This folder contains materials to reproduce the 3 submissions files in ./subs subfolder that contributed to the final solution

1. Hardware:

* CPU : 8 cores
* Memory: 16 GB
* GPU: 1 GTX 2080 Ti

2. Software:

* CUDA 10.0 CuDNN 7.4
* Anaconda Python 3.7 2019.03
* pytorch==1.1.0
* pytorch\_geometric
* openbabel
* torch\_contrib

3. Re-run Training:

* Require:
  + Competition data in ../data
  + Unzip xyz files in the path at kaggle\_champs.constants.STRUCT\_DATA\_PATH
* Run all 3 notebooks entirely to recreate 3 submissions
* Estimated time on listed hardware: ~ 100h