/Users/zhangjiatao$ conda install pytorch torchvision torchaudio cpuonly -c pytorch
WARNING: The conda.compat module is deprecated and will be removed in a future release.
Collecting package metadata: done
Solving environment: done
==> WARNING: A newer version of conda exists. <==
 current version: 4.6.11
 latest version: 4.9.2
Please update conda by running
    $ conda update -n base -c defaults conda
## Package Plan ##
 environment location: /home/zhangjiatao/anaconda3/envs/kg
  added / updated specs:
   - cpuonly
    - pytorch
    - torchaudio
    - torchvision
The following packages will be downloaded:
    package
                                          build
                                       mk1
                                                         6 KB https://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/free
    ca-certificates-2020.11.8 ha878542_0
                                                        145 KB https://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud/conda-forge
    certifi-2020.11.8
                              py37h89c1867_0
                                                        150 KB https://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud/conda-forge
    cpuonly-1.0
    freetype-2.10.4
                                     h7ca028e 0
                                                        912 KB https://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud/conda-forge
                                                        264 KB https://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud/conda-forge
    jpeg-9d
                                      h36c2ea0 0
    1cms2-2.11
                                      hcbb858e 1
                                                        434 KB https://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud/conda-forge
```

♦OpenKE简介

◆ OpenKE是THUNLP基于TensorFlow、PyTorch开发的用于将知识 图谱嵌入到低维连续向量空间进行表示的开源框架。OpenKE提供 了快速且稳定的各类接口,也实现了诸多经典的知识表示学习模 型。该框架易于扩展,基于框架设计新的知识表示模型也十分的 方便。

◆OpenKE配置

◈下载地址:

◈下载: https://github.com/thunlp/OpenKE

◆文档: http://139.129.163.161/static/index.html

◈运行样例:

Clone the OpenKE-PyTorch branch:

\$ git clone -b OpenKE-PyTorch https://github.com/thunlp/OpenKE

\$ cd OpenKE

\$ cd openke

Compile C++ files

\$ bash make.sh

Quick Start

\$ cd ../

\$ cp examples/train_transe_FB15K237.py ./

\$ python train_transe_FB15K237.py

运行前的一些准备:

benchmarks同级目录下手动创建一个checkpoint文件夹来存放模型参数

修改py文件中的参数(根据配置选择性修改)

1.第39、45行改成: use_gpu=False

2.超参: nbatches=50 dim=100 train_times=10

修改参数或给虚拟机多分配cpu都可以加快速度

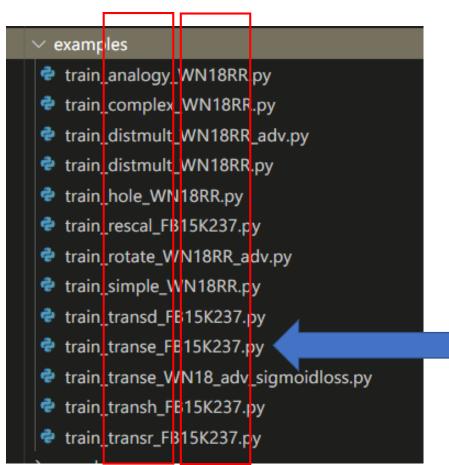
♦OpenKE简介

- ◆OpenKE结构
 - ◆./base/.Cpp和.h文件,封装数据处理操作,向上层提供 调用接口
 - ♦ Config.py 封装了训练、验证和预测相关的方法
 - ◈使用ctypes模块调用下层的C++数据处理接口
 - ◆使用torch中的optim、autograd模块统一进行模型反向传播和参数更新
 - ◆Models.py作为所有实现模型的父类,继承自nn.Module, 定义了四个通用方法
 - ◆example_train_transe.py训练入口文件,最上层

◆示例-选择表示学习模型及数据集

◆examples目录下示例脚本

选择模型 选择数据集



选择该脚本作为示例, 将该文件复制到 OpenKE根目录下

◆示例脚本参数说明

```
train_dataloader = TrainDataLoader(
    in_path = "./benchmarks/FB15K237/",
                                                                                                                            训练、
                                                                                                                            测试数
    sampling_mode = "normal",
                                                                                                                            据参数
    neg\_ent = 25,
    neg_rel = 0)
test_dataloader = TestDataLoader("./benchmarks/FB15K237/", "link")
transe = TransE(
    ent_tot = train_dataloader.get_ent_tot(),
    rel_tot = train_dataloader.get_rel_tot(),
    norm_flag = True)
model = NegativeSampling(
    model = transe,
    loss = MarginLoss(margin = 5.0),
    batch_size = train_dataloader.get_batch_size()
trainer = Trainer(model = model, data_loader = train_dataloader, train_times = 1000, alpha = 1.0, use_gpu = True)
trainer.run()
transe.save_checkpoint('./checkpoint/transe.ckpt')
# test the model
transe.load_checkpoint('./checkpoint/transe.ckpt')
tester = Tester(model = transe, data_loader = test_dataloader, use_gpu = True)
tester.run_link_prediction(type_constrain = False)
```

◆Examples配置模型参数

```
# dataloader for training
train_dataloader = TrainDataLoader(
    in_path = "./benchmarks/FB15K237/",
    nbatches = 100,
    threads = 8,
    sampling_mode = "normal",
    bern_flag = 1,
    filter_flag = 1,
    neg_ent = 25,
    neg_rel = 0)

# dataloader for test
test_dataloader = TestDataLoader("./benchmarks/FB15K237/", "link")
```

• in_path: 训练集路径

• nbatches: 批次数

• threads: 线程数

sampling_mode: 采样模型

• bern flag: 负采样策略

• neg_ent: 打乱实体构造负例数量

· neg_rel: 打乱关系构造负例数量

◈示例

◆Examples配置模型参数

```
# define the model
transe = TransE(
    ent_tot = train_dataloader.get_ent_tot(),
    rel_tot = train_dataloader.get_rel_tot(),
    dim = 200,
    p_norm = 1,
    norm_flag = True)

# define the loss function
model = NegativeSampling(
    model = transe,
    loss = MarginLoss(margin = 5.0),
    batch_size = train_dataloader.get_batch_size()
)
```

- dim: Embedding size
- p_norm: 能量函数为1/2范数 margin: Margin loss中margin值

◆Examples配置模型参数

```
# train the model
trainer = Trainer(model = model, data_loader = train_dataloader, train_times = 1000, alpha = 1.0, use_gpu = True)
trainer.run()
transe.save_checkpoint('./checkpoint/transe.ckpt')

# test the model
transe.load_checkpoint('./checkpoint/transe.ckpt')
tester = Tester(model = transe, data_loader = test_dataloader, use_gpu = True)
tester.run_link_prediction(type_constrain = False)
```

- train_times: epoch-训练轮次
- alpha: 学习率
- use_gpu: 训练过程是否使用gpu加速

◈运行脚本

```
(zjt_py) test-Super-Server% python train_transe_FB15K237.py
Input Files Path : ./benchmarks/FB15K237/
The toolkit is importing datasets.
The total of relations is 237.
The total of entities is 14541.
The total of train triples is 272115.
Input Files Path : ./benchmarks/FB15K237/
The total of test triples is 20466.
The total of valid triples is 17535.
Finish initializing...
Epoch 19 | loss: 5.382204: 2%|

⊗ 0 ∧ 1 № 0
```

◈输出测试结果

Hit@N: Hit@N 是用于排序任务(如搜索、推荐等)的评测指标。将知识图谱数据层事实性知识补全和知识图谱本体补全视为一个排序任务,即给定知识图谱三元组的任意两部分预测剩余的部分,例如给定三元组的主语和谓语预测三元组的宾语。

当预测出所有缺失部分时,按照相关性对预测结果进行排序并取前N个结果。假定所有需要预测的三元组个数为K,而所有预测结果中正确结果在前N个结果的个数为K。则计算Hit@N 如公式下所示:

$$Hits@N = \frac{K_j}{K}$$

metric:	MRR	MR	hit@10	hit@3	hit@1
l(raw):	0.201013	458.071143	0.557167	0.395924	0.07311
r(raw):	0.261077	445.237366	0.554550	0.397278	0.07297
averaged(raw):	0.261045	451.954254	0.555868	0.396601	0.07304
l(filter):	0.402197	354.581635	0.801112	0.622960	0.13332
r(filter):	0.400600	334.621826	0.795553	0.616048	0.13311
averaged(filter): 0.798332	0.401399	344.601746	0.798332	0.619504	0.13322

◈示例

◈输出测试结果

• MRR(Mean Reciprocal Rank): 首先计算每一个预测三元组中预测结果的位置 排名得分 rankj如公式下所示:

$$MRR = \frac{1}{K} \sum_{j=1}^{K} rank_j$$

其中 Ri 是预测正确结果的排名,然后针对所有 K个三元组计算 MRR 如公式如下所示:

$$rank_j = \frac{1}{R_j}$$

metric:	MRR	MR	hit@10	hit@3	hit@1
l(raw):	0.201013	458.071143	0.557187	0.395924	0.073113
r(raw):	0.261077	445.237366	0.554550	0.397278	0.072971
averaged(raw):	0.261045	451.954254	0.555868	0.396601	0.073042
l(filter):	0.402197	354.581635	0.801112	0.622960	0.133329
r(filter):	0.400600	334.621826	0.795553	0.616048	0.133115
averaged(filter): 0.798332 0.7983324527740479	0.401399	344.601746	0.798332	0.619504	0.133222

◈示例

◈输出测试结果

• MR(Mean Rank):与 MRR 类似,MR 也是评估整体排序质量的指标,MR 的计算公式如下所示:

其中Rj是预测三元组正确结果的排名。

$$MR = \frac{1}{K} \sum_{j=1}^{K} R_j$$

	237366 0.			0.073113
		554550 0.	397278	0 072071
.045 451.	05/05/ 0			0.072971
	954254 0.	555868 0.	.396601	0.073042
197 354.	581635 0.	801112 0.	.622960	0.133329
600 334.	621826 0.	795553 0.	616048	0.133115
.399 344.	601746 0.	798332 0.	619504	0.133222
١	600 334.	334.621826 0.	600 334.621826 0.795553 0.	600 334.621826 0.795553 0.616048

◈课堂作业

- ◆阅读OpenKE README文档及样例程序,了解数据集结构及模型参数意义,训练满足以下条件的TransE、TransH模型,并获取测试性能,要求:
 - **Embedding size = 100**
 - ◆数据集为WN18RR
- ◆其他参数可自行调整,
- ◆将代码运行过程与实验结果(链接预测)截图形成实验报告。