

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/open-source>

The version of Anaconda should be chosen based on Python 3.x rather than Python 2.x, etc.

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 Anaconda (<https://www.anaconda.com/distribution>).

Make sure installation completely and environment variables are set rightly.

2. Download "spec-list.txt" and create an independent environment

```
#> conda create --name AIGen --file spec-list.txt
#> conda activate AIGen
```

Note: If some errors happen like: *CondaHTTPError: HTTP 404 NOT FOUND for url <<https://conda.anaconda.org/conda-forge/linux-64/xxxx-xxxx>>*, you can delete corresponding soft package in "spec-list.txt". Then repeat above steps. The missing soft package can be installed without version number via similar below step:

```
#> conda install -c conda-forge xxxx
```

3. Install the necessary libraries

```
#> conda install -c conda-forge openblas
#> conda install -c conda-forge openssl
#> pip install editdistance==0.3.1
```

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.