[31]:
```
import numpy as np
import torch
import torch.nn as nn
from skorch import NeuralNetClassifier
import skorch.callbacks
from sklearn.datasets import make_classification
from sklearn.model_selection import train_test_split
from skopt import BayesSearchCV
from skopt.space import Real, Integer

# Neural network model
class NeuralNetwork(nn.Module):
    def __init__(self, input_size, hidden_size, output_size, dropout_rate=0.5):
        super(NeuralNetwork, self).__init__()
        self.fc1 = nn.Linear(input_size, hidden_size)
        self.relu = nn.ReLU()
        self.dropout = nn.Dropout(dropout_rate)
        self.fc2 = nn.Linear(hidden_size, output_size)

    def forward(self, x):
        x = self.fc1(x)
        x = self.relu(x)
        x = self.dropout(x)
        x = self.fc2(x)
        return x

# Function to create a model with specified parameters
def create_model(input_size, output_size):
    return NeuralNetClassifier(
        module=NeuralNetwork,
        module__input_size=input_size,
        module__hidden_size=100,  # Default which will be overwritten by␣
 ↪hyperparameter search
        module__output_size=output_size,
        module__dropout_rate=0.5,  # Default
        criterion=nn.CrossEntropyLoss,
        optimizer=torch.optim.Adam,
        optimizer__lr=0.001,  # Default
        max_epochs=20,
        batch_size=32,
        iterator_train__shuffle=True,
        callbacks=[('early_stopping', skorch.callbacks.
 ↪EarlyStopping(patience=5))]
    )

# Function to optimize hyperparameters using BayesSearchCV
def optimize_hyperparameters(X_train, y_train):
```

```
    model = create_model(input_size=X_train.shape[1],␣
↪output_size=len(set(y_train)))
    search = BayesSearchCV(
        estimator=model,
        search_spaces={
            'optimizer__lr': Real(1e-4, 1e-1, prior='log-uniform'),
            'module__hidden_size': Integer(32, 256),
            'module__dropout_rate': Real(0.1, 0.7),
        },
        n_iter=10,
        cv=3,  # Number of cross-validation folds
        verbose=1,
        n_jobs=1  # Set to 1 to avoid multiprocessing issues
    )
    search.fit(X_train.astype(np.float32), y_train)
    return search.best_params_

if __name__ == "__main__":
    X, y = make_classification(n_samples=1000, n_features=20, n_classes=2,␣
↪random_state=42)
    X_train, X_valid, y_train, y_valid = train_test_split(X, y, test_size=0.2,␣
↪random_state=42)

    best_params = optimize_hyperparameters(X_train, y_train)
    print("Best Parameters:", best_params)
```

```
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4774       0.8318        0.3849
0.1618
      2        0.3314       0.8598        0.3350
0.0462
      3        0.2699       0.8505        0.3514  0.0437
      4        0.2238       0.8692        0.3495  0.0428
      5        0.2394       0.8411        0.3874  0.0462
      6        0.2163       0.8411        0.3901  0.0477
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4517       0.8318        0.4349
0.0534
      2        0.3595       0.8224        0.4204  0.0475
      3        0.2581       0.8318        0.4209  0.0446
      4        0.2514       0.8318        0.3914  0.0500
      5        0.2093       0.8318        0.4406  0.0321
      6        0.1923       0.8318        0.4648  0.0342
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      7        0.2027       0.8505        0.5220  0.0324
      8        0.1809       0.8505        0.5412  0.0339
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4516       0.8318        0.4364
0.0329
      2        0.3100       0.8224        0.4214  0.0310
      3        0.2720       0.8505        0.4292  0.0361
      4        0.2563       0.8318        0.4604  0.0333
      5        0.2111       0.8131        0.4517  0.0312
      6        0.1994       0.8224        0.5041  0.0424
Stopping since valid_loss has not improved in the last 5 epochs.
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.9875       0.7757        0.9963
0.0331
      2        0.8426       0.8785        0.5673
0.0325
      3        1.1480       0.8411        0.8351  0.0364
      4        1.1647       0.8318        1.0225  0.0316
      5        0.7276       0.8411        0.7115  0.0362
      6        0.8681       0.8037        1.1388  0.0320
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.8345       0.8411        0.8864
0.0323
      2        0.8252       0.8131        1.0606  0.0314
      3        1.0101       0.8037        1.3406  0.0357
      4        1.0520       0.8318        1.1713  0.0404
      5        0.9740       0.8318        0.9944  0.0407
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.9239       0.8131        1.2600
0.0353
      2        0.9059       0.8318        1.0087
0.0331
      3        1.0176       0.8318        1.1252  0.0326
      4        0.7439       0.8037        1.0778  0.0324
      5        0.7708       0.8037        1.1004  0.0321
      6        0.8085       0.8411        1.1549  0.0322
Stopping since valid_loss has not improved in the last 5 epochs.
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
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      1        0.6431       0.8131        0.5368
0.0317
      2        0.3523       0.7290        0.7395  0.0290
      3        0.4897       0.8131        0.6685  0.0294
      4        0.3095       0.7944        0.7928  0.0310
      5        0.2530       0.7944        0.7050  0.0410
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.5885       0.7850        0.6467
0.0316
      2        0.4427       0.8037        0.6040
0.0365
      3        0.3425       0.8318        0.7065  0.0316
      4        0.3455       0.7944        0.5448  0.0302
      5        0.2620       0.7664        0.7075  0.0304
      6        0.2786       0.8037        0.7855  0.0300
      7        0.2578       0.8224        0.6089  0.0321
      8        0.2184       0.7944        0.8412  0.0297
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.6869       0.7944        0.5734
0.0314
      2        0.3445       0.8318        0.5745  0.0298
      3        0.2623       0.7944        0.5628  0.0302
      4        0.2231       0.8318        0.6114  0.0302
      5        0.2140       0.8131        0.7725  0.0324
      6        0.2665       0.7944        0.8947  0.0295
      7        0.2491       0.8037        1.2029  0.0299
Stopping since valid_loss has not improved in the last 5 epochs.
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4683       0.8318        0.4944
0.0337
      2        0.3702       0.8224        0.4048  0.0300
      3        0.3329       0.8131        0.4892  0.0302
      4        0.2972       0.8318        0.4267  0.0306
      5        0.3121       0.8505        0.3801  0.0322
      6        0.2110       0.8037        0.4916  0.0299
      7        0.2240       0.8131        0.6064  0.0292
      8        0.2175       0.8318        0.5466  0.0345
      9        0.2690       0.8131        0.5958  0.0422
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4340       0.7944        0.4836
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0.0306
      2        0.3745       0.8411        0.4646
0.0324
      3        0.2885       0.8224        0.4892  0.0303
      4        0.3438       0.8598        0.5011  0.0300
      5        0.3017       0.8505        0.5018  0.0293
      6        0.3324       0.8318        0.6008  0.0309
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4764       0.8411        0.5556
0.0325
      2        0.4070       0.8318        0.5440  0.0317
      3        0.3044       0.8224        0.4831  0.0291
      4        0.3587       0.8318        0.5538  0.0467
      5        0.3248       0.8411        0.5159  0.0375
      6        0.2531       0.8131        0.4695  0.0348
      7        0.2952       0.8224        0.6950  0.0348
      8        0.2368       0.8224        0.6389  0.0331
      9        0.2357       0.7944        0.6973  0.0317
     10        0.2435       0.7944        0.7404  0.0318
Stopping since valid_loss has not improved in the last 5 epochs.
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.5377       0.8505        0.3855
0.0335
      2        0.3316       0.8598        0.3307
0.0281
      3        0.3113       0.8598        0.3464  0.0324
      4        0.2689       0.8411        0.3507  0.0297
      5        0.2414       0.8318        0.3530  0.0311
      6        0.2173       0.8318        0.3599  0.0300
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.5240       0.7850        0.4000
0.0412
      2        0.3258       0.8224        0.3768
0.0333
      3        0.2921       0.8411        0.3742
0.0306
      4        0.2439       0.8411        0.3943  0.0289
      5        0.2311       0.8131        0.4000  0.0299
      6        0.2375       0.8505        0.3932  0.0310
      7        0.2232       0.8598        0.3990  0.0323
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
```

```
-------  ------------  -----------  ------------  ------
      1        0.5789       0.8131        0.4216
0.0352
      2        0.3405       0.8224        0.4350  0.0306
      3        0.3116       0.8318        0.4473  0.0291
      4        0.2550       0.8411        0.4212
0.0306
      5        0.2424       0.8411        0.3987  0.0341
      6        0.2314       0.8411        0.4334  0.0324
      7        0.2191       0.8411        0.4296  0.0325
      8        0.1962       0.8411        0.4456  0.0337
      9        0.1797       0.8411        0.4566  0.0303
Stopping since valid_loss has not improved in the last 5 epochs.
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.6825       0.6916        0.6391
0.0305
      2        0.6909       0.7290        0.6192  0.0320
      3        0.6534       0.7570        0.6018
0.0314
      4        0.6213       0.7850        0.5857
0.0344
      5        0.6029       0.8037        0.5710
0.0338
      6        0.5916       0.8224        0.5567
0.0314
      7        0.5849       0.8318        0.5437
0.0309
      8        0.5829       0.8505        0.5317
0.0340
      9        0.5316       0.8598        0.5206
0.0313
     10        0.5307       0.8598        0.5097  0.0315
     11        0.5387       0.8692        0.4991  0.0423
     12        0.5112       0.8879        0.4898
0.0342
     13        0.5204       0.8879        0.4808  0.0311
     14        0.4876       0.8879        0.4721  0.0317
     15        0.4910       0.8879        0.4636  0.0316
     16        0.4730       0.8972        0.4557
0.0354
     17        0.4805       0.8972        0.4487  0.0382
     18        0.4661       0.8879        0.4425  0.0381
     19        0.4490       0.8879        0.4366  0.0471
     20        0.4493       0.8879        0.4307  0.0384
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
```

```
      1        0.7533       0.4579        0.7237
0.0286
      2        0.7238       0.5234        0.6981
0.0320
      3        0.7245       0.6262        0.6741  0.0394
      4        0.6723       0.6636        0.6516
0.0288
      5        0.6563       0.7009        0.6307
0.0330
      6        0.6324       0.7290        0.6127
0.0305
      7        0.6121       0.7570        0.5960
0.0306
      8        0.6014       0.7757        0.5810
0.0318
      9        0.5698       0.7757        0.5669  0.0301
     10        0.5694       0.7850        0.5540
0.0339
     11        0.5590       0.7944        0.5418
0.0337
     12        0.5531       0.8224        0.5306
0.0320
     13        0.5129       0.8318        0.5201
0.0310
     14        0.5134       0.8224        0.5102  0.0367
     15        0.4922       0.8224        0.5013  0.0462
     16        0.4925       0.8224        0.4926  0.0312
     17        0.4908       0.8318        0.4848  0.0380
     18        0.4698       0.8131        0.4770  0.0378
     19        0.4629       0.8037        0.4699  0.0319
     20        0.4672       0.7944        0.4634  0.0302
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.7109       0.5794        0.6842
0.0309
      2        0.6944       0.6262        0.6599
0.0308
      3        0.6613       0.6729        0.6376
0.0305
      4        0.6504       0.7196        0.6185
0.0321
      5        0.6355       0.7477        0.6011
0.0306
      6        0.6079       0.7570        0.5857
0.0344
      7        0.5984       0.7757        0.5718
0.0311
      8        0.5612       0.7850        0.5591
```

```
0.0304
      9        0.5743       0.7850        0.5469  0.0295
     10        0.5388       0.7757        0.5360  0.0340
     11        0.5320       0.7664        0.5255  0.0354
     12        0.5241       0.7664        0.5160  0.0321
     13        0.5220       0.7757        0.5074  0.0306
     14        0.4826       0.7944        0.4990
0.0307
     15        0.4871       0.7944        0.4911  0.0323
     16        0.4878       0.8131        0.4845  0.0373
     17        0.4649       0.8131        0.4777  0.0303
     18        0.4523       0.8131        0.4718  0.0361
     19        0.4593       0.8131        0.4659  0.0304
     20        0.4416       0.8131        0.4602  0.0299
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4613       0.8692        0.3578
0.0273
      2        0.3144       0.8692        0.3259  0.0304
      3        0.2795       0.8318        0.3516  0.0334
      4        0.2354       0.8411        0.3637  0.0306
      5        0.2240       0.8411        0.3754  0.0371
      6        0.2019       0.8411        0.3951  0.0337
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4675       0.7944        0.3785
0.0322
      2        0.3163       0.8411        0.3732
0.0298
      3        0.2646       0.8411        0.3664  0.0310
      4        0.2467       0.8318        0.3758  0.0355
      5        0.2362       0.8318        0.3809  0.0310
      6        0.2135       0.7944        0.3999  0.0315
      7        0.1989       0.8318        0.4056  0.0305
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4949       0.8318        0.4102
0.0341
      2        0.3048       0.8224        0.4293  0.0309
      3        0.2814       0.8411        0.4157  0.0312
      4        0.2535       0.8318        0.4246  0.0334
      5        0.2332       0.8318        0.4263  0.0352
Stopping since valid_loss has not improved in the last 5 epochs.
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
```

```
-------  ------------  -----------  ------------  ------
      1        0.6068       0.8505        0.5045
0.0364
      2        0.4546       0.8505        0.4243  0.0308
      3        0.3876       0.8505        0.3778  0.0327
      4        0.3476       0.8692        0.3545
0.0304
      5        0.3116       0.8692        0.3415  0.0303
      6        0.3015       0.8598        0.3308  0.0327
      7        0.2899       0.8505        0.3278  0.0298
      8        0.2663       0.8598        0.3329  0.0296
      9        0.2669       0.8411        0.3402  0.0312
     10        0.2493       0.8411        0.3392  0.0318
     11        0.2331       0.8318        0.3402  0.0297
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.6087       0.7757        0.4982
0.0330
      2        0.4275       0.8037        0.4304
0.0348
      3        0.3548       0.8131        0.3983
0.0288
      4        0.3140       0.8224        0.3815
0.0302
      5        0.2897       0.8318        0.3729
0.0289
      6        0.2643       0.8318        0.3692  0.0368
      7        0.2854       0.8411        0.3660  0.0316
      8        0.2676       0.8318        0.3661  0.0294
      9        0.2613       0.8318        0.3708  0.0292
     10        0.2418       0.8411        0.3705  0.0333
     11        0.2297       0.8505        0.3754  0.0367
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.6248       0.8037        0.5067
0.0296
      2        0.4438       0.8131        0.4232
0.0303
      3        0.3626       0.8224        0.3993
0.0322
      4        0.3297       0.8224        0.3972  0.0301
      5        0.2892       0.8131        0.3997  0.0296
      6        0.2799       0.8131        0.4054  0.0292
      7        0.2730       0.8131        0.4096  0.0315
      8        0.2556       0.8224        0.4146  0.0299
Stopping since valid_loss has not improved in the last 5 epochs.
```

```
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.6171       0.8224        0.5132
0.0309
      2        0.4671       0.8692        0.4324
0.0305
      3        0.3875       0.8692        0.3811  0.0304
      4        0.3461       0.8598        0.3569  0.0302
      5        0.3224       0.8692        0.3388  0.0307
      6        0.2975       0.8692        0.3313  0.0318
      7        0.2863       0.8692        0.3277  0.0462
      8        0.2762       0.8598        0.3290  0.0296
      9        0.2670       0.8411        0.3340  0.0313
     10        0.2556       0.8505        0.3326  0.0304
     11        0.2508       0.8411        0.3312  0.0327
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.6040       0.7570        0.5373
0.0356
      2        0.4598       0.7757        0.4609
0.0330
      3        0.3862       0.8131        0.4177
0.0316
      4        0.3338       0.8131        0.3988  0.0348
      5        0.3087       0.8037        0.3881  0.0337
      6        0.2842       0.8224        0.3817
0.0341
      7        0.2697       0.8411        0.3798
0.0379
      8        0.2644       0.8131        0.3804  0.0319
      9        0.2519       0.8318        0.3810  0.0304
     10        0.2407       0.8224        0.3850  0.0320
     11        0.2270       0.8224        0.3893  0.0299
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.6328       0.8037        0.5283
0.0306
      2        0.4655       0.8037        0.4383  0.0325
      3        0.3773       0.8131        0.3961
0.0306
      4        0.3308       0.8224        0.3803
0.0312
      5        0.3071       0.8224        0.3788  0.0302
      6        0.2885       0.8224        0.3775  0.0356
      7        0.2709       0.8224        0.3837  0.0295
```

```
      8        0.2545       0.8224        0.3845  0.0314
      9        0.2597       0.8224        0.3869  0.0311
     10        0.2463       0.8224        0.3895  0.0329
Stopping since valid_loss has not improved in the last 5 epochs.
Fitting 3 folds for each of 1 candidates, totalling 3 fits
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4499       0.8692        0.3514
0.0825
      2        0.3041       0.8411        0.3904  0.0412
      3        0.2742       0.8131        0.3956  0.0421
      4        0.2335       0.8318        0.4066  0.0397
      5        0.2439       0.8224        0.4104  0.0416
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4856       0.8598        0.3744
0.0414
      2        0.3132       0.8131        0.4617  0.0371
      3        0.2819       0.8131        0.4207  0.0429
      4        0.2322       0.8131        0.4249  0.0486
      5        0.2037       0.8505        0.4398  0.0375
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.4694       0.8131        0.5142
0.0421
      2        0.3223       0.8224        0.5106
0.0462
      3        0.3008       0.8318        0.4228
0.0457
      4        0.2799       0.8318        0.4583  0.0497
      5        0.2295       0.8411        0.4723  0.0374
      6        0.1945       0.8411        0.4996  0.0394
      7        0.1988       0.8224        0.5272  0.0409
Stopping since valid_loss has not improved in the last 5 epochs.
  epoch    train_loss    valid_acc    valid_loss     dur
-------  ------------  -----------  ------------  ------
      1        0.6143       0.8187        0.4987
0.0791
      2        0.4343       0.8250        0.3978
0.0669
      3        0.3557       0.8250        0.3598  0.0653
      4        0.3208       0.8438        0.3506
0.0607
      5        0.3037       0.8562        0.3481
0.0595
      6        0.2960       0.8500        0.3475  0.0647
```

```
      7        0.2781       0.8562        0.3467  0.0630
      8        0.2708       0.8562        0.3482  0.0624
      9        0.2664       0.8562        0.3460  0.0684
     10        0.2582       0.8625        0.3442
0.0703
     11        0.2568       0.8500        0.3459  0.0580
     12        0.2417       0.8625        0.3491  0.0615
     13        0.2345       0.8625        0.3507  0.0603
     14        0.2241       0.8562        0.3487  0.0601
Stopping since valid_loss has not improved in the last 5 epochs.
Best Parameters: OrderedDict([('module__dropout_rate', 0.13851697056139806),
('module__hidden_size', 214), ('optimizer__lr', 0.0011736445950409776)])
```