smallTraining

July 24, 2023

```
[1]: import torch
     import json
     import os
     import random
     import numpy as np
     import torch
     from sklearn import preprocessing
     import torch.multiprocessing as mp
     import torch
     from torch.utils.data import DataLoader
     import copy
     from torch import nn
     %matplotlib inline
     import matplotlib.pyplot as plt
     from dnaDataloader import expermentDataloader
     from dnaDataloader import addData
     from scipy import stats as st
     from dnaModelUtil import train
     device = torch.device("cuda:1" if torch.cuda.is_available() else "cpu")
     cpu = torch.device("cpu")
     batch size = 25
     device
```

```
[1]: device(type='cuda', index=1)
```

```
[2]: try:
    mp.set_start_method('spawn')
except RuntimeError:
    pass # throws error if run twice without resetting the kernal, if its_
    already set we dont care that this errors
```

0.1 Eval with small traing sets

The goal here is to eval the model while training on small sets of data. That is how well can MLP learn from 100-200 examples of single-molecule experiments. A verity of samples have been provided and preprocessed (converted from excel to csv and had empty frames added) to the folder

```
[4]: datasets = []
     featIn = 0
     for d in folders:
         data = expermentDataloader(
             f"{d}/index.csv",
             f"{d}",
         )
         rawData = [d for d in data]
         featIn = len(rawData[0][0])
         trainValidData = []
         testData = []
         addData(testData, trainValidData, rawData, rhsSize=300)
         np.random.shuffle(trainValidData)
         trainData = []
         validData = []
         addData(trainData, validData, trainValidData,

¬rhsSize=int(len(trainValidData)*(1/3)))
         datasets.append({"name": f"{os.path.basename(d)}",
                          "train":DataLoader(trainData, batch_size=batch_size,__
      ⇒shuffle=True) ,
                          "valid":DataLoader(validData, batch_size=batch_size,_
      ⇒shuffle=True) ,
                          "test":DataLoader(testData, batch_size=len(testData), ___
      ⇔shuffle=True) ,
                          "model": {}}
                         )
```

```
[5]: print(f"datasets:")
  for d in datasets:
     print(d)
  print(f"{len(datasets)}")
  print(f"featIn: {featIn}")
```

datasets:

```
{'name': '1800_nM_AR_out', 'train': <torch.utils.data.dataloader.DataLoader
object at 0x7f52ee8cceb0>, 'valid': <torch.utils.data.dataloader.DataLoader
object at 0x7f52e3f4bf10>, 'test': <torch.utils.data.dataloader.DataLoader
object at 0x7f52e3f620b0>, 'model': {}}
```

```
{'name': '800_nM_AR_out', 'train': <torch.utils.data.dataloader.DataLoader
    object at 0x7f5456899d50>, 'valid': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3f10550>, 'test': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3f10610>, 'model': {}}
    {'name': '1200 nM AR out', 'train': <torch.utils.data.dataloader.DataLoader
    object at 0x7f5456899c60>, 'valid': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3f7c430>, 'test': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3fbbeb0>, 'model': {}}
    {'name': '400_nM_AR_out', 'train': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3f7fdf0>, 'valid': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3fb8040>, 'test': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3ff3fa0>, 'model': {}}
    {'name': '50_nM_AR_out', 'train': <torch.utils.data.dataloader.DataLoader object
    at 0x7f52e3fbbfa0>, 'valid': <torch.utils.data.dataloader.DataLoader object at
    0x7f52e3ff0070>, 'test': <torch.utils.data.dataloader.DataLoader object at
    0x7f52e3e23fa0>, 'model': {}}
    {'name': '100_nM_AR_out', 'train': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3ff3eb0>, 'valid': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3e20190>, 'test': <torch.utils.data.dataloader.DataLoader
    object at 0x7f52e3e5bd30>, 'model': {}}
    featIn: 12000
[6]: for d in datasets:
         print(f"-- {d['name']} --")
         print(f"train: {len(d['train'])}")
         print(f"valid: {len(d['valid'])}")
         print(f"test : {len(d['test'])}")
    -- 1800_nM_AR_out --
    train: 8
    valid: 4
    test : 1
    -- 800_nM_AR_out --
    train: 8
    valid: 4
    test: 1
    -- 1200_nM_AR_out --
    train: 8
    valid: 4
    test : 1
    -- 400_nM_AR_out --
    train: 8
    valid: 4
    test: 1
    -- 50_nM_AR_out --
    train: 8
    valid: 4
```

```
test: 1
     -- 100_nM_AR_out --
     train: 8
     valid: 4
     test: 1
 [7]: manager = mp.Manager()
      return_dict = manager.dict()
 []:
 [8]: processes = []
      devices = [torch.device("cuda:0"),torch.device("cuda:1"),torch.device("cuda:
      epochs = 10000
      error_margin = 20
      for d in datasets:
         processes.append(mp.Process(target=train, args=(d["train"], d["valid"], u
       →d["name"], featIn, return_dict, epochs, error_margin, devices[0])))
         devices.append(devices.pop(0))
      processes
 [8]: [<Process name='Process-2' parent=1575574 initial>,
       <Process name='Process-3' parent=1575574 initial>,
       <Process name='Process-4' parent=1575574 initial>,
       <Process name='Process-5' parent=1575574 initial>,
       <Process name='Process-6' parent=1575574 initial>,
       <Process name='Process-7' parent=1575574 initial>]
 [9]: print(return_dict)
     {}
[10]: processesList = list(range(len(processes)))
      while processesList:
         run = processesList[:4]
         processesList = processesList[4:]
         for i in run:
             processes[i].start()
         for i in run:
             processes[i].join()
             processes[i].terminate()
      print(return_dict)
     training 1800_nM_AR_out on cuda:0...
     training 800 nM AR out on cuda:1...
     training 1200_nM_AR_out on cuda:2...
```

```
training 400_nM_AR_out on cuda:3...
    training 50_nM_AR_out on cuda:0...
    training 100_nM_AR_out on cuda:1...
    {'1800_nM_AR_out': {'path': './Models/smallTrain/1800_nM_AR_out.pt', 'acc':
        0.54}, '800_nM_AR_out': {'path': './Models/smallTrain/800_nM_AR_out.pt', 'acc':
        0.3700000000000005}, '1200_nM_AR_out': {'path':
        './Models/smallTrain/1200_nM_AR_out.pt', 'acc': 0.53}, '400_nM_AR_out': {'path':
        './Models/smallTrain/400_nM_AR_out.pt', 'acc': 0.43000000000000005},
        '50_nM_AR_out': {'path': './Models/smallTrain/50_nM_AR_out.pt', 'acc':
        0.8500000000000001}, '100_nM_AR_out': {'path':
        './Models/smallTrain/100_nM_AR_out.pt', 'acc': 0.52}}

[11]: results = dict(return_dict)
    with open("./Models/smallTrain/results.json", 'w') as file:
        json_object = json.dumps(results, indent=4)
        file.write(json_object)
```