An example of packaging deep learning model "AIGenMols" for MolAICal

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1. Introduction

Sometimes, the "AIGenMols" have not good compatibility in Linux operating system. In this case, it needs to generate the binary "AIGenMols" again. In this tutorial, the ORGAN (https://github.com/gablg1/ORGAN) is chosen for the installation of "AIGenMols". Besides, you can build the "AIGenMols" from your trained deep learning model.

2. Materials

2.1. Software requirement
1) MolAICal: https://molaical.github.io
2) Anaconda: https://www.anaconda.com

2.2. Example files
1) All the necessary tutorial files are downloaded from:
https://github.com/MolAICal/specialtopic/tree/master/012-AIGenMols

3. Procedure

1. Install Anconda (https://www.anaconda.com/distribution).
Make sure installation completely and environment variables are set rightly.

2. Create an independent environment
#> conda create -n AIGen python=3.6.7
#> conda activate AIGen

3. Install the necessary libraries
#> conda install tensorflow==1.13.1
#> conda install future==0.16.0
#> pip install editdistance==0.3.1
#> conda install tqdm
#> conda install dill
#> conda install pyinstaller==3.4

4. Finally, produce binary "deep learning model".
Decompress "organ.zip"
#> unzip organ.zip
#> cd organ
#> pyinstaller --add-data="organ/NP_score.pkl.gz:organ" --add-data="organ/SA_score.pkl.gz:organ" --add-data="organ/data/FDA-H.csv:organ/data" --add-data="organ/checkpoints/FDA-H/FDA-H_99.ckpt.data-00000-of-00001:organ/checkpoints/FDA-H" --add-data="organ/checkpoints/FDA-H/FDA-H_99.ckpt.index:organ/checkpoints/FDA-H" --add-data="organ/checkpoints/FDA-H/FDA-H_99.ckpt.meta:organ/checkpoints/FDA-H" --add-data="organ/data/FDA1884.csv:organ/data" --add-

data="organ/checkpoints/FDA1884/FDA1884_119.ckpt.data-00000-of-00001:organ/checkpoints/FDA1884" --add-data="organ/checkpoints/FDA1884/FDA1884_119.ckpt.index:organ/checkpoints/FDA1884" --add-data="organ/checkpoints/FDA1884/FDA1884_119.ckpt.meta:organ/checkpoints/FDA1884" --add-data="organ/data/zinc.csv:organ/data" --add-data="organ/checkpoints/ZINC/ZINC_99.ckpt.data-00000-of-00001:organ/checkpoints/ZINC" --add-data="organ/checkpoints/ZINC/ZINC_99.ckpt.index:organ/checkpoints/ZINC" --add-data="organ/checkpoints/ZINC/ZINC_99.ckpt.meta:organ/checkpoints/ZINC" -F main.py

Open folder "organ/dist"
#> cd dist

You will see file named "main", rename it as "AIGenMols"
#> mv main AIGenMols
#> chmod +x AIGenMols

The deep binary deep learning model named "AIGenMols" is produced completely. Put it into MolAICal software folder directly.

Analysis of install process:

--add-data="organ/data/zinc.csv:organ/data" --add-data="organ/checkpoints/ZINC/ZINC_99.ckpt.data-00000-of-00001:organ/checkpoints/ZINC" --add-data="organ/checkpoints/ZINC/ZINC_99.ckpt.index:organ/checkpoints/ZINC" --add-data="organ/checkpoints/ZINC/ZINC_99.ckpt.meta:organ/checkpoints/ZINC" -F main.py
----
You can replace above data by trained deep learning model.

Notice:
1. When you install Anaconda, the install path of Anaconda should have no blank space for packaging "AIGenMols". For example, /home/test install/anaconda. The blank space between the characters "test" and "install" may lead to the failure of the packaging process.

2. The command usage of "AIGenMols" should be like as below:

AIGenMols -f test.txt -s FDAFrag -n 100
AIGenMols -f test.txt -s ZINCMol -n 100

-f: represents file name which contains generated results of molecules with SMILES format
-s: represents selection of deep learning model
-n: represents the number of generated molecules

This is just an example for packaging "AIGenMols". You can use the similar way for your trained model. We will update deep learning model.