# HYPER-PARAMETER OPTIMIZATION PROJECT

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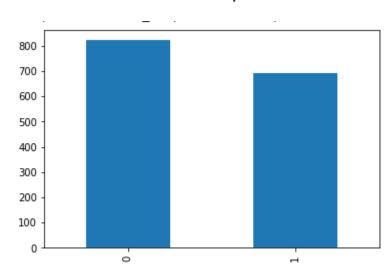
# **Abstract**

This project is a hyper-parameter-optimization of the neural network, which has been implemented on Bace molecular data set . I use ray , pytorch ,schedulers and search-algorithms and more objects in this project.

### Introduction of dataset

Type of data set is molecular. The number of records is 1513, target variables are 0 or 1 and the number of features is 200.

Distribution of labels plot:



In this case the distribution of labels are balance. There is an balance between the class of one and zero labels in Bace dataset.

# **Preprocessing**

Data partitioning, Feature selection, and Missing are the important things for prepare the data for final processing.

# **Import libraries**

```
%%capture
try:
    import ray
except:
    !pip install -U ray
   import ray
try:
   import optuna
except:
   %pip install optuna
    import optuna
    %%capture
try:
    from featurewiz import featurewiz
    !pip install featurewiz==0.1.70
import numpy as np
import pandas as pd
import torch
import torch.nn as nn
from torch.utils.data import TensorDataset
from pandas import read csv
from sklearn.impute import SimpleImputer
import io
import matplotlib as mpl
import matplotlib.pyplot as plt
import random
from functools import partial
import os
import torch.nn.functional as F
import torch.optim as optim
from torch.utils.data import random split
from torchsummary import summary
from ray import tune
from ray.tune import CLIReporter
from ray.tune.schedulers import ASHAScheduler
```

### **Data reading**

```
from google.colab import files
uploaded = files.upload()

dataX = pd.read_csv(io.BytesIO(uploaded['bace_global_cdf_rdkit.csv']))
dataY = pd.read_csv(io.BytesIO(uploaded1['bace(lables).csv']))
```

### **Data splitting**

```
from sklearn.model_selection import train_test_split
Y = dataY.iloc[:, 1]
X = dataX.iloc[:,1:201]
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=
0.15,random_state=1234)
```

#### Feature selection

I used Corrolation matrix and featurewiz library to select important features of Bace data set, then I've observed that featurewiz is better.

```
from featurewiz import FeatureWiz
features = FeatureWiz(corr limit=0.70, feature engg='',
category encoders='', dask xgboost flag=False, nrows=None, verbose=2)
X_train = features.fit_transform(X_train, Y_train)
X test = features.transform(X test)
features.features ### provides the list of selected features ###
###################
######### FAST FEATURE ENGG AND SELEC
T I O N ! #######
# Be judicious with featurewiz. Don't use it to create too many un-
interpretable features! #
##################
Skipping feature engineering since no feature engg input...
Skipping category encoding since no category encoders specified in
input...
**INFO: featurewiz can now read feather formatted files. Loading train
data...
   Shape of your Data Set loaded: (1286, 201)
   Loaded train data. Shape = (1286, 201)
   Some column names had special characters which were removed...
No test data filename given...
############
################################ C L A S S I F Y I N G V A R I A B L E S
```

##################### ############ Classifying variables in data set... 200 Predictors classified... 33 variable(s) to be removed since ID or low-information variables more than 33 variables to be removed; too many to print... train data shape before dropping 33 columns = (1286, 201) train data shape after dropping columns = (1286, 168) Converted pandas dataframe into a Dask dataframe ... GPU active on this device Tuning XGBoost using GPU hyper-parameters. This will take time... After removing redundant variables from further processing, features left = 167No interactions created for categorical vars since feature engg does not specify it #### Single Label Binary Classification problem ####

##### Searching for Uncorrelated List Of Variables (SULOV) in 167
features ###########

there are no null values in dataset... Removing (62) highly correlated variables:

############

#### How SULOV Method Works by Removing Highly Correlated Features

In SULOV, we repeatedly remove features with lower mutual info scores among highly correlated pairs (see figure), SULOV selects the feature with higher mutual info score related to target when choosing between a pair Bigger circle denotes higher mutual info score with target Thicker line denotes higher correlation between two variables fr COO2classnumpyfloat64 (selected)
fr nitro arom nonorthoclassnumpyfloat64 (selected) fr ketoneslassnumpyfloat64 (removed)
fr\_Ndealkylation1classnumpyfloat64 (selected) fr\_amideclassnumpyfloat64 (removed)
fr\_amideclassnumpyfloat64 (selected) fr\_ketone\_Tablication1classnumpyfloat64 (selected) fr\_ketone\_Toplissclassnumpyfloat64 (selected) NumSaturatedCarbocyclesclassnumpyfloat64 (selected) NumAromaticCarbocyclesclassnumpyfloat64 (removed) fr\_etherclassnumpyfloat64 (selected) NumHDonorsclassnumpyfloat64 (removed) NumHAcceptorsclassnumpyfloat64 (selected) fr\_guanidoclassnumpyfloat64 (removed) fr\_C\_O\_noCOOclassnumpyfloat64 (removed) SlogP\_VSA12classnumpyfloat64 (removed) NumRotatableBondsclassnumpyfloat64 (removed) SMR\_VSA2classnumpyfloat64 (selected) NHOHCountclassnumpyfloat64 (selected) fr\_COOclassnumpyfloat64 (removed) Chi3vclassnumpyfloat64 (removed) fr\_phenolclassnumpyfloat64 (selected) Chi4nclassnumpyfloat64 (removed) ol\_noOrthoHbondclassnumpyfloat64 (removed) fr\_C\_Oclassnumpyfloat64 (selecte nitro\_aromclassnumpyfloat64 (removed) fr\_Al\_OHclassnumpyfloat64 (remo SlogP\_VSA7classnumpyfloat64 (se r\_NH1classnumpyfloat64 (selected) nitrileclassnumpyfloat64 (removed) Chi3nclassnumpyfloat64 (rem cCarbocyclesclassnumpyfloat64 (removed) fr\_Nhpyrroleclassnumpyfloat64 COOclassnumpyfloat64 (removed) Kappa3classnumpyfloat64 (re OHclassnumpyfloat64 (removed) SlogP\_VSA11classnumpyfloat64 tialChargeclassnumpyfloat64 (selected) FpDensityMorgan2classnumpyfloa |Chargeclassnumpyfloat64 (removed) PEOE\_VSA14classnumpyfloat64 Chi1vclassnumpyfloat64 (re alChargeclassnumpyfloat64 (selected) tialChargeclassnumpyfloat64 (removed) MolMRclassnumpyfloat64 (rei VSA1classnumpyfloat64 (selected) Chi1nclassnumpyfloat64 (ren gP\_VSA2classnumpyfloat64 (removed) gedclassnumpyfloat64 (select TPSAclassnumpyfloat64 (selected) NumValenceElectronsclassnumpyfloat64 SlogP\_VSA3classnumpyfloat64 (selected) Chi0vclassnumpyfloat64 (remove SMR\_VSA7classnumpyfloat64 (selected) FpDensityMorgan3classnumpyfloat64 (rem Chi1classnumpyfloat64 (removed) NumHeteroatomsclassnumpyfloat64 (remo EState\_VSA1classnumpyfloat64 (removed) HeavyAtomCountclassnumpyfloat64 (removed EState VSA2classnumpyfloat64 (selected) Chi2nclassnumpyffoat64 (removed) MinEStateIndexclassnumpyfloat64 (selected) NOCountclassnumpyfloat64 (removed) SMR\_VSA6classnumpyfloat64 (selected) FpDensityMorgan1classnumpyfloat64 (selected) SlogP\_VSA5classnumpyfloat64 (selected) Kappa2classnumpyfloat64 (removed) EState\_VSA10classnumpyfloat64 (removed) Chi0nclassnumpyfloat64 (removed) Chioclassnumpyfloat64 (removed)

Chioclassnumpyfloat64 (removed)

SMR VSA5classnumpyfloat64 (removed)

ExactMolVic lassnumpyfloat64 (removed)

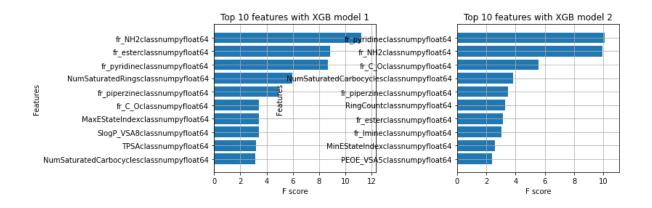
Halfic lassnumpyfloat64 (removed)

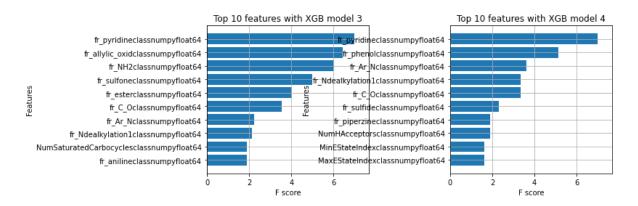
Republic lassnumpyfloat64 (removed)

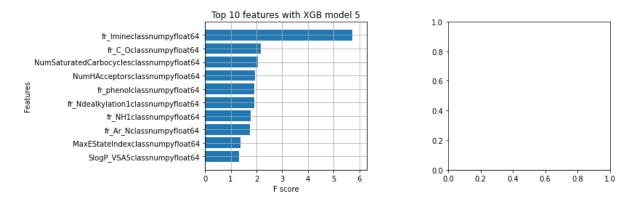
Time taken for SULOV method = 4 seconds Adding 0 categorical variables to reduced numeric variables of 105 Final list of selected vars after SULOV = 105 Readying dataset for Recursive XGBoost by converting all features to numeric... ############# RECURSIVE XGBOOST: FEATURE SELECTI O N ###### ############ using regular XGBoost Train and Test loaded into Dask dataframes successfully after feature engg completed Current number of predictors = 105 XGBoost version: 1.6.1 Number of booster rounds = 100 using 105 variables... Time taken for regular XGBoost feature selection = 2 seconds using 84 variables... Time taken for regular XGBoost feature selection = 5 seconds using 63 variables... Time taken for regular XGBoost feature selection = 7 seconds using 42 variables... Time taken for regular XGBoost feature selection = 8 seconds using 21 variables... Time taken for regular XGBoost feature selection = 9 seconds Total time taken for XGBoost feature selection = 12 seconds ############ ##### FEATURE SELECTION COMPLETED ####### ############ Selected 56 important features. Too many to print... Time taken for feature selection = 15 seconds Returning 2 dataframes: dataname and test data with 56 important features. Time taken to create entire pipeline = 17 second(s) ["('fr\_NH2', <class 'numpy.float64'>)", '('fr\_ester', <class 'numpy.float64'>)" "('fr\_pyridine', <class 'numpy.float64'>)", "('NumSaturatedRings', <class 'numpy.float64'>)", "('fr\_piperzine', <class 'numpy.float64'>)", "('fr\_C\_O', <class 'numpy.float64'>)", "('MaxEStateIndex', <class 'numpy.float64'>)", "('SlogP\_VSA8', <class 'numpy.float64'>)", "('TPSA', <class 'numpy.float64'>)", "('NumSaturatedCarbocycles', <class 'numpy.float64'>)", "('PEOE\_VSA4', <class 'numpy.float64'>)", "('SMR\_VSA10', <class 'numpy.float64'>)"

"('fr\_aryl\_methyl', <class 'numpy.float64'>)",

```
"('NumHAcceptors', <class 'numpy.float64'>)",
"('MinEStateIndex', <class 'numpy.float64'>)",
"('SlogP_VSA5', <class 'numpy.float64'>)",
"('MaxPartialCharge', <class 'numpy.float64'>)",
"('SlogP_VSA4', <class 'numpy.float64'>)",
"('VSA_EState10', <class 'numpy.float64'>)",
"('PEOE_VSA12', <class 'numpy.float64'>)",
"('SlogP_VSA1', <class 'numpy.float64'>)",
"('PEOE_VSA11', <class 'numpy.float64'>)",
"('PEOE_VSA2', <class 'numpy.float64'>)",
"('SMR_VSA6', <class 'numpy.float64'>)"
"('fr_bicyclic', <class 'numpy.float64'>)",
"('RingCount', <class 'numpy.float64'>)",
"('fr_Imine', <class 'numpy.float64'>)",
"('PEOE_VSA5', <class 'numpy.float64'>)"
"('fr_phenol', <class 'numpy.float64'>)",
"('fr_NH0', <class 'numpy.float64'>)",
"('fr_para_hydroxylation', <class 'numpy.float64'>)",
"('fr_allylic_oxid', <class 'numpy.float64'>)",
"('fr_sulfone', <class 'numpy.float64'>)",
"('fr_Ar_N', <class 'numpy.float64'>)",
"('fr_Ndealkylation1', <class 'numpy.float64'>)",
"('fr_aniline', <class 'numpy.float64'>)",
"('fr_Ndealkylation2', <class 'numpy.float64'>)",
"('fr_oxazole', <class 'numpy.float64'>)",
"('fr_imidazole', <class 'numpy.float64'>)",
"('qed', <class 'numpy.float64'>)",
"('fr_unbrch_alkane', <class 'numpy.float64'>)",
"('fr_sulfide', <class 'numpy.float64'>)",
"('SlogP_VSA3', <class 'numpy.float64'>)",
"('SMR_VSA7', <class 'numpy.float64'>)",
"('MaxAbsPartialCharge', <class 'numpy.float64'>)",
"('NHOHCount', <class 'numpy.float64'>)",
"('Chi4v', <class 'numpy.float64'>)"
"('SMR_VSA1', <class 'numpy.float64'>)",
"('fr ketone_Topliss', <class 'numpy.float64'>)",
"('fr_NH1', <class 'numpy.float64'>)"
"('fr_ether', <class 'numpy.float64'>)",
"('FpDensityMorgan1', <class 'numpy.float64'>)",
"('SlogP_VSA7', <class 'numpy.float64'>)",
"('fr_COO2', <class 'numpy.float64'>)"
"('SMR_VSA2', <class 'numpy.float64'>)"
"('fr Nhpyrrole', <class 'numpy.float64'>)"]
```







It should be noted that the feature selection section is processed only based on the information in the training set.

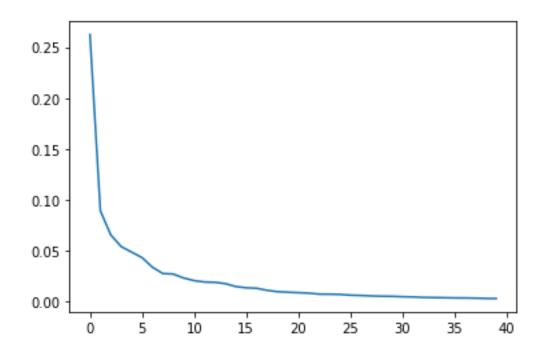
56 features were selected as influencing features on the target variable in the Bace dataset.

#### **PCA**

I have used PCA but the result of our model is not good in this way, cause of that ignored it.

```
from sklearn.decomposition import PCA as sklearnPCA
pca = sklearnPCA(n components=40)
```

```
pca.fit(X_train)
X_train=pca.transform(X_train)
X_test=pca.transform(X_test)
plt.plot(np.arange(40),pca.explained_variance_ratio_)
plt.show()
```



# **Scailing data**

```
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn import preprocessing
import random
np.random.seed(1234)

from sklearn import preprocessing
scaler_data = preprocessing.MinMaxScaler()
X_train = scaler_data.fit_transform(X_train)
X_test = scaler_data.transform(X_test)
scaler labels = preprocessing.MinMaxScaler()
```

I have not used MinMaxScaler method on lables, because they are 0 or 1.

#### Transform to torch tensor

```
device = torch.device('cuda:0' if torch.cuda.is_available() el
se 'cpu')

tensor_x = torch.tensor(X_train, dtype=torch.float).to(device)

tensor_x2 = torch.tensor(X_test, dtype=torch.float).to(device)

tensor_y = torch.tensor(Y_train, dtype=torch.float).to(device)

tensor_y2 = torch.tensor(Y_test, dtype=torch.float).to(device)

tensor_y2 = torch.tensor(Y_test, dtype=torch.float).to(device)

# create your dataset

trainset = TensorDataset(tensor_x, tensor_y)

testset = TensorDataset(tensor_x2, tensor_y2)
```

### **Loading the Data**

```
def load_data(data_dir=None):
    return trainset, testset
```

# **Missing values**

Bace data set has not any missing values.

### **Accuracy and error measurement**

I used ROC\_AUC score for Bace data set ,cause that is a classification project.

```
from sklearn.metrics import roc auc score
def compute score(model, data loader, device="cpu"):
   model.eval()
   metric = roc auc score
    with torch.no grad():
        prediction all= torch.empty(0, device=device)
        labels all= torch.empty(0, device=device)
        for i, (feats, labels) in enumerate(data loader):
            feats=feats.to(device)
            labels=labels.to(device)
            prediction = model(feats).to(device)
            prediction = torch.sigmoid(prediction).to(device)
            prediction all = torch.cat((prediction all, predic
tion), 0)
            labels all = torch.cat((labels all, labels), 0)
        try:
            t = metric(labels all.int().cpu(), prediction all.
cpu()).item()
        except ValueError:
           t = 0
    return t
```

# **Configurable neaural network**

We can tune those parameters that are configurable (Learning rate, Hidden dim, Number of layers, Activation functions).

Note: In this case I define a loop for assigning Hidden\_dim in our Nueral Network model.

```
class Net(nn.Module):
    def init (self, config):
        super(). init ()
        self.config = config
        self.hidden dim1 = int(self.config.get("hidden dim1", 100))
        self.hidden dim2 = int(self.config.get("hidden dim2", 100))
        self.hidden dim3 = int(self.config.get("hidden dim3", 100))
        hidden dim={}
        self.act1 = self.config.get("act1", "relu")
        self.act2 = self.config.get("act2", "relu")
        self.act3 = self.config.get("act3", "relu")
        self.linear1 = nn.Linear(200, self.hidden dim1)
        self.linear2 = nn.Linear(self.hidden dim1, self.hidden dim2)
        self.linear3 = nn.Linear(self.hidden dim2, self.hidden dim3)
        self.linear4 = nn.Linear(self.hidden dim3, 1)
        for i in range (4, num layers):
          self.config.update("hidden dim"+str(i):tune.quniform(150,300,
10))
          self.config.update("linear"+str(i):nn.Linear("hidden dim"+str
(i-1), "hidden dim"+str(i)))
          self.config.update("act"+str(i):tune.choice("relu", "selu", "ta
nh"))
        self.linear("num layers") = nn.Linear(self.hidden dim("num laye
rs")), 1)
    @staticmethod
    def activation func(act str):
        if act str=="tanh":
            return eval("torch."+act str)
        elif act str=="selu" or act str=="relu":
            return eval("torch.nn.functional."+act str)
    def forward(self, x):
        output = self.linear1(x)
        output = self.activation func(self.act1)(output)
        output = self.linear2(output)
        output = self.activation func(self.act2)(output)
        output = self.linear3(output)
        output = self.activation func(self.act3)(output)
        output = self.linear4(output)
        output = self.linear("linear") (output)
        output = self.activation func(self.act)(output)
        output =torch.sigmoid(output)
        predictY=output
        return predictY
```

### The train function

We wrap the training script in a function "trainable\_func".

As you can guess, the "config" parameter will receive the hyperparameters we would like to train with. The "checkpoint\_dir" parameter is used to restore checkpoints. The "data\_dir" specifies the directory where we load and store the data, so multiple runs can share the same data source.

In this function I defined a loss function (criterion=nn.BCELoss()) And an optimizer(SGD).

We also split the training data into a training and validation subset. We thus train on 70% of the data and calculate the validation loss on the remaining 15%. The batch sizes with which we iterate through the training and test sets are configurable as well.

Here we first save a checkpoint and then report some metrics back to Ray Tune. Specifically we send the validation loss and accuracy back to Ray Tune. Ray Tune can then use these metrics to decide which hyperparameter configuration lead to the best results. These metrics can also be used to stop bad performing trials early in order to avoid wasting resources on those trials.

Also, by saving the checkpoint we can later load the trained models and validate them.

```
def trainable_func(config, checkpoint_dir=None, data_dir=None,
    epochs=10):
    net = Net(config)

    device = "cpu"
    if torch.cuda.is_available():
        device = "cuda:0"
        if torch.cuda.device_count() > 1:
            net = nn.DataParallel(net)
    net.to(device)
```

```
1.1.1
    Define a loss function
    ## Classification
    #criterion = nn.CrossEntropyLoss()
    criterion=nn.BCELoss()
    # Define an optimizer
    optimizer = torch.optim.SGD(net.parameters(), lr=config.ge
t("lr",0.0003))
    if checkpoint dir:
        model state, optimizer state = torch.load(
            os.path.join(checkpoint dir, "checkpoint"))
        net.load state dict(model state)
        optimizer.load state dict(optimizer state)
    # Load data
    trainset, testset = load data(data dir)
    # Split the dataset into training and validation sets
    train size = int(len(trainset) * 0.825)
    train subset, val subset = random split(trainset, [train s
ize, len(trainset) - train size])
    # Define data loaders (which combines a dataset and a samp
ler, and provides an iterable over the given dataset)
    trainloader = torch.utils.data.DataLoader(
        train subset,
        batch size=int(config.get("batch_size",32)),
        shuffle=True,
        num workers=2)
    valloader = torch.utils.data.DataLoader(
        val subset,
        batch size=int(config.get("batch size", 32)),
        shuffle=True,
        num workers=2)
    for epoch in range (epochs): # loop over the dataset multi
ple times
        epoch train loss = 0.0
        # epoch steps = 0
        net.train() # Prepare model for training
        for i, data in enumerate (trainloader):
            # get the inputs; data is a list of [inputs, label
s]
            inputs, labels = data
```

```
inputs, labels = inputs.to(device), labels.to(devi
ce)
            # zero the parameter gradients
            optimizer.zero grad()
            # forward + backward + optimize
            outputs = net(inputs)
            loss = criterion(outputs, labels)
            loss.backward()
            optimizer.step()
            Compute train loss without scaling to print
        score = compute score(net, valloader, device="cpu")
        with tune.checkpoint dir(epoch) as checkpoint dir:
            path = os.path.join(checkpoint dir, "checkpoint")
            torch.save((net.state dict(), optimizer.state dict
()), path)
        tune.report(score=score)
    print("Finished Training")
```

#### Test set score

Commonly the performance of a machine learning model is tested on a hold-out test set with data that has not been used for training the model. We also wrap this in a function.

I have defined this function for applying best model's score on the test set:

```
def test_score(config, net , device="cpu"):
    trainset, testset = load_data()

    testloader = torch.utils.data.DataLoader(testset, batch_si
ze=int(config.get("batch_size",32)), shuffle=False, num_worker
s=2)
    best_trained_model=net
    criterion = nn.CrossEntropyLoss()

    test_score = compute_score(best_trained_model, testloader,
    device)
    print("Best_trial_test_set_score: {}".format(test_score))
```

### **Configuring the search space**

Ray Tune will now randomly sample a combination of parameters from these search spaces. It will then train a number of models in parallel and find the best performing one among these. We also use the "ASHAScheduler" which will terminate bad performing trials early.

### **Main function**

At the first, I should say that I have used some search algorithms and schedulers (You can see them on my github, 6nd version file) and choose the best ones. I used the search algorithm of OptunaSearch, which is based on Bayesian optimization. In addition, ASHAScheduler as a scheduler plays an active role in reducing computational costs for me.

This is a part where the functions are finally one by one called. The optimization of the hyper-parameters begins:

```
def main (num samples=10, max num epochs=100, gpus per trial=2)
    # define data directory here if you want to load data from
 files
    data dir = os.path.abspath("./data")
    load data(data dir)
    # define the search space of hyperparameters
    confiq = {
        "act1 ": tune.choice(["relu", "tanh", "selu"]),
        "act2" : tune.choice(["relu", "tanh", "selu"]),
        "act3" : tune.choice(["relu","tanh","selu"]),
        "11": tune.choice([2**2,2**3,2**4,2**5,2**6,2**7,2**8]
), #tune.sample from(lambda : 2**np.random.randint(2, 8)),
        "12": tune.choice([2**2,2**3,2**4,2**5,2**6,2**7,2**8]
), #tune.sample from(lambda : 2**np.random.randint(2, 8)),
        "13": tune.choice([2**2,2**3,2**4,2**5,2**6,2**7,2**8]
), #tune.sample from(lambda : 2**np.random.randint(2, 8)),
        "lr": tune.quniform(0.0005, 0.001, 0.0001),
        "batch size": tune.choice([8, 16, 32]),
        "hidden dim1" : tune.guniform(150, 300, 10),
        "hidden dim2" : tune.quniform(150, 300, 10),
        "hidden dim3" : tune.quniform(150, 300, 10),
        "num layers" :tune.uniform(4,10)
    }
    # Optuna search algorithm
    from ray.tune.suggest.optuna import OptunaSearch
    from ray.tune.suggest import ConcurrencyLimiter
```

```
search alg = OptunaSearch(
        metric="score", #or accuracy, etc.
        mode="max", #or max
         seed = 42,
    search alg = ConcurrencyLimiter(search alg, max concurrent
=10)
    scheduler = ASHAScheduler(
        metric ="score",
        mode="max",
        max t=max num epochs,
        reduction factor=2,
        grace period=4,
        brackets=5
    reporter = CLIReporter(
        parameter_columns=["11", "12", "lr", "batch size"],
        metric columns=["score", "training iteration"]
    result = tune.run(
        partial(trainable func, data dir=data dir, epochs=max
num epochs),
        scheduler=scheduler,
        search alg=search alg,
        num samples=num samples,
        config=config,
        verbose=2,
        checkpoint score attr="score",
        checkpoint freq=0,
        keep checkpoints num=1,
        progress reporter=reporter,
        resources per trial={"cpu": 0.5, "gpu": gpus per trial
},
        stop={"training iteration": max num epochs},
        )
   best trial = result.get best trial("score", "max", "last")
    print("Best trial config: {}".format(best trial.config))
   print("Best trial final validation score: {}".format(
        best trial.last result["score"]))
   best trained model = Net(best trial.config)
    device = "cpu"
    if torch.cuda.is available():
```

```
device = "cuda:0"
        if gpus per trial > 1:
             best trained model = nn.DataParallel(best trained
model)
    best trained model.to(device)
   best checkpoint dir = best trial.checkpoint.value
   model state, optimizer state = torch.load(os.path.join(
       best checkpoint dir, "checkpoint"))
   best trained model.load state dict(model state)
    test score value = test score(best trial.config, best trained model
, device)
   print("Best trial test set score: {}".format(test score value))
if name == " main ":
    main(num samples=100, max num epochs=10, gpus per trial=0)
Best trial final validation score: 0.8190438871473355
Best trial test set score: 0.808862171931479
Best trial config = {'act1 ': 'tanh', 'act2': 'tanh', 'act3':
'tanh''lr': 0.0008, 'batch size': 16, 'hidden dim1': 130.0, 'h
idden dim2': 170.0, 'hidden dim3': 100.0, 'num layares':4}
```

# Train the neural network from the beginning and check the results

```
import random
random.seed(1234)
Best_trial_config = {'act1 ': 'tanh', 'act2': 'tanh', 'act3':
'tanh''lr': 0.0008, 'batch_size': 16, 'hidden_dim1': 130.0, 'h
idden_dim2': 170.0, 'hidden_dim3': 100.0, 'num_layares':4}
epochs = 10
config = {'act1 ': 'tanh', 'act2': 'tanh', 'act3': 'tanh''lr':
    0.0008, 'batch_size': 16, 'hidden_dim1': 130.0, 'hidden_dim2':
    170.0, 'hidden_dim3': 100.0, 'num_layares':4}

net = Net(Best_trial_config)
criterion = nn.CrossEntropyLoss()

# # Define an optimizer
optimizer = optim.Adam(net.parameters(), lr=config.get("lr",0.0003))
```

```
trainset, testset = load data()
    # Split the dataset into training and validation sets
train size = int(len(trainset) * 0.825)
train subset, val subset = random split(trainset, [train size,
len(trainset) - train size])
    # Define data loaders (which combines a dataset and a samp
ler, and provides an iterable over the given dataset)
trainloader = torch.utils.data.DataLoader(
    train subset,
   batch size=int(config.get("batch size", 32)),
    shuffle=False,
    num workers=2)
valloader = torch.utils.data.DataLoader(
    val subset,
   batch size=int(config.get("batch size", 32)),
    shuffle=False,
    num workers=2)
for epoch in range(epochs): # loop over the dataset multiple
times
        epoch train loss = 0.0
        # epoch steps = 0
        net.train() # Prepare model for training
        for i, data in enumerate(trainloader):
            # get the inputs; data is a list of [inputs, label
s]
            inputs, labels = data
            inputs, labels = inputs.to(device), labels.to(devi
ce)
            # zero the parameter gradients
            optimizer.zero grad()
            # forward + backward + optimize
            outputs = net(inputs)
            loss = criterion(outputs, labels)
            loss.backward()
            optimizer.step()
            Compute train loss without scaling to print
            1.1.1
        score = compute score(net, valloader, device="cpu")
        with tune.checkpoint dir(epoch) as checkpoint dir:
            path = os.path.join(checkpoint dir, "checkpoint")
```

Best trial final validation score: 0.8190438871473355

Best trial **test set score**: 0.808862171931479

Final result with best hyperparameters on test score: 0.788749847528569

## **Conclusion**

In this part I compare results of each search algorithms and schedulers in a table:

scheduler	MedianStoppingRule	MedianStoppingRule	HyperBandForBOHB
search algorithm	HyperOptSearch	OptunaSearch	OptunaSearch
validation	0.6823	0.6912	0.7651
score			
test set score	0.6654	0.7054	0.7421
rank	4	3	2

scheduler search algorithm	AsyncHyperBandScheduler HyperOptSearch	ASHAscheduler OptunaSearch
validation score	-	<mark>0.8190</mark>
test set score	-	0.8088
rank	Error	1

### Final words

I have learned significant and essential lessons from Dr.Taheri in this term.

Special Thanks to Professor Dr. Taheri for their efforts, guidance and patience.

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