! nvidia-smi

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Tue May 24 07:22:31 2022
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NVIDIA-SMI 460.32.03 Driver Version: 460.32.03 CUDA Version: 11.2
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GPU Name Persistence-M Bus-Id Disp.A | Volatile Uncorr. ECC |
| Fan Temp Perf Pwr:Usage/Cap| Memory-Usage | GPU-Util Compute M. |
                                    MIG M. |
______
 0 Tesla T4 Off | 00000000:00:04.0 Off |
| N/A 43C P8 11W / 70W | 0MiB / 15109MiB |
                               0% Default |
                                     N/A
Processes:
GPU GI CI
           PID Type Process name
                                  GPU Memory
    ID ID
                                  Usage
|-----|
No running processes found
```

!pip install pytorch-tabnet optuna

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Collecting optuna
    Downloading optuna-2.10.0-py3-none-any.whl (308 kB)
                                   308 kB 19.8 MB/s
Requirement already satisfied: scikit learn>0.21 in /usr/local/lib/python3.7/dist-
Requirement already satisfied: numpy<2.0,>=1.17 in /usr/local/lib/python3.7/dist-p
Requirement already satisfied: tqdm<5.0,>=4.36 in /usr/local/lib/python3.7/dist-pa
Requirement already satisfied: scipy>1.4 in /usr/local/lib/python3.7/dist-packages
Requirement already satisfied: torch<2.0,>=1.2 in /usr/local/lib/python3.7/dist-pa
Requirement already satisfied: joblib>=0.11 in /usr/local/lib/python3.7/dist-packa
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.7/di
Requirement already satisfied: typing-extensions in /usr/local/lib/python3.7/dist-
Requirement already satisfied: PyYAML in /usr/local/lib/python3.7/dist-packages (f
Collecting colorlog
    Downloading colorlog-6.6.0-py2.py3-none-any.whl (11 kB)
Collecting cmaes>=0.8.2
    Downloading cmaes-0.8.2-py3-none-any.whl (15 kB)
Requirement already satisfied: packaging>=20.0 in /usr/local/lib/python3.7/dist-pa
Collecting alembic
    Downloading alembic-1.7.7-py3-none-any.whl (210 kB)
                               210 kB 58.2 MB/s
Requirement already satisfied: sqlalchemy>=1.1.0 in /usr/local/lib/python3.7/dist-
Collecting cliff
    Downloading cliff-3.10.1-py3-none-any.whl (81 kB)
                   | 81 kB 11.4 MB/s
Requirement already satisfied: pyparsing!=3.0.5,>=2.0.2 in /usr/local/lib/python3.
Requirement already satisfied: greenlet!=0.4.17 in /usr/local/lib/python3.7/dist-p
Requirement already satisfied: importlib-metadata in /usr/local/lib/python3.7/dist
Collecting Mako
    Downloading Mako-1.2.0-py3-none-any.whl (78 kB)
                                                         | 78 kB 2.9 MB/s
Requirement already satisfied: importlib-resources in /usr/local/lib/python3.7/dis
Collecting autopage>=0.4.0
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Collecting cmd2>=1.0.0

146 kB 52.8 MB/s

Downloading autopage-0.5.0-py3-none-any.whl (29 kB)

Downloading cmd2-2.4.1-py3-none-any.whl (146 kB)

```
Collecting pbr!=2.1.0,>=2.0.0
          Downloading pbr-5.9.0-py2.py3-none-any.whl (112 kB)
                                              112 kB 58.0 MB/s
        Requirement already satisfied: PrettyTable>=0.7.2 in /usr/local/lib/python3.7/dist
        Collecting stevedore>=2.0.1
          Downloading stevedore-3.5.0-py3-none-any.whl (49 kB)
                                         49 kB 6.3 MB/s
        Collecting pyperclip>=1.6
          Downloading pyperclip-1.8.2.tar.gz (20 kB)
        Requirement already satisfied: wcwidth>=0.1.7 in /usr/local/lib/python3.7/dist-pac
        Requirement already satisfied: attrs>=16.3.0 in /usr/local/lib/python3.7/dist-pack
        Requirement already satisfied: zipp>=0.5 in /usr/local/lib/python3.7/dist-packages
        Requirement already satisfied: MarkupSafe>=0.9.2 in /usr/local/lib/python3.7/dist-
        Building wheels for collected packages: pyperclip
          Building wheel for pyperclip (setup.py) ... done
          Created wheel for pyperclip: filename=pyperclip-1.8.2-py3-none-any.whl size=1113
          Stored in directory: /root/.cache/pip/wheels/9f/18/84/8f69f8b08169c7bae2dde6bd7d
        Successfully built pyperclip
        Installing collected packages: pyperclip, pbr, stevedore, Mako, cmd2, autopage, cd
        Successfully installed Mako-1.2.0 alembic-1.7.7 autopage-0.5.0 cliff-3.10.1 cmaes- ▼
   import pandas as pd
   import numpy as np
   from pytorch tabnet.tab model import TabNetClassifier
   from sklearn.metrics import accuracy_score,classification_report
   import optuna as opt
   import torch
   import os
   import joblib
   def make save cv model(i, model name, model, best params, optim, output path="./drive/MyDrive/S
        ''' This function saves cross validation model in the corresponding directory ( if the
       if os.path.exists(os.path.join(output_path,f"{i}_{model_name}_{optim}")):
           joblib.dump(model, os.path.join(output path,f"{i} {model name} {optim}/{i} model.z
           with open(os.path.join(output_path,f"{i}_{model_name}_{optim}/model_params.txt"),"
               file.write(str(best_params))
       else:
           os.mkdir(os.path.join(output_path,f"{i}_{model_name}_{optim}"))
           joblib.dump(model, os.path.join(output_path,f"{i}_{model_name}_{optim})/{i}_model.z
           with open(os.path.join(output path,f"{i} {model name} {optim}/model params.txt"),"
               file.write(str(best params))
   def train(fold_dict,fold,model_name,sc_df,tar_col,optim,optim_trial,k_folds=10,tar_cols=""
        ''' this function is used to train the model with parameters optimization using optuna
       y = sc df[tar col]
https://colab.research.google.com/drive/1Mnt281Zpg1sWltZGLmDRu72WPMAnaUeY#scrollTo=l2B4NzJSvEUT&printMode=true
```

```
x = sc df.drop([tar col],axis=1)
model name = model name
def objective(trial):
  train_index = fold_dict[fold]["train"]
  test_index = fold_dict[fold]["test"]
  clf = TabNetClassifier(n_d=trial.suggest_int("n_d", 8, 64),
                          n_a =trial.suggest_int("n_a", 8, 64),
                          n_steps = trial.suggest_int("n_steps",3,10),
                          gamma =trial.suggest_float("gamma", 1.0, 2.0),
                          n_independent = trial.suggest_int("n_independent",1,5),
                          n_shared = trial.suggest_int("n_shared",1,5),
                          momentum = trial.suggest float("momentum", 0.01, 0.4),
                          optimizer fn = torch.optim.Adam,
                          # scheduler_fn = torch.optim.lr_scheduler,
                          # scheduler_params = {"gamma" :trial.suggest_float("sch-gamm")
                          verbose = verbose,
                          device_name = "auto"
  # print(f" train_index :: {train_index}")
  # print(f" test_index :: {test_index}")
  X_train,X_test = x.iloc[train_index,:], x.iloc[test_index,:]
  # print(X_train.shape, X_test.shape)
  X_train, X_test = X_train.to_numpy(dtype=np.float64), X_test.to_numpy(dtype=np.float
  Y_train, Y_test = y.iloc[train_index], y.iloc[test_index]
  Y_train, Y_test = Y_train.to_numpy(dtype=np.float64), Y_test.to_numpy(dtype=np.float
  print(Y_train.shape, Y_test.shape)
  clf.fit(X_train, Y_train,
          eval_set=[(X_test, Y_test)],
          eval_metric=['accuracy'])
  Y_pred = clf.predict(X_test)
  print(classification_report(Y_test, Y_pred, labels=[x for x in range(6)]))
  acc = accuracy_score(Y_pred, Y_test)
  return acc
print(f"Starting optimization for fold : [{fold}/{k_folds}]")
study = opt.create study(direction='maximize')
study.optimize(objective, n trials=optim trial)
best params = study.best params
print(f" Best params for fold : [{fold}/{k_folds}]")
print(best_params)
joblib.dump(best_params,f"./drive/MyDrive/SOLAR_CELL/ML_PROCESSED_DATA/outputs/{model_
with open(f"./drive/MyDrive/SOLAR_CELL/ML_PROCESSED_DATA/outputs/{model_name}/best_par
print(f"Saved best_params at : outputs/{model_name}/best_params/fold_{fold}_best_param
train_index = fold_dict[fold]["train"]
test index = fold dict[fold]["test"]
X_train,X_test = x.iloc[train_index,:], x.iloc[test_index,:]
# print(X_train.shape, X_test.shape)
X train, X test = X train.to numpy(dtype=np.float64), X test.to numpy(dtype=np.float64
Y train, Y test = y.iloc[train index], y.iloc[test index]
Y_train, Y_test = Y_train.to_numpy(dtype=np.float64), Y_test.to_numpy(dtype=np.float64
clf_model = TabNetClassifier(**study.best_params)
clf_model.fit(X_train,Y_train)
Y_pred = clf_model.predict(X_test)
clf_report = classification_report(Y_test, Y_pred, labels=[x for x in range(6)])
with open(f"./drive/MyDrive/SOLAR_CELL/ML_PROCESSED_DATA/outputs/classification_report
```

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accuracy = accuracy_score(Y_pred, Y_test)
    with open(f"./drive/MyDrive/SOLAR CELL/ML PROCESSED DATA/outputs/{model name}/{model n
    try:
        print("[++] Saving the model and parameters in corresponding directories")
        make_save_cv_model(fold,model_name,clf_model,best_params,optim=optim)
    except:
        print("[-] Failed to save the model")
use_df = pd.read_csv("./drive/MyDrive/SOLAR_CELL/ML_PROCESSED_DATA/outputs/data/trainable_
tar_col = "PCE_categorical"
model_name = "pytorch_tabnet"
optimizer = "Adam"
fold_dict = joblib.load("./drive/MyDrive/SOLAR_CELL/ML_PROCESSED_DATA/inputs/fold_vals/fol
fold = 6
train(fold_dict = fold_dict,
      fold = fold,
      model_name=model_name,
      sc_df=use_df,
      tar_col=tar_col,
      optim=optimizer,
      optim trial = 15)
print(f"[++] Ended the training process for fold {fold}")
     פעטנוו 4ס ן בעסטאס טייש פעטנוו 4ס ן דער אייטטאס טייש פעטנוו 4ס ן דער אייטטאס אייטטאס אייטטאס אייטטאס אייטטאס אייטטאס
     epoch 46 | loss: 0.47144 | 0:02:00s
     epoch 47 | loss: 0.46496 | 0:02:03s
     epoch 48 | loss: 0.46084 | 0:02:05s
     epoch 49 | loss: 0.45356 | 0:02:08s
     epoch 50 | loss: 0.44674 | 0:02:10s
     epoch 51 | loss: 0.44621 | 0:02:13s
     epoch 52 | loss: 0.4578 | 0:02:16s
     epoch 53 | loss: 0.45311 | 0:02:18s
     epoch 54 | loss: 0.44346 | 0:02:21s
     epoch 55 | loss: 0.44408 | 0:02:23s
     epoch 56 | loss: 0.44867 | 0:02:26s
     epoch 57 | loss: 0.43741 | 0:02:28s
     epoch 58 | loss: 0.44922 | 0:02:31s
     epoch 59 | loss: 0.44798 | 0:02:33s
     epoch 60 | loss: 0.44962 | 0:02:36s
     epoch 61 | loss: 0.43741 | 0:02:38s
     epoch 62 | loss: 0.4282 | 0:02:41s
     epoch 63 | loss: 0.41778 | 0:02:44s
     epoch 64 | loss: 0.41568 | 0:02:46s
     epoch 65 | loss: 0.41298 | 0:02:49s
     epoch 66 | loss: 0.41474 | 0:02:51s
     epoch 67 | loss: 0.42709 | 0:02:54s
     epoch 68 | loss: 0.42211 | 0:02:56s
     epoch 69 | loss: 0.41249 | 0:02:59s
     epoch 70 | loss: 0.40765 | 0:03:01s
     epoch 71 | loss: 0.40954 | 0:03:04s
     epoch 72 | loss: 0.40961 | 0:03:06s
     epoch 73 | loss: 0.39756 | 0:03:09s
     epoch 74 | loss: 0.39453 | 0:03:11s
     epoch 75 | loss: 0.39214 | 0:03:14s
     epoch 76 | loss: 0.40054 | 0:03:16s
     epoch 77 | loss: 0.39724 | 0:03:19s
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epoch 78 | loss: 0.40694 |
                            0:03:21s
epoch 79 | loss: 0.40329 |
                            0:03:24s
epoch 80 | loss: 0.39786 |
                           0:03:26s
epoch 81 | loss: 0.39452 |
                           0:03:29s
epoch 82 | loss: 0.39643 |
                           0:03:31s
epoch 83 | loss: 0.39305 |
                            0:03:34s
epoch 84 | loss: 0.3882 |
                            0:03:36s
epoch 85 | loss: 0.388 |
                           0:03:39s
epoch 86 | loss: 0.3891 |
                           0:03:41s
epoch 87 | loss: 0.37989 | 0:03:44s
epoch 88 | loss: 0.39215 | 0:03:46s
epoch 89 | loss: 0.38917 |
                           0:03:49s
epoch 90 | loss: 0.38255 |
                           0:03:51s
epoch 91 | loss: 0.37401 |
                           0:03:54s
epoch 92 | loss: 0.37217 |
                           0:03:56s
epoch 93 | loss: 0.37285 | 0:03:59s
epoch 94 | loss: 0.37109 |
                           0:04:01s
epoch 95 | loss: 0.37071 | 0:04:04s
epoch 96 | loss: 0.36848 |
                           0:04:06s
epoch 97 | loss: 0.36445 |
                           0:04:09s
epoch 98 | loss: 0.36235 | 0:04:11s
epoch 99 | loss: 0.36406 | 0:04:14s
[++] Saving the model and parameters in corresponding directories
[++] Ended the training process for fold 6
```

Fold 0 has started running on 20-05-22

Fold 0 has completed sucessfully on 17:00 20-05-22

Fold 1 has started running at 15:15 21-05-22

Fold 2 has started running at 09:45 22-05-22

Fold 2 has completed sucessfully on 10:58 22-05-22

Fold 3 has started running at 18:40 22-05-22

Fold 3 has completed sucessfully on 22-05-22

Fold 4 completed sucessfully on 21:04 on 22-05-22

Fold 5 started at 18:21 on 23-05-22

Fold 5 completed sucessfully on 19:44 on 23-05-22

Fold 6 started at 12:53 on 24-05-22

Fold 6 has completed at 14:14 on 24-05-22

✓ 1h 19m 58s completed at 2:13 PM