

ipy_evaluate_after

July 25, 2023

Connected to pgt_hug (Python 3.10.11)

```
[ ]: import os
os.chdir("..")
import random
from argparse import ArgumentParser

# Third party imports
import numpy as np
import torch
import yaml
from utils.modeling_graphormer_improved import (
    GraphormerConfig,
    GraphormerForGraphClassification,
    BetterGraphormerConfig
)

from transformers import (    Trainer,
    TrainingArguments,)

from utils.modeling_graphormer_improved_3d import
    Graphormer3DForGraphClassification, Graphormer3DConfig
from utils.graphormer_data_collator_improved_3d import Graphormer3DDataCollator

# Local application imports
from utils import data as data_utils
from utils import graphormer_data_collator_improved as graphormer_collator_utils
from utils import setup as setup_utils
from utils import evaluate as evaluate_utils
```

```
/home/alexander/miniconda3/envs/pgt_hug/lib/python3.10/site-
packages/tqdm/auto.py:21: TqdmWarning: IProgress not found. Please update
jupyter and ipywidgets. See
https://ipywidgets.readthedocs.io/en/stable/user\_install.html
    from .autonotebook import tqdm as notebook_tqdm
/home/alexander/miniconda3/envs/pgt_hug/lib/python3.10/site-
packages/torch/cuda/__init__.py:107: UserWarning: CUDA initialization: CUDA
```

unknown error - this may be due to an incorrectly set up environment, e.g. changing env variable CUDA_VISIBLE_DEVICES after program start. Setting the available devices to be zero. (Triggered internally at /opt/conda/conda-bld/pytorch_1682343995026/work/c10/cuda/CUDAFunctions.cpp:109.)

```
return torch._C._cuda_getDeviceCount() > 0
```

```
[ ]: import wandb
run = wandb.init()
```

Failed to detect the name of this notebook, you can set it manually with the WANDB_NOTEBOOK_NAME environment variable to enable code saving.

wandb: Currently logged in as: [alexanderkrauck](#). Use ``wandb login --relogin`` to force relogin

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

```
[ ]: dataset = data_utils.prepare_cv_dataset_for_training(seed=72,
    ↪memory_mode="full", dataset_name = "qm9", data_dir=data_dir,
    ↪model_type="graphormer3d", num_folds=10, train_split=0.9)[0]
target_scaler = data_utils.get_regression_target_scaler(dataset["train"],
    ↪num_classes=19)
evaluation_func = evaluate_utils.prepare_evaluation_for_training(
    False, dataset_name = "qm9", target_scaler=target_scaler
)

artifact_names = ["alexanderkrauck/pretrained_graph_transformer/
    ↪model-19-07-2023_09-54-17_81_qm9_no_pretrain_3d:v0",
    "alexanderkrauck/pretrained_graph_transformer/
    ↪model-19-07-2023_03-20-20_80_qm9_no_pretrain_3d:v0",
    "alexanderkrauck/pretrained_graph_transformer/
    ↪model-18-07-2023_13-12-46_79_qm9_no_pretrain_3d:v0",
    "alexanderkrauck/pretrained_graph_transformer/
    ↪model-17-07-2023_23-04-39_78_qm9_no_pretrain_3d:v0",
    "alexanderkrauck/pretrained_graph_transformer/
    ↪model-17-07-2023_08-56-48_77_qm9_no_pretrain_3d:v0",
    "alexanderkrauck/pretrained_graph_transformer/
    ↪model-17-07-2023_03-08-54_76_qm9_no_pretrain_3d:v0",
    "alexanderkrauck/pretrained_graph_transformer/
    ↪model-16-07-2023_19-58-48_75_qm9_no_pretrain_3d:v0",
```

```

"alexanderkrauck/pretrained_graph_transformer/
↳model-16-07-2023_17-02-10_74_qm9_no_pretrain_3d:v0",
"alexanderkrauck/pretrained_graph_transformer/
↳model-16-07-2023_10-32-26_73_qm9_no_pretrain_3d:v0",
"alexanderkrauck/pretrained_graph_transformer/
↳model-16-07-2023_08-42-30_72_qm9_no_pretrain_3d:v0"]

```

```

-----
NameError                                Traceback (most recent call last)
/mnt/92669E5D669E4241/pretrained-graph-transformer/scripts/ipy_evaluate_after.py
↳in line 2
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/script. /
↳ipy_evaluate_after.py?line=128'>129</a> # %%
----> <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/script. /
↳ipy_evaluate_after.py?line=129'>130</a> dataset = data_utils.
↳prepare_cv_dataset_for_training(seed=72, memory_mode="full", dataset_name =
↳"qm9", data_dir=data_dir, model_type="graphormer3d", num_folds=10,
↳train_split=0.9) [0]
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/script. /
↳ipy_evaluate_after.py?line=130'>131</a> target_scaler = data_utils.
↳get_regression_target_scaler(dataset["train"], num_classes=19)
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/script. /
↳ipy_evaluate_after.py?line=131'>132</a> evaluation_func = evaluate_utils.
↳prepare_evaluation_for_training(
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/script. /
↳ipy_evaluate_after.py?line=132'>133</a>                False, dataset_name = "qm9",
↳target_scaler=target_scaler
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/script. /
↳ipy_evaluate_after.py?line=133'>134</a>                )

NameError: name 'data_dir' is not defined

```

```
[ ]: do_evaluation(artifact_names, target_scaler, model_type = "graphormer3d")
```

Cell was canceled due to an error in a previous cell.

```
[ ]: data_dir = "data/"
```

```
[ ]: dataset = data_utils.prepare_cv_dataset_for_training(seed=72,
↳memory_mode="full", dataset_name = "qm9", data_dir=data_dir,
↳model_type="graphormer3d", num_folds=10, train_split=0.9) [0]
target_scaler = data_utils.get_regression_target_scaler(dataset["train"],
↳num_classes=19)
evaluation_func = evaluate_utils.prepare_evaluation_for_training(
    False, dataset_name = "qm9", target_scaler=target_scaler
    )

```

```

artifact_names = ["alexanderkrauck/pretrained_graph_transformer/
↳model-19-07-2023_09-54-17_81_qm9_no_pretrain_3d:v0",
                  "alexanderkrauck/pretrained_graph_transformer/
↳model-19-07-2023_03-20-20_80_qm9_no_pretrain_3d:v0",
                  "alexanderkrauck/pretrained_graph_transformer/
↳model-18-07-2023_13-12-46_79_qm9_no_pretrain_3d:v0",
                  "alexanderkrauck/pretrained_graph_transformer/
↳model-17-07-2023_23-04-39_78_qm9_no_pretrain_3d:v0",
                  "alexanderkrauck/pretrained_graph_transformer/
↳model-17-07-2023_08-56-48_77_qm9_no_pretrain_3d:v0",
                  "alexanderkrauck/pretrained_graph_transformer/
↳model-17-07-2023_03-08-54_76_qm9_no_pretrain_3d:v0",
                  "alexanderkrauck/pretrained_graph_transformer/
↳model-16-07-2023_19-58-48_75_qm9_no_pretrain_3d:v0",
                  "alexanderkrauck/pretrained_graph_transformer/
↳model-16-07-2023_17-02-10_74_qm9_no_pretrain_3d:v0",
                  "alexanderkrauck/pretrained_graph_transformer/
↳model-16-07-2023_10-32-26_73_qm9_no_pretrain_3d:v0",
                  "alexanderkrauck/pretrained_graph_transformer/
↳model-16-07-2023_08-42-30_72_qm9_no_pretrain_3d:v0"]

```

100%| | 133247/133247 [00:37<00:00, 3586.98it/s]

```
[ ]: do_evaluation(artifact_names, target_scaler, model_type = "graphormer3d")
```

```

-----
NameError                                Traceback (most recent call last)
/mnt/92669E5D669E4241/pretrained-graph-transformer/scripts/ipy_evaluate_after.p
↳in line 2
      <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/script: /
↳ipy_evaluate_after.py?line=145'>146</a> # %%
----> <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/script: /
↳ipy_evaluate_after.py?line=146'>147</a> do_evaluation(artifact_names,
↳target_scaler, model_type = "graphormer3d")

NameError: name 'do_evaluation' is not defined

```

```

[ ]: def do_evaluation(art_names, target_scaler = None, model_type="graphormer"):
    eval_results_list = []
    for artifact_name in art_names:
        artifact = run.use_artifact(artifact_name, type='model')
        artifact_dir = artifact.download()

        if model_type == "graphormer":
            config = BetterGraphormerConfig.from_pretrained(artifact_dir)
        else:

```

```

        config = Graphormer3DConfig.from_pretrained(artifact_dir)
        config.classification_task = "regression"
        model_params = torch.load(artifact_dir + "/pytorch_model.bin", torch.
↪device('cpu'))
        model = Graphormer3DForGraphClassification(config)
        model.load_state_dict(model_params)

        if model_type == "graphormer":
            collator = graphormer_collator_utils.
↪GraphormerDataCollator(model_config=model.config,
↪on_the_fly_processing=False, collator_mode="classification",
↪target_scaler=target_scaler)
        else:
            collator = Graphormer3DDataCollator(model_config=model.config,
↪on_the_fly_processing=False, collator_mode="classification",
↪target_scaler=target_scaler)

        trainer = Trainer(
            model=model,                                # the instantiated
↪Transformers model to be trained
            args=training_args,                        # training arguments, defined
↪above
            compute_metrics=evaluation_func,
            data_collator=collator,
                # evaluation dataset
        )
        eval_results = trainer.evaluate(eval_dataset=dataset["test"])
        eval_results_list.append(eval_results)

    for key in eval_results_list[0].keys():
        print(key)
        listed_results = [eval_result[key] for eval_result in eval_results_list]
        print(listed_results)
        print(np.mean(listed_results), np.std(listed_results))

```

```
[ ]: do_evaluation(artifact_names, target_scaler, model_type = "graphormer3d")
```

wandb: 3 of 3 files downloaded.

```

-----
NameError                                Traceback (most recent call last)
/mnt/92669E5D669E4241/pretrained-graph-transformer/scripts/ipy_evaluate_after.p
↪in line 2
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/script. /
↪ipy_evaluate_after.py?line=145'>146</a> # %%

```

```

----> <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts/
↳ipy_evaluate_after.py?line=146'>147</a> do_evaluation(artifact_names,
↳target_scaler, model_type = "graphormer3d")

/mnt/92669E5D669E4241/pretrained-graph-transformer/scripts/ipy_evaluate_after.p
↳in line 24, in do_evaluation(art_names, target_scaler, model_type)

    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=77'>78</a> else:
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=78'>79</a>     collator =
↳Graphormer3DDataCollator(model_config=model.config,
↳on_the_fly_processing=False, collator_mode="classification",
↳target_scaler=target_scaler)
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=80'>81</a> trainer = Trainer(
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=81'>82</a>     model=model,
↳# the instantiated Transformers model to be trained
----> <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=82'>83</a>     args=training_args,
↳# training arguments, defined above
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=83'>84</a>     compute_metrics=evaluation_func,
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=84'>85</a>     data_collator=collator,
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=85'>86</a>     # evaluation dataset
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=86'>87</a> )
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=87'>88</a> eval_results = trainer.
↳evaluate(eval_dataset=dataset["test"])
    <a href='file:///mnt/92669E5D669E4241/pretrained-graph-transformer/scripts
↳ipy_evaluate_after.py?line=88'>89</a> eval_results_list.append(eval_results)

```

NameError: name 'training_args' is not defined

```

[ ]: training_args = TrainingArguments(
    output_dir='./logs',           # output directory
    num_train_epochs=3,           # total number of training epochs
    per_device_train_batch_size=16, # batch size per device during training
    per_device_eval_batch_size=64,  # batch size for evaluation
    warmup_steps=500,             # number of warmup steps for learning rate
    ↳scheduler
    weight_decay=0.01,            # strength of weight decay
    logging_dir='./logs',
    report_to = []                # directory for storing logs
)

```

```
[ ]: do_evaluation(artifact_names, target_scaler, model_type = "graphormer3d")
```

```
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:15<00:00, 13.24it/s]  
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:14<00:00, 14.35it/s]  
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:15<00:00, 13.84it/s]  
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:16<00:00, 12.87it/s]  
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:15<00:00, 13.76it/s]  
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:14<00:00, 14.40it/s]  
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:15<00:00, 13.11it/s]  
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:14<00:00, 14.13it/s]  
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:14<00:00, 14.51it/s]  
wandb: 3 of 3 files downloaded.  
100%|      | 209/209 [00:14<00:00, 14.19it/s]
```

eval_loss

```
[0.005854427348822355, 0.01204886194318533, 0.005342952907085419,  
0.004156446550041437, 0.008993885479867458, 0.003990353550761938,  
0.009239076636731625, 0.013214043341577053, 0.006194186396896839,  
0.010027782991528511]  
0.007906201714649796 0.003096790027337427
```

eval_A_mse

```
[0.000914114657300008, 0.0007978163521294533, 0.0002700756967271643,  
0.00017639641156535875, 0.0008543083224694186, 0.0011566838583766798,  
0.0002068842170004036, 0.000652347317443348, 0.00037641652773603914,  
0.0020539664808493646]  
0.0007459009841597238 0.0005393585448828886
```

eval_A_mae

```
[0.018620968595682918, 0.01350489867695476, 0.006461579569785815,  
0.006335355178369119, 0.010840740675223375, 0.027301189428335478,  
0.007111944012695311, 0.016130001043301742, 0.007197881904811104,  
0.019798869024923085]  
0.013330342811008273 0.00671914505995056
```

eval_B_mse

```
[0.004822522189361953, 0.017675600654715035, 0.011262123322006877,  
0.0054944773751818155, 0.008317343170711696, 0.0028273046242378534,  
0.011373264794865985, 0.05322412828242933, 0.010193938407745032,  
0.006488484076682865]  
0.013167918689793843 0.013943152778904155
```

eval_B_mae

[0.04018267003108103, 0.04045400356194452, 0.030175383696639597,
 0.028155039694712235, 0.03915430738904339, 0.034834100290227876,
 0.037500947549145174, 0.10480769598220781, 0.03324832600688628,
 0.04206752319205697]
 0.04305799973939449 0.021040665923378644
 eval_C_mse
 [0.009214693489340394, 0.046860929513761, 0.0186936110366182,
 0.010551650318178049, 0.014544465093098034, 0.0038511034733746136,
 0.023470773167641863, 0.03493042745418407, 0.013668274205820754,
 0.003993714119966182]
 0.01797796418719832 0.013075663027637331
 eval_C_mae
 [0.0297255423040463, 0.0331350476057179, 0.024460848543918258,
 0.023078015058451345, 0.030132576227488113, 0.031371903749615286,
 0.028209757982849352, 0.08706163664742621, 0.025436642690356823,
 0.03356882664046557]
 0.03461807974503352 0.01780429474264251
 eval_mu_mse
 [0.040292966651770006, 0.07690955016642624, 0.02720630813938101,
 0.024907091812925584, 0.07016366620168862, 0.025347262746418176,
 0.06781527725271352, 0.06943607089453291, 0.041948204257375506,
 0.07503683885256021]
 0.05190632369757918 0.02081433802625241
 eval_mu_mae
 [0.12870258658288236, 0.18946038797629625, 0.10370855070627957,
 0.0997274108356861, 0.17148217217096015, 0.10333102121009234,
 0.17109198837748307, 0.1758893903685288, 0.12962282447193044,
 0.18388074233586593]
 0.1456897075036005 0.03436988669755535
 eval_alpha_mse
 [0.004026224499288659, 0.005845046290098411, 0.0029897219407577164,
 0.0028373943672054193, 0.004485902601765464, 0.0031556633550554563,
 0.004397457802568061, 0.0056105072140282385, 0.0033624609496337495,
 0.007074480405566613]
 0.004378485942596778 0.001338068711559313
 eval_alpha_mae
 [0.0388023234175692, 0.048906321405033294, 0.032673119731823935,
 0.031343452319125636, 0.04212787341571641, 0.03504395474727753,
 0.041681988825794734, 0.05048553781594561, 0.03564716966841655,
 0.05170403643929596]
 0.04084157777859988 0.0070717103390548685
 eval_homo_mse
 [0.022141707730721476, 0.03322348416975513, 0.016811102955327072,
 0.015098411275040271, 0.03169187010326489, 0.01577171798119943,
 0.029561097984807876, 0.03750026690337606, 0.020368423644653223,
 0.040869141251650774]
 0.026303722399979617 0.008967618665463225
 eval_homo_mae

[0.10536426672429382, 0.1350412788819698, 0.09248895035430867,
 0.08692040203677558, 0.1285302584744301, 0.08923174010949374,
 0.12519098752074267, 0.14305859732081455, 0.1017097246960141,
 0.14937706668259199]
 0.1156913272801435 0.022094249054027747
 eval_lumo_mse
 [0.007934106068444264, 0.011817610329269, 0.0067804361276254865,
 0.005274542297399396, 0.010436686109574681, 0.005950611655026669,
 0.010357160661695789, 0.012442240600635734, 0.007291114718413207,
 0.014737061766796794]
 0.009302157033488101 0.0029640424470876404
 eval_lumo_mae
 [0.061562433438442775, 0.07420004189220539, 0.05171901558504844,
 0.047712393925768225, 0.0685711006963483, 0.05118406448603401,
 0.06765363265538395, 0.07620987596510712, 0.055720268153493624,
 0.08707113357282821]
 0.06416039603706601 0.012141822093124033
 eval_gap_mse
 [0.011712419063748994, 0.018022710347066276, 0.01006985543643543,
 0.008234684544401988, 0.01637707655106474, 0.009248291797070572,
 0.015190959086453284, 0.019790702156594047, 0.011333144653754061,
 0.02205579018276881]
 0.014203563381935822 0.004526294896034804
 eval_gap_mae
 [0.07404915102662141, 0.09236086392532074, 0.06341885990748759,
 0.059015576448141885, 0.08581919054265555, 0.06354313025922324,
 0.08353835718131386, 0.09797171397746351, 0.06934362100179227,
 0.10638669649452011]
 0.07954471607645403 0.015334344279621033
 eval_r2_mse
 [0.0013194514918062525, 0.0032281044030132537, 0.001064570688375215,
 0.0009106901307037937, 0.0031637117079747487, 0.0010326423473698972,
 0.0026816989669669407, 0.0035201421383814187, 0.0012257714969091534,
 0.002159735150053455]
 0.002030651852155413 0.0009856019372789244
 eval_r2_mae
 [0.02653584857714753, 0.0400610220694293, 0.023288932863236203,
 0.021917502346491383, 0.040209965716394125, 0.02349987824947079,
 0.03673514131050992, 0.042210504787856214, 0.025408580676099753,
 0.03317136650167027]
 0.031303874309830546 0.007607108870530253
 eval_zpve_mse
 [0.0010276198851715435, 0.001513832946592096, 0.0008999779400328267,
 0.0005978519818834162, 0.0013408419776533864, 0.0007632974776766776,
 0.0013215185746225616, 0.0016546514668997565, 0.0009019191761088887,
 0.0022792708665122724]
 0.0012300782293153424 0.000475126567625426
 eval_zpve_mae

[0.021263091940652352, 0.024843489008865016, 0.019282759162902594,
 0.01626628211837057, 0.021902851739027986, 0.019605546912420783,
 0.02170257613264077, 0.025312501278317582, 0.01933365309845285,
 0.03384307448487994]
 0.022335582587653047 0.004603618284738407
 eval_u0_mse
 [0.0006529889091708424, 0.0010434486752339649, 0.00030646211532970474,
 0.000374563445666555, 0.0006813366579365584, 0.0005325060708459995,
 0.0006204094715094411, 0.000960643187917635, 0.0005748820941449196,
 0.0010014551101817347]
 0.0006748695737937355 0.00024162665490979314
 eval_u0_mae
 [0.01653035324993822, 0.021519224776699517, 0.011873911248315975,
 0.012825272361330804, 0.014979359569661526, 0.016480320918211118,
 0.014057200432123228, 0.01894786386297334, 0.014022076527469814,
 0.01998189166652086]
 0.01612174746132444 0.0030199805516549446
 eval_u298_mse
 [0.0006561112985516652, 0.0010458815752807497, 0.0003061971597235298,
 0.00037504394175592214, 0.0006785472028349293, 0.000531194007681987,
 0.0006193783468483794, 0.0009617942561495694, 0.0005756680698029224,
 0.0009969113070084337]
 0.0006746727165638088 0.0002415427929632252
 eval_u298_mae
 [0.016532938128358658, 0.021492860104095197, 0.011871685359218391,
 0.0128119084898923, 0.014979495459630402, 0.016457353411448765,
 0.014053427160580903, 0.018952174871974047, 0.014018190437117026,
 0.01979775853321622]
 0.01609677919555319 0.002994568504291084
 eval_h298_mse
 [0.0006549360311689623, 0.0010449565315187094, 0.00030620187470520435,
 0.0003747068884807917, 0.0006773393559521162, 0.000532091039725485,
 0.0006197882594101799, 0.0009667990559345029, 0.000573647473819797,
 0.0010071994996959913]
 0.000675766601041174 0.0002434553023352543
 eval_h298_mae
 [0.01657416202701055, 0.021483446588090288, 0.011884254557242688,
 0.012822122473946538, 0.01497815405193829, 0.016460260678982895,
 0.014050443537423303, 0.018978850502272986, 0.014026420692003633,
 0.019987227904100513]
 0.016124534301301167 0.0030166928599032273
 eval_g298_mse
 [0.0006529507256202339, 0.0010448764179172374, 0.0003067924633496608,
 0.00037515495057679, 0.0006823723004142136, 0.0005314390307995475,
 0.0006187243848436387, 0.0009609875109431583, 0.000575553579891724,
 0.0009992032822031271]
 0.0006748054646559331 0.00024153580747648395
 eval_g298_mae

[0.016520424896922865, 0.02150457616889522, 0.011874588295453568,
 0.012818724440164615, 0.014980757105335068, 0.01645876524625465,
 0.014052539409949816, 0.018933492593455593, 0.014040263506242075,
 0.01982921878719656]
 0.016101335044987005 0.002995977898767529
 eval_cv_mse
 [0.0022026275797888636, 0.003564516199917909, 0.001580131675335199,
 0.001406399456230064, 0.002693030148543403, 0.0019045384423348746,
 0.0026621397308875406, 0.003242400424880164, 0.0019416243109965905,
 0.003791150434725913]
 0.0024988558403640517 0.00078815401619822
 eval_cv_mae
 [0.033192704305866655, 0.04374403345699941, 0.028863998715273745,
 0.02704530758878831, 0.03750162105479647, 0.03261610936639266,
 0.03679183913598338, 0.041033233787893135, 0.03204750546852979,
 0.04445168098988593]
 0.03572880338704095 0.005700383106011709
 eval_u0_atom_mse
 [0.0007443612805375011, 0.0013105154946036913, 0.0006606151162847488,
 0.0004907946763209666, 0.001015101162539476, 0.0006645475402661926,
 0.0009975355646818396, 0.001292172928610081, 0.0006883344538989415,
 0.0014846785444934398]
 0.0009348656762236878 0.0003199991535178171
 eval_u0_atom_mae
 [0.017638323838178743, 0.02385885776420733, 0.016538560273756043,
 0.014263013402468244, 0.019367492865806225, 0.017886391153366838,
 0.018657807656205738, 0.02245281541835607, 0.016722143593891695,
 0.02628347698057374]
 0.019366888294681063 0.0035251409957952158
 eval_u298_atom_mse
 [0.000743983843715321, 0.0013084817417638676, 0.0006602542886095132,
 0.0004902857367414861, 0.0010139762996124399, 0.0006635952784527226,
 0.0009970103214450268, 0.0012914740487415138, 0.0006883346154579119,
 0.0014804845241741618]
 0.0009337880698713965 0.0003191286671132392
 eval_u298_atom_mae
 [0.017635291138958075, 0.023830854872069675, 0.016523726403841667,
 0.01425041887629183, 0.019329498056641605, 0.017876223082851216,
 0.018646583778565973, 0.02243927555210928, 0.016713640997194384,
 0.026220092329058094]
 0.01934656050875818 0.003512422705048531
 eval_h298_atom_mse
 [0.0007423198334451637, 0.0013042753051258173, 0.0006590929440003053,
 0.00048822326216946146, 0.0010117005799753433, 0.0006616063835599512,
 0.0009945048352752281, 0.001291574191035548, 0.0006862500981613534,
 0.0014796135747549655]
 0.0009319161007503138 0.00031920564489292604
 eval_h298_atom_mae

[0.017612791589567717, 0.023776307856055418, 0.016508328147487372,
 0.01422182223229782, 0.019292666204207415, 0.017847486115738567,
 0.018603960428170238, 0.022462441827654753, 0.01667656366588534,
 0.02617726247668143]
 0.019317963054374606 0.0035105073115063844
 eval_g298_atom_mse
 [0.0007780136539658093, 0.001366723377767811, 0.0006825724372615972,
 0.0005141235203842792, 0.001054552520099539, 0.0006906164942420611,
 0.0010368634543884757, 0.0013374996483537544, 0.0007155795077036682,
 0.0015387004443469434]
 0.000971524505851394 0.00033129199962527074
 eval_g298_atom_mae
 [0.018097580593019177, 0.024522909041425615, 0.016881441268053386,
 0.014653170752145462, 0.0200316737791867, 0.0182519817377504,
 0.019281492817126114, 0.023016953517971266, 0.017191192215440593,
 0.026789037312783093]
 0.01987174330349018 0.0035899952722146192
 eval_mean_mae
 [0.03763912907401265, 0.04830002240169867, 0.031078868125793344,
 0.02927279950416937, 0.04285325027339428, 0.03417270637648359,
 0.041505927152878284, 0.054018660901138396, 0.03463824681431727,
 0.05107299907100602]
 0.04045526096948919 0.008119726880185477
 eval_A_unscaled_mse
 [3341.3875847295562, 2916.2792254199467, 987.2148741914239, 644.7864808843635,
 3122.7758796464777, 4228.057351609227, 756.2293728549529, 2384.5425531395117,
 1375.9253200668313, 7507.918116214131]
 2726.511675875642 1971.5315944760434
 eval_A_unscaled_mae
 [35.601259276802416, 25.81989205524591, 12.353834812468495, 12.112507502001112,
 20.726312755434275, 52.196894459060466, 13.597260620972571, 30.83880121202529,
 13.761564472593049, 37.85327605446694]
 25.48616032210705 12.846271964044155
 eval_B_unscaled_mse
 [0.013294913673911673, 0.04872877245840874, 0.03104785098531425,
 0.015147386678408922, 0.022929570132443285, 0.007794420076692774,
 0.03135424830591913, 0.14673031913707, 0.028103040206581335,
 0.017887700150975943]
 0.0363018221805726 0.038439018886832564
 eval_B_unscaled_mae
 [0.06671821322031989, 0.06716873295029761, 0.050102386829425326,
 0.04674786240809918, 0.06501074869070307, 0.05783759866918927,
 0.06226555525392242, 0.17401986687562965, 0.05520461768676926,
 0.06984777761511644]
 0.0714923360199472 0.03493535448031149
 eval_C_unscaled_mse
 [0.012067183839605701, 0.061367162458709414, 0.02448039202160243,
 0.013818010419681465, 0.019046838074738285, 0.00504324898426037,

0.030736370134758637, 0.04574346031853111, 0.017899415704056686,
 0.005230005408958775]
 0.02354320873649029 0.01712335491223474
 eval_C_unscaled_mae
 [0.03401671118136692, 0.03791841428394713, 0.027992007706275114,
 0.026409548323545397, 0.03448250414618169, 0.03590074377897601,
 0.032282109557093104, 0.09962983316023574, 0.029108667181388638,
 0.03841481497608796]
 0.03961553542950977 0.02037451915901723
 eval_mu_unscaled_mse
 [0.09458136839977478, 0.18053301268586783, 0.06386250702318796,
 0.05846546088372534, 0.16469811133507536, 0.059498693535151,
 0.15918564079176423, 0.1629901966612762, 0.09846677749683082,
 0.17613711509500943]
 0.1218418883907663 0.04885836735653684
 eval_mu_unscaled_mae
 [0.1971857144244741, 0.2902729775402297, 0.1588922600961836,
 0.15279274090928777, 0.26272847686368234, 0.15831384980141563,
 0.26213067430798964, 0.26948079212653364, 0.19859561617953497,
 0.28172437281221013]
 0.2232117475061542 0.05265823159128986
 eval_alpha_unscaled_mse
 [0.2701010398327267, 0.39211749026325465, 0.20056679888726767,
 0.19034787321361868, 0.30093875506005435, 0.21169906503475247,
 0.2950053632302053, 0.37638329595519976, 0.22557219224551756,
 0.47459463625646897]
 0.2937326509979066 0.08976492067592702
 eval_alpha_unscaled_mae
 [0.31781315477429045, 0.4005706765636672, 0.2676114574032694,
 0.2567207499045719, 0.3450513060291191, 0.2870299868381836, 0.3413992033689024,
 0.4135052949750219, 0.29197065082551193, 0.42348554189339016]
 0.3345158022575928 0.057921335914462926
 eval_homo_unscaled_mse
 [1.089383409807729e-05, 1.6346124369249578e-05, 8.271148689525269e-06,
 7.4284956163424405e-06, 1.559256267250152e-05, 7.759765829320198e-06,
 1.4544211886162672e-05, 1.845032366476326e-05, 1.0021369194277481e-05,
 2.0107826949693346e-05]
 1.2941566296991303e-05 4.412114381293483e-06
 eval_homo_unscaled_mae
 [0.0023371047642613205, 0.0029953760742318057, 0.0020515148675305747,
 0.0019279978339430879, 0.0028509539150611946, 0.0019792659885852553,
 0.0027768849182830354, 0.0031732097073365034, 0.0022560425902712062,
 0.0033133607573335292]
 0.0025661711416837514 0.0004900766851572937
 eval_lumo_unscaled_mse
 [1.744516295897162e-05, 2.5984040799131696e-05, 1.4908524211227744e-05,
 1.1597431390595882e-05, 2.294772613976962e-05, 1.3083942931582478e-05,
 2.2772868760863285e-05, 2.7357450333437078e-05, 1.6031381930675064e-05,

3.2403202065656845e-05]
 2.045317315219113e-05 6.51720587890971e-06
 eval_lumo_unscaled_mae
 [0.0028867175730239655, 0.0034793062724093092, 0.0024251508844108254,
 0.0022372768257061726, 0.0032153602453117674, 0.0024000665889306926,
 0.003172339348423747, 0.003573549215778432, 0.0026127732103040837,
 0.004082843302660792]
 0.0030085383466959786 0.0005693408834236922
 eval_gap_unscaled_mse
 [2.6421994388829955e-05, 4.065735043751997e-05, 2.271654194794086e-05,
 1.8576588361204744e-05, 3.694497352783957e-05, 2.0863181266018078e-05,
 3.426921727669282e-05, 4.464575486508752e-05, 2.556639110373629e-05,
 4.975555436670538e-05]
 3.204175475415752e-05 1.0210847145025015e-05
 eval_gap_unscaled_mae
 [0.003517058448840176, 0.004386796351130107, 0.0030121591132446224,
 0.00280301961705281, 0.004076091220442578, 0.0030180616769873683,
 0.003967760248754662, 0.004653290703265526, 0.0032935632514384584,
 0.005052970880949974]
 0.0037780771512106286 0.0007283240727898511
 eval_r2_unscaled_mse
 [103.2963276058599, 252.71962388390085, 83.34235729869214, 71.29548137418611,
 247.67845161974023, 80.84281952380444, 209.94299050891132, 275.5824397029228,
 95.9623396930564, 169.07986439192587]
 158.9742695603 77.16011815630912
 eval_r2_unscaled_mae
 [7.424696455943996, 11.209021711660869, 6.516212569251357, 6.132488561219691,
 11.250694913087111, 6.5752370224054, 10.278444079867903, 11.810443157817437,
 7.109286907909053, 9.281305556617903]
 8.758783093578073 2.128458737737655
 eval_zpve_unscaled_mse
 [1.1371257502967674e-06, 1.6751504694543708e-06, 9.958821278048445e-07,
 6.615607043165629e-07, 1.4837256681883412e-06, 8.446366304451564e-07,
 1.4623431452611359e-06, 1.830975490977124e-06, 9.980302168080077e-07,
 2.5221566173560264e-06]
 1.361158682090834e-06 5.257573777021141e-07
 eval_zpve_unscaled_mae
 [0.0007073175636019387, 0.0008264194030325673, 0.0006414418947530632,
 0.000541098524751158, 0.0007285992467436337, 0.0006521792917424801,
 0.0007219370783153879, 0.0008420213789688807, 0.0006431348245407647,
 0.0011257913788037413]
 0.0007429940585253615 0.00015313955825557265
 eval_u0_unscaled_mse
 [1.0506276208744003, 1.6788596067431352, 0.49308301463007753,
 0.6026546431551705, 1.0962384918637176, 0.8567770338163295, 0.9982095342919913,
 1.5456293825019791, 0.9249578545874392, 1.6112939801588395]
 1.0858331162623078 0.3887659184901221
 eval_u0_unscaled_mae

[0.663061187378406, 0.8631738171679162, 0.4762834193146381, 0.5144440710827413,
 0.6008481814837034, 0.661054467677863, 0.5638589586754429, 0.7600319634785119,
 0.5624499057293963, 0.8015088389430464]
 0.6466714810931665 0.12113674199901298
 eval_u298_unscaled_mse
 [1.055640402987261, 1.682755777789215, 0.4926513548080056, 0.6034211107813262,
 1.0917382399516748, 0.8546568432447653, 0.9965397370569008, 1.5474645263176892,
 0.9262126212349084, 1.6039661220281578]
 1.0855046736199905 0.3886267940191784
 eval_u298_unscaled_mae
 [0.6631613776079291, 0.8621116309012989, 0.4761914461000751, 0.5139051536835183,
 0.6008505008780193, 0.6601296950113003, 0.5637044585736751, 0.7602007122420693,
 0.5622910567926724, 0.7941186455559662]
 0.6456664677346523 0.12011679131453981
 eval_h298_unscaled_mse
 [1.0537492381597244, 1.6812673687549604, 0.4926588396519093, 0.6028787953406909,
 1.0897947693085528, 0.8560997323493763, 0.9971992222270798, 1.5555170789206514,
 0.9229612640981959, 1.6205195902106555]
 1.0872645899021796 0.3917040223966077
 eval_h298_unscaled_mae
 [0.6648147494015586, 0.8617338571034149, 0.47669561899433105,
 0.5143148425641112, 0.6007965211531616, 0.660246033605213, 0.5635848967224324,
 0.7612707598018503, 0.5626208394550014, 0.8017187170535488]
 0.6467796835854623 0.12100424434222566
 eval_g298_unscaled_mse
 [1.0505937228674231, 1.6811999813631782, 0.49362734020536375,
 0.6036219303307149, 1.0979327592764005, 0.8550819767420328, 0.9955238808713351,
 1.546222996489198, 0.9260622125659798, 1.6077121187197658]
 1.0857578919431392 0.388629681803873
 eval_g298_unscaled_mae
 [0.6626717103705014, 0.8625973200734168, 0.4763166862905109, 0.5141879556436577,
 0.6009120588230118, 0.6601982259900777, 0.5636792524015344, 0.7594653039508821,
 0.5631867745912127, 0.7953950352378255]
 0.645861032337263 0.12017549395004848
 eval_cv_unscaled_mse
 [0.03630448022965563, 0.05875161065595781, 0.026044282878985702,
 0.023180769801942086, 0.04438746379607744, 0.03139126021549877,
 0.04387832035794606, 0.05344238044534811, 0.032002533697020934,
 0.06248707331377612]
 0.04118701753922087 0.012990632550266367
 eval_cv_unscaled_mae
 [0.13475727647949146, 0.1775940483405904, 0.1171833833822149,
 0.10979978745150447, 0.15225079924549936, 0.13241635220647036,
 0.14936920324741843, 0.16658861620939375, 0.13010794091203198,
 0.18046699363209756]
 0.14505344011067128 0.023142682573407097
 eval_u0_atom_unscaled_mse
 [42.61430500365518, 75.02634443306113, 37.81989914395752, 28.097760398243363,

58.114040495176205, 38.04502891987497, 57.10842478010108, 73.97626227106667,
 39.406812017723134, 84.99711304266336]
 53.52059905055226 18.319788702187587
 eval_u0_atom_unscaled_mae
 [4.220298051055542, 5.708676193683668, 3.9571605810936132, 3.41269288569671,
 4.634034864476811, 4.279654215571983, 4.464229654929377, 5.37225581041352,
 4.001086199637103, 6.288813310892257]
 4.633890176745059 0.8434555287672795
 eval_u298_atom_unscaled_mse
 [43.35187441033439, 76.24508777302098, 38.472978540613944, 28.568909056553498,
 59.08432039729347, 38.66765813562144, 58.0957119859952, 75.25408044547491,
 40.10921644772888, 86.26769782595112]
 54.41175350185879 18.595590566046138
 eval_u298_atom_unscaled_mae
 [4.257011582239468, 5.752566561911369, 3.9886908784078807, 3.439932220600611,
 4.665979210228976, 4.315171756099833, 4.5011298046952914, 5.416653459434024,
 4.034534659201566, 6.329310809727532]
 4.670098094254655 0.8478687930588497
 eval_h298_atom_unscaled_mse
 [43.87143655366955, 77.08327977705858, 38.95267362017044, 28.854212280494682,
 59.791950885717974, 39.10122521388565, 58.77567132859882, 76.33262129561085,
 40.55767112045459, 87.44582661923555]
 55.07665686948967 18.86520366583243
 eval_h298_atom_unscaled_mae
 [4.281772092269844, 5.7801606072763425, 4.0132690314259, 3.4574075403100646,
 4.690158847634836, 4.33882726838696, 4.522730285858668, 5.460750725135371,
 4.054168403063097, 6.3638450456976114]
 4.69630898470587 0.8534253525549219
 eval_g298_atom_unscaled_mse
 [37.7141202488787, 66.25177271010888, 33.087604145750085, 24.9220696837446,
 51.119307631457154, 33.47754689227913, 50.26183353594934, 64.8351471045278,
 34.68761722833838, 74.58832572092338]
 47.09453449019574 16.059348250347973
 eval_g298_atom_unscaled_mae
 [3.984546408248918, 5.3992132898947816, 3.716787801027256, 3.226189782897444,
 4.410375799369198, 4.018540188692743, 4.245208406473479, 5.067645730861652,
 3.78498538018797, 5.898145659665869]
 4.375163844731931 0.7904102592004584
 eval_runtime
 [15.8175, 14.5964, 15.1303, 16.2683, 15.2147, 14.5441, 15.9734, 14.8132,
 14.4273, 14.7625]
 15.15477 0.6195126230352374
 eval_samples_per_second
 [842.356, 912.829, 880.615, 819.016, 875.733, 916.108, 834.138, 899.469,
 923.528, 902.559]
 880.6350999999999 35.23941282271882
 eval_steps_per_second
 [13.213, 14.319, 13.813, 12.847, 13.737, 14.37, 13.084, 14.109, 14.486, 14.158]

13.8136 0.5528312943385172