Hyperparameter Tuning for PyTorch With `spotPython`: Regression

In this tutorial, we will show how `spotPython` can be integrated into the `PyTorch` training workflow.

This document refers to the following software versions:

- `python`: 3.10.10
- `torch`: 2.0.1
- `torchvision`: 0.15.0
- `spotPython`: 0.2.15

`spotPython` can be installed via pip[1].

```
!pip install spotPython
```

Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time, initial design size and the device that is used.

```
MAX_TIME = 10
INIT_SIZE = 20
DEVICE = "cpu" # "cuda:0"
```

Initialization of the `fun_control` Dictionary

`spotPython` uses a Python dictionary for storing the information required for the hyperparameter tuning process. This dictionary is called `fun_control` and is initialized with the function `fun_control_init`. The function `fun_control_init` returns a skeleton dictionary. The dictionary is filled with the required information for the hyperparameter tuning process. It stores the hyperparameter tuning settings, e.g., the deep learning network architecture that should be tuned, the classification (or regression) problem, and the data that is used for the tuning. The dictionary is used as an input for the SPOT function.

```
from spotPython.utils.init import fun_control_init
fun_control = fun_control_init(task="regression",
 tensorboard_path="runs/24_spot_torch_regression")
```

[1]Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

PyTorch Data Loading

```python
# Create dataset
import pandas as pd
import numpy as np
from sklearn import datasets as sklearn_datasets
from sklearn.preprocessing import MinMaxScaler
from sklearn.model_selection import train_test_split
X, y = sklearn_datasets.make_regression(
    n_samples=1000, n_features=10, noise=1, random_state=123)
y = y.reshape(-1, 1)

# Normalize the data
X_scaler = MinMaxScaler()
X_scaled = X_scaler.fit_transform(X)
y_scaler = MinMaxScaler()
y_scaled = y_scaler.fit_transform(y)

# combine the features and target into a single dataframe named train_df
train_df = pd.DataFrame(np.hstack((X_scaled, y_scaled)))

target_column = "y"
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column,
    axis=1),
    train_df[target_column],
    random_state=42,
    test_size=0.25)
trainset = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
testset = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
trainset.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
testset.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
print(trainset.shape)
print(testset.shape)
```

```python
import torch
from spotPython.torch.dataframedataset import DataFrameDataset
```

```
dtype_x = torch.float32
dtype_y = torch.float32
train_df = DataFrameDataset(train_df, target_column=target_column,
    dtype_x=dtype_x, dtype_y=dtype_y)
train = DataFrameDataset(trainset, target_column=target_column,
    dtype_x=dtype_x, dtype_y=dtype_y)
test = DataFrameDataset(testset, target_column=target_column,
    dtype_x=dtype_x, dtype_y=dtype_y)
n_samples = len(train)
```

- Now we can test the data loading:

```
from spotPython.torch.traintest import create_train_val_data_loaders
trainloader, testloader = create_train_val_data_loaders(train, 2, True, 0)
for i, data in enumerate(trainloader, 0):
    inputs, labels = data
    print(inputs.shape)
    print(labels.shape)
    print(inputs)
    print(labels)
    break
```

- Since this works fine, we can add the data loading to the `fun_control` dictionary:

```
# add the dataset to the fun_control
fun_control.update({"data": train_df, # full dataset,
               "train": train,
               "test": test,
               "n_samples": n_samples,
               "target_column": target_column,})
```

Specification of the Preprocessing Model

After the training and test data are specified and added to the `fun_control` dictionary, `spotPython` allows the specification of a data preprocessing pipeline, e.g., for the scaling of the data or for the one-hot encoding of categorical variables. The preprocessing model is called `prep_model` ("preparation" or pre-processing) and includes steps that are not subject to the hyperparameter tuning process. The preprocessing model is specified in the `fun_control` dictionary. The preprocessing model can be implemented as a `sklearn` pipeline. The following code shows a typical preprocessing pipeline:

```
categorical_columns = ["cities", "colors"]
one_hot_encoder = OneHotEncoder(handle_unknown="ignore",
                                    sparse_output=False)
prep_model = ColumnTransformer(
        transformers=[
             ("categorical", one_hot_encoder, categorical_columns),
         ],
         remainder=StandardScaler(),
     )
```

```
fun_control.update({"prep_model": None})
```

Select `algorithm` and `core_model_hyper_dict`

Implementing a Configurable Neural Network With spotPython

`spotPython` includes the `Net_lin_reg` class which is implemented in the file `netregression.py`.

```
from torch import nn
import spotPython.torch.netcore as netcore


class Net_lin_reg(netcore.Net_Core):
    def __init__(
        self, _L_in, _L_out, l1, dropout_prob, lr_mult,
        batch_size, epochs, k_folds, patience, optimizer,
        sgd_momentum
    ):
        super(Net_lin_reg, self).__init__(
            lr_mult=lr_mult,
            batch_size=batch_size,
            epochs=epochs,
            k_folds=k_folds,
            patience=patience,
            optimizer=optimizer,
            sgd_momentum=sgd_momentum,
        )
        l2 = max(l1 // 2, 4)
        self.fc1 = nn.Linear(_L_in, l1)
        self.fc2 = nn.Linear(l1, l2)
        self.fc3 = nn.Linear(l2, _L_out)
        self.relu = nn.ReLU()
        self.softmax = nn.Softmax(dim=1)
        self.dropout1 = nn.Dropout(p=dropout_prob)
        self.dropout2 = nn.Dropout(p=dropout_prob / 2)

    def forward(self, x):
        x = self.fc1(x)
        x = self.relu(x)
        x = self.dropout1(x)
        x = self.fc2(x)
        x = self.relu(x)
        x = self.dropout2(x)
        x = self.fc3(x)
        return x
```

The `Net_Core` class

`Net_lin_reg` inherits from the class `Net_Core` which is implemented in the file `netcore.py`. It implements the additional attributes that are common to all neural network models. The `Net_Core` class is implemented in the file `netcore.py`. It implements hyperparameters as attributes, that are not used by the `core_model`, e.g.:

- optimizer (`optimizer`),
- learning rate (`lr`),
- batch size (`batch_size`),
- epochs (`epochs`),
- k_folds (`k_folds`), and
- early stopping criterion "patience" (`patience`).

Users can add further attributes to the class. The class `Net_Core` is shown below.

```
from torch import nn


class Net_Core(nn.Module):
    def __init__(self, lr_mult, batch_size, epochs, k_folds, patience,
    optimizer, sgd_momentum):
        super(Net_Core, self).__init__()
        self.lr_mult = lr_mult
        self.batch_size = batch_size
        self.epochs = epochs
        self.k_folds = k_folds
        self.patience = patience
        self.optimizer = optimizer
        self.sgd_momentum = sgd_momentum
```

:::{.callout-note}

We see that the class `Net_lin_reg` has additional attributes and does not inherit from `nn` directly. It adds an additional class, `Net_core`, that takes care of additional attributes that are common to all neural network models, e.g., the learning rate multiplier `lr_mult` or the batch size `batch_size`.

`spotPython`'s `core_model` implements an instance of the `Net_lin_reg` class. In addition to the basic neural network model, the `core_model` can use these additional attributes. `spotPython` provides methods for handling these additional attributes to guarantee 100% compatibility with the `PyTorch` classes. The method `add_core_model_to_fun_control` adds the hyper-parameters and additional attributes to the `fun_control` dictionary. The method is shown below.

```
from spotPython.torch.netregression import Net_lin_reg
from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
core_model = Net_lin_reg
fun_control = add_core_model_to_fun_control(core_model=core_model,
                              fun_control=fun_control,
                              hyper_dict=TorchHyperDict,
                              filename=None)
```

The Search Space

Configuring the Search Space With spotPython

The `hyper_dict` Hyperparameters for the Selected Algorithm

`spotPython` uses `JSON` files for the specification of the hyperparameters. Users can specify their individual `JSON` files, or they can use the `JSON` files provided by `spotPython`. The `JSON` file for the `core_model` is called `torch_hyper_dict.json`.

`spotPython` can handle numerical, boolean, and categorical hyperparameters. They can be specified in the `JSON` file in a similar way as the numerical hyperparameters as shown below.

Each entry in the JSON file represents one hyperparameter with the following structure: type, default, transform, lower, and upper.

```
"factor_hyperparameter": {
    "levels": ["A", "B", "C"],
    "type": "factor",
    "default": "B",
    "transform": "None",
    "core_model_parameter_type": "str",
    "lower": 0,
    "upper": 2},
```

The corresponding entries for the Net_lin_reg class are shown below.

```
    "Net_lin_reg":
    {
        "_L_in": {
            "type": "int",
            "default": 10,
            "transform": "None",
            "lower": 10,
            "upper": 10},
        "_L_out": {
            "type": "int",
            "default": 1,
            "transform": "None",
            "lower": 1,
            "upper": 1},
        "l1": {
            "type": "int",
            "default": 3,
            "transform": "transform_power_2_int",
            "lower": 3,
            "upper": 8},
        "dropout_prob": {
            "type": "float",
            "default": 0.01,
            "transform": "None",
            "lower": 0.0,
            "upper": 0.9},
        "lr_mult": {
            "type": "float",
            "default": 1.0,
            "transform": "None",
            "lower": 0.1,
            "upper": 10.0},
        "batch_size": {
            "type": "int",
            "default": 4,
            "transform": "transform_power_2_int",
            "lower": 1,
            "upper": 4},
        "epochs": {
            "type": "int",
            "default": 4,
            "transform": "transform_power_2_int",
            "lower": 4,
            "upper": 9},
        "k_folds": {
            "type": "int",
            "default": 1,
            "transform": "None",
            "lower": 1,
            "upper": 1},
        "patience": {
            "type": "int",
            "default": 2,
            "transform": "transform_power_2_int",
            "lower": 1,
            "upper": 5
        },
        "optimizer": {
            "levels": ["Adadelta",
                       "Adagrad",
                       "Adam",
                       "AdamW",
                       "SparseAdam",
                       "Adamax",
                       "ASGD",
                       "NAdam",
                       "RAdam",
                       "RMSprop",
                       "Rprop",
                     "SGD"],
            "type": "factor",
            "default": "SGD",
            "transform": "None",
            "class_name": "torch.optim",
            "core_model_parameter_type": "str",
            "lower": 0,
            "upper": 12},
        "sgd_momentum": {
            "type": "float",
            "default": 0.0,
            "transform": "None",
            "lower": 0.0,
            "upper": 1.0}
    },
```

Modifying the Hyperparameters

`spotPython` provides functions for modifying the hyperparameters, their bounds and factors as well as for activating and de-activating hyperparameters without re-compilation of the Python source code. These functions are described in the following.

Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

After specifying the model, the corresponding hyperparameters, their types and bounds are loaded from the `JSON` file `torch_hyper_dict.json`. After loading, the user can modify the hyperparameters, e.g., the bounds. `spotPython` provides a simple rule for de-activating hyperparameters: If the lower and the upper bound are set to identical values, the hyperparameter is de-activated. This is useful for the hyperparameter tuning, because it allows to specify a hyperparameter in the `JSON` file, but to de-activate it in the `fun_control` dictionary. This is done in the next step.

Modify Hyperparameters of Type numeric and integer (boolean)

Since the hyperparameter `k_folds` is not used in the `PyTorch` tutorial, it is de-activated here by setting the lower and upper bound to the same value. Note, `k_folds` is of type "integer".

```python
# modify the hyperparameter levels

from spotPython.hyperparameters.values import modify_hyper_parameter_bounds

fun_control = modify_hyper_parameter_bounds(fun_control, "epochs", bounds=[2, 16])
fun_control = modify_hyper_parameter_bounds(fun_control, "patience", bounds=[3, 7])
```

Modify Hyperparameter of Type factor

In a similar manner as for the numerical hyperparameters, the categorical hyperparameters can be modified. New configurations can be chosen by adding or deleting levels. For example, the hyperparameter `optimizer` can be re-configured as follows:

In the following setting, two optimizers (`"SGD"` and `"Adam"`) will be compared during the `spotPython` hyperparameter tuning. The hyperparameter `optimizer` is active.

```python
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
fun_control = modify_hyper_parameter_levels(fun_control, "optimizer",
    ["SGD", "Adam"])
```

The hyperparameter `optimizer` can be de-activated by choosing only one value (level), here: `"SGD"`.

```python
fun_control = modify_hyper_parameter_levels(fun_control, "optimizer", ["SGD"])
```

As discussed in Section , there are some issues with the LBFGS optimizer. Therefore, the usage of the LBFGS optimizer is not deactivated in `spotPython` by default. However, the LBFGS optimizer can be activated by adding it to the list of optimizers. `Rprop` was removed, because it does perform very poorly (as some pre-tests have shown). However, it can also be activated by adding it to the list of optimizers. Since `SparseAdam` does not support dense gradients, `Adam` was used instead. Therefore, there are 10 default optimizers:

```python
fun_control = modify_hyper_parameter_levels(fun_control, "optimizer",
    ["Adadelta", "Adagrad", "Adam", "AdamW", "Adamax", "ASGD", "NAdam"])


fun_control.update({
               "_L_in": n_features,
               "_L_out": 1,})
```

Optimizers

Table 1 shows some of the optimizers available in `PyTorch`:

Table 1: Optimizers available in PyTorch (selection). “mom” denotes `momentum`, “weight” `weight_decay`, “damp” `dampening`, “nest” `nesterov`, “lr_sc” `learning rate for scaling delta`, “mom_dec” for `momentum_decay`, and “step_s” for `step_sizes`. The default values are shown in the table.

Optimizer	lr	mom	weight	damp	nest	rho	lr_sc	lr_decay	betas	lambd	alpha	mom_decay	etas	step_s
Adadelta	-	-	0.	-	-	0.9	1.0	-	-	-	-	-	-	-
Adagrad	1e-2	-	0.	-	-	-	-	0.	-	-	-	-	-	-
Adam	1e-3	-	0.	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-
AdamW	1e-3	-	1e-2	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-
SparseAdam	1e-3	-	-	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-
Adamax	2e-3	-	0.	-	-	-	-	-	(0.9, 0.999)	-	-	-	-	-
ASGD	1e-2	0.9	0.	-	False	-	-	-	-	1e-4	0.75	-	-	-
LBFGS	1.	-	-	-	-	-	-	-	-	-	-	-	-	-
NAdam	2e-3	-	0.	-	-	-	-	-	(0.9,0.999)	-	-	0	-	-
RAdam	1e-3	-	0.	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-
RMSprop	1e-2	0.	0.	-	-	-	-	-	(0.9,0.999)	-	-	-	-	-
Rprop	1e-2	-	-	-	-	-	-	-	-	-	(0.5,1.2)	(1e-6, 50)	-	-
SGD	required	0.	0.	0.	False	-	-	-	-	-	-	-	-	-

`spotPython` implements an `optimization` handler that maps the optimizer names to the corresponding `PyTorch` optimizers.

A note on LBFGS

We recommend deactivating `PyTorch`'s LBFGS optimizer, because it does not perform very well. The `PyTorch` documentation, see https://pytorch.org/docs/stable/generated/torch.optim.LBFGS.html#torch.optim.LBFGS, states:

> This is a very memory intensive optimizer (it requires additional `param_bytes * (history_size + 1)` bytes). If it doesn't fit in memory try reducing the history size, or use a different algorithm.

Furthermore, the LBFGS optimizer is not compatible with the `PyTorch` tutorial. The reason is that the LBFGS optimizer requires the `closure` function, which is not implemented in the `PyTorch` tutorial. Therefore, the `LBFGS` optimizer is recommended here.

Since there are 10 optimizers in the portfolio, it is not recommended tuning the hyperparameters that effect one single optimizer only.

A note on the learning rate

`spotPython` provides a multiplier for the default learning rates, `lr_mult`, because optimizers use different learning rates. Using a multiplier for the learning rates might enable a simultaneous tuning of the learning rates for all optimizers. However, this is not recommended, because the learning rates are not comparable across optimizers. Therefore, we recommend fixing the learning rate for all optimizers if multiple optimizers are used. This can be done by setting the lower and upper bounds of the learning rate multiplier to the same value as shown below.

Thus, the learning rate, which affects the `SGD` optimizer, will be set to a fixed value. We choose the default value of `1e-3` for the learning rate, because it is used in other `PyTorch` examples (it is also the default value used by `spotPython` as defined in the `optimizer_handler()` method). We recommend tuning the learning rate later, when a reduced set of optimizers is fixed. Here, we will demonstrate how to select in a screening phase the optimizers that should be used for the hyperparameter tuning.

For the same reason, we will fix the `sgd_momentum` to `0.9`.

```
fun_control = modify_hyper_parameter_bounds(fun_control,
    "lr_mult", bounds=[1e-3, 1e-3])
fun_control = modify_hyper_parameter_bounds(fun_control,
    "sgd_momentum", bounds=[0.9, 0.9])
```

Evaluation

The evaluation procedure requires the specification of two elements:

1. the way how the data is split into a train and a test set and
2. the loss function (and a metric).

Hold-out Data Split and Cross-Validation

As a default, `spotPython` provides a standard hold-out data split and cross validation.

Hold-out Data Split

If a hold-out data split is used, the data will be partitioned into a training, a validation, and a test data set. The split depends on the setting of the `eval` parameter. If `eval` is set to `train_hold_out`, one data set, usually the original training data set, is split into a new training and a validation data set. The training data set is used for training the model. The validation data set is used for the evaluation of the hyperparameter configuration and early stopping to prevent overfitting. In this case, the original test data set is not used. The following splits are performed in the hold-out setting: $\{\text{train}_0, \text{test}\} \rightarrow \{\text{train}_1, \text{validation}_1, \text{test}\}$, where $\text{train}_1 \cup \text{validation}_1 = \text{train}_0$.

Note

`spotPython` returns the hyperparameters of the machine learning and deep learning models, e.g., number of layers, learning rate, or optimizer, but not the model weights. Therefore, after the SPOT run is finished, the corresponding model with the optimized architecture has to be trained again with the best hyperparameter configuration. The training is performed on the training data set. The test data set is used for the final evaluation of the model.
Summarizing, the following splits are performed in the hold-out setting:

1. Run `spotPython` with `eval` set to `train_hold_out` to determine the best hyperparameter configuration.
2. Train the model with the best hyperparameter configuration ("architecture") on the training data set:
   - `train_tuned(model_spot, train, "model_spot.pt")`.
3. Test the model on the test data:
   - `test_tuned(model_spot, test, "model_spot.pt")`

These steps will be exemplified in the following sections.

In addition to this `hold-out` setting, `spotPython` provides another hold-out setting, where an explicit test data is specified by the user that will be used as the validation set. To choose this option, the `eval` parameter is set to `test_hold_out`. In this case, the training data set is used for the model training. Then, the explicitly defined test data set is used for the evaluation of the hyperparameter configuration (the validation).

Cross-Validation

The cross validation setting is used by setting the `eval` parameter to `train_cv` or `test_cv`. In both cases, the data set is split into k folds. The model is trained on $k-1$ folds and evaluated on the remaining fold. This is repeated k times, so that each fold is used exactly once for evaluation. The final evaluation is performed on the test data set. The cross validation setting is useful for small data sets, because it allows to use all data for training and evaluation. However, it is computationally expensive, because the model has to be trained k times.

Note

Combinations of the above settings are possible, e.g., cross validation can be used for training and hold-out for evaluation or *vice versa*. Also, cross validation can be used for training and testing. Because cross validation is not used in the `PyTorch` tutorial (PyTorch 2023), it is not considered further here.

Overview of the Evaluation Settings

Settings for the Hyperparameter Tuning

Table 2 provides an overview of the training evaluations.

Table 2: Overview of the evaluation settings.

eval	train	test	function	comment
`"train_hold_out"`	✓		`train_one_epoch()`, `validate_one_epoch()` for early stopping	splits the `train` data set internally
`"test_hold_out"`	✓	✓	`train_one_epoch()`, `validate_one_epoch()` for early stopping	use the `test data set` for `validate_one_epoch()`
`"train_cv"`	✓		`evaluate_cv(net, train)`	CV using the `train` data set

eval	train	test	function	comment
"test_cv"		✓	evaluate_cv(net, test)	CV using the test data set . Identical to "train_cv", uses only test data.

- "train_cv" and "test_cv" use sklearn.model_selection.KFold() internally.

Settings for the Final Evaluation of the Tuned Architecture

Training of the Tuned Architecture

train_tuned(model, train): train the model with the best hyperparameter configuration (or simply the default) on the training data set. It splits the traindata into new train and validation sets using create_train_val_data_loaders(), which calls torch.utils.data.random_split() internally. Currently, 60% of the data is used for training and 40% for validation. The train data is used for training the model with train_one_epoch(). The validation data is used for early stopping using validate_one_epoch() on the validation data set.

Testing of the Tuned Architecture

test_tuned(model, test): test the model on the test data set. No data splitting is performed. The (trained) model is evaluated using the validate_one_epoch() function.

Note: During training, shuffle is set to True, whereas during testing, shuffle is set to False.

Loss Functions and Metrics

The key "loss_function" specifies the loss function which is used during the optimization. There are several different loss functions under PyTorch's nn package. For example, a simple loss is MSELoss, which computes the mean-squared error between the output and the target. In this tutorial we will use CrossEntropyLoss, because it is also used in the PyTorch tutorial.

Loss Function

The loss function is specified by the key "loss_function". We will use MSE loss for the regression task.

```
from torch.nn import MSELoss
loss_torch = MSELoss()
fun_control.update({"loss_function": loss_torch})
```

In addition to the loss functions, `spotPython` provides access to a large number of metrics.

- The key `"metric_sklearn"` is used for metrics that follow the `scikit-learn` conventions.
- The key `"river_metric"` is used for the river based evaluation (Montiel et al. 2021) via `eval_oml_iter_progressive`, and
- the key `"metric_torch"` is used for the metrics from `TorchMetrics`.

`TorchMetrics` is a collection of more than 90 PyTorch metrics[2].

```
from torchmetrics import MeanAbsoluteError
metric_torch = MeanAbsoluteError()
fun_control.update({"metric_torch": metric_torch})
```

Calling the SPOT Function

Now, the dictionary `fun_control` contains all information needed for the hyperparameter tuning. Before the hyperparameter tuning is started, it is recommended to take a look at the experimental design. The method `gen_design_table` generates a design table as follows:

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control))
```

This allows to check if all information is available and if the information is correct. Table 3 shows the experimental design for the hyperparameter tuning. Hyperparameter transformations are shown in the column "transform", e.g., the `l1` default is `5`, which results in the value $2^5 = 32$ for the network, because the transformation `transform_power_2_int` was selected in the `JSON` file. The default value of the `batch_size` is set to `4`, which results in a batch size of $2^4 = 16$.

[2]https://torchmetrics.readthedocs.io/en/latest/.

Table 3: Experimental design for the hyperparameter tuning. The table shows the hyperparameters, their types, default values, lower and upper bounds, and the transformation function. The transformation function is used to transform the hyperparameter values from the unit hypercube to the original domain. The transformation function is applied to the hyperparameter values before the evaluation of the objective function.

name	type	default	lower	upper	transform
_L_in	int	10	10	10	None
_L_out	int	1	1	1	None
l1	int	3	3	8	transform_power_2_int
dropout_prob	float	0.01	0	0.9	None
lr_mult	float	1.0	0.001	0.001	None
batch_size	int	4	1	4	transform_power_2_int
epochs	int	4	2	16	transform_power_2_int
k_folds	int	1	1	1	None
patience	int	2	3	7	transform_power_2_int
optimizer	factor	SGD	0	6	None
sgd_momentum	float	0.0	0.9	0.9	None

The objective function `fun_torch` is selected next. It implements an interface from `PyTorch`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hypertorch import HyperTorch
fun = HyperTorch().fun_torch
```

```
fun_control.update({
               "device": "cpu",
               })
```

The `spotPython` hyperparameter tuning is started by calling the `Spot` function. Here, we will run the tuner for approximately 30 minutes (`max_time`). Note: the initial design is always evaluated in the `spotPython` run. As a consequence, the run may take longer than specified by `max_time`, because the evaluation time of initial design (here: `init_size`, 10 points) is performed independently of `max_time`.

```
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                   lower = lower,
                   upper = upper,
                   fun_evals = inf,
                   fun_repeats = 1,
                   max_time = MAX_TIME,
                   noise = False,
                   tolerance_x = np.sqrt(np.spacing(1)),
                   var_type = var_type,
                   var_name = var_name,
                   infill_criterion = "y",
                   n_points = 1,
                   seed=123,
                   log_level = 50,
                   show_models= False,
                   show_progress= True,
                   fun_control = fun_control,
                   design_control={"init_size": INIT_SIZE,
                                   "repeats": 1},
                   surrogate_control={"noise": True,
                                      "cod_type": "norm",
                                      "min_theta": -4,
                                      "max_theta": 3,
                                      "n_theta": len(var_name),
                                      "model_fun_evals": 10_000,
                                      "log_level": 50
                                      })
spot_tuner.run(X_start=X_start)
```

During the run, the following output is shown:

```
config: {'_L_in': 10, '_L_out': 1, 'l1': 64, 'dropout_prob': 0.4475780541539,
    'lr_mult': 0.001, 'batch_size': 16, 'epochs': 512, 'k_folds': 1,
    'patience': 32,'optimizer': 'Adagrad', 'sgd_momentum': 0.9}
Epoch: 1
...
Epoch: 7002
Loss on hold-out set: 1.6959798782529844e-05
MeanAbsoluteError value on hold-out data: 0.0018855303060263395
Epoch: 7003
Loss on hold-out set: 1.6984027051769603e-05
MeanAbsoluteError value on hold-out data: 0.001883985591121018
Early stopping at epoch 7002
Returned to Spot: Validation loss: 1.6984027051769603e-05
```

Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard.

Tensorboard: Start Tensorboard

Start TensorBoard through the command line to visualize data you logged. Specify the root log directory as used in `fun_control = fun_control_init(task="regression", tensorboard_path="runs/24_spot_torch_regression")` as the `tensorboard_path`. The argument logdir points to directory where TensorBoard will look to find event files that it can display. TensorBoard will recursively walk the directory structure rooted at logdir, looking for *.tfevents.* files.

tensorboard –logdir=runs

Go to the URL it provides OR to http://localhost:6006/.

The following figures show some screenshots of Tensorboard.

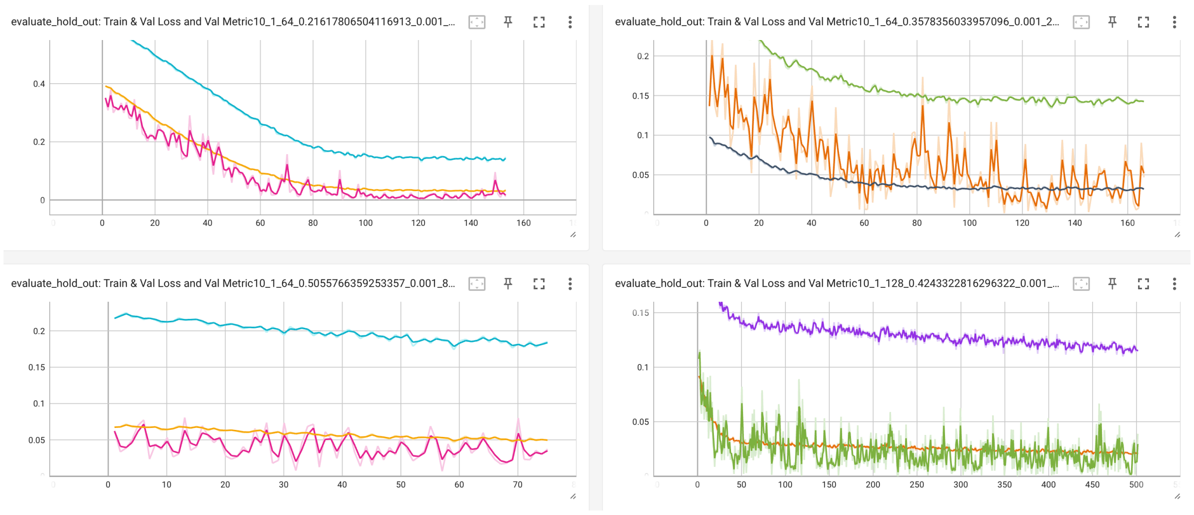
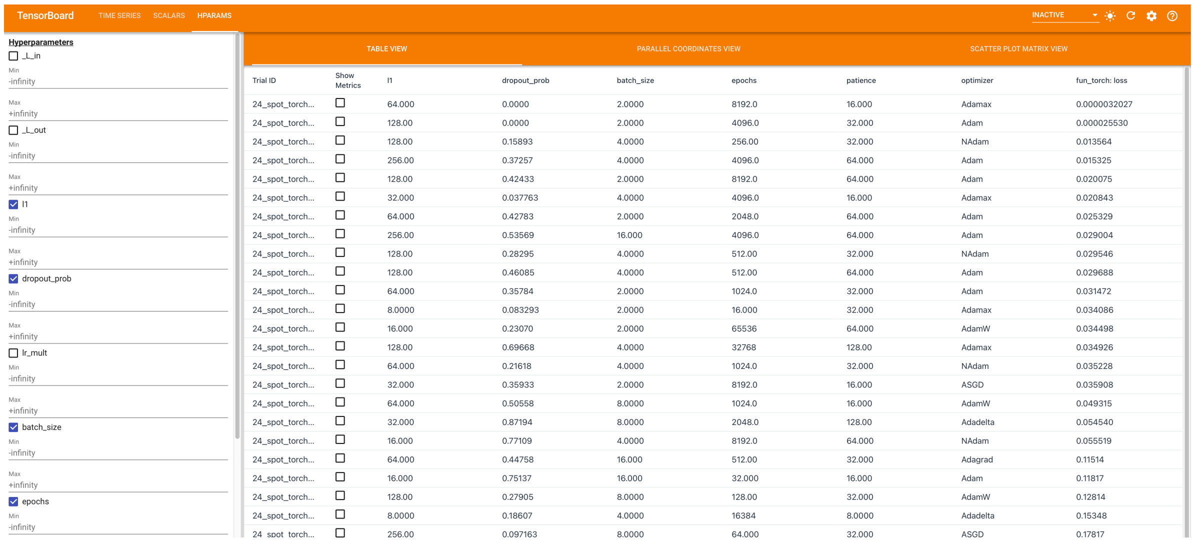

evaluate_hold_out: Train & Val Loss and Val Metric10_1_64_0.21617806504116913_0.001_...
evaluate_hold_out: Train & Val Loss and Val Metric10_1_64_0.3578356033957096_0.001_2...
evaluate_hold_out: Train & Val Loss and Val Metric10_1_64_0.5055766359253357_0.001_8...
evaluate_hold_out: Train & Val Loss and Val Metric10_1_128_0.4243322816296322_0.001_...

Figure 1: Tensorboard

Results

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The following code generates the progress plot from Figure 4.

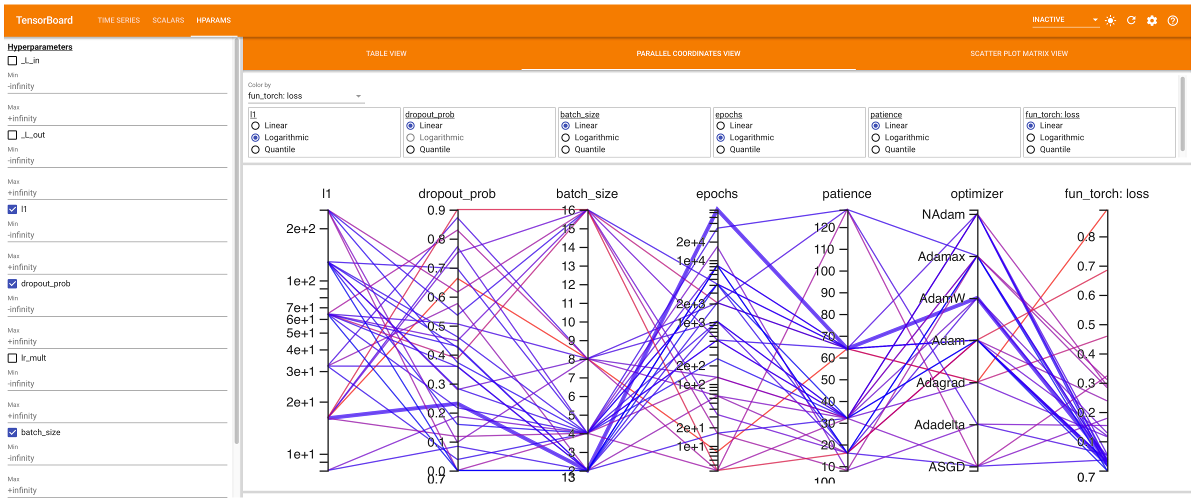


Hyperparameters

- [ ] _L_in — Min -infinity, Max +infinity
- [ ] _L_out — Min -infinity, Max +infinity
- [✓] l1 — Min -infinity, Max +infinity
- [✓] dropout_prob — Min -infinity, Max +infinity
- [ ] lr_mult — Min -infinity, Max +infinity
- [✓] batch_size — Min -infinity, Max +infinity
- [✓] epochs — Min -infinity

Trial ID	Show Metrics	l1	dropout_prob	batch_size	epochs	patience	optimizer	fun_torch: loss
24_spot_torch...	☐	64.000	0.0000	2.0000	8192.0	16.000	Adamax	0.0000032027
24_spot_torch...	☐	128.00	0.0000	2.0000	4096.0	32.000	Adam	0.000025530
24_spot_torch...	☐	128.00	0.15893	4.0000	256.00	32.000	NAdam	0.013564
24_spot_torch...	☐	256.00	0.37257	4.0000	4096.0	64.000	Adam	0.015325
24_spot_torch...	☐	128.00	0.42433	2.0000	8192.0	64.000	Adam	0.020075
24_spot_torch...	☐	32.000	0.037763	4.0000	4096.0	16.000	Adamax	0.020843
24_spot_torch...	☐	64.000	0.42783	2.0000	2048.0	64.000	Adam	0.025329
24_spot_torch...	☐	256.00	0.53569	16.000	4096.0	64.000	Adam	0.029004
24_spot_torch...	☐	128.00	0.28295	4.0000	512.00	32.000	NAdam	0.029546
24_spot_torch...	☐	128.00	0.46085	4.0000	512.00	64.000	Adam	0.029688
24_spot_torch...	☐	64.000	0.35784	2.0000	1024.0	32.000	Adam	0.031472
24_spot_torch...	☐	8.0000	0.083293	2.0000	16.000	32.000	Adamax	0.034086
24_spot_torch...	☐	16.000	0.23070	2.0000	65536	64.000	AdamW	0.034498
24_spot_torch...	☐	128.00	0.69668	4.0000	32768	128.00	Adamax	0.034926
24_spot_torch...	☐	64.000	0.21618	4.0000	1024.0	32.000	NAdam	0.035228
24_spot_torch...	☐	32.000	0.35933	2.0000	8192.0	16.000	ASGD	0.035908
24_spot_torch...	☐	64.000	0.50558	8.0000	1024.0	16.000	AdamW	0.049315
24_spot_torch...	☐	32.000	0.87194	8.0000	2048.0	128.00	Adadelta	0.054540
24_spot_torch...	☐	16.000	0.77109	4.0000	8192.0	64.000	NAdam	0.055519
24_spot_torch...	☐	64.000	0.44758	16.000	512.00	32.000	Adagrad	0.11514
24_spot_torch...	☐	16.000	0.75137	16.000	32.000	16.000	Adam	0.11817
24_spot_torch...	☐	128.00	0.27905	8.0000	128.00	32.000	AdamW	0.12814
24_spot_torch...	☐	8.0000	0.18607	4.0000	16384	8.0000	Adadelta	0.15348
24_spot_torch...	☐	256.00	0.097163	8.0000	64.000	32.000	ASGD	0.17817

Figure 2: Tensorboard



Hyperparameters

- [ ] _L_in — Min -infinity, Max +infinity
- [ ] _L_out — Min -infinity, Max +infinity
- [✓] l1 — Min -infinity, Max +infinity
- [✓] dropout_prob — Min -infinity, Max +infinity
- [ ] lr_mult — Min -infinity, Max +infinity
- [✓] batch_size — Min -infinity, Max +infinity

Color by: fun_torch: loss

l1	dropout_prob	batch_size	epochs	patience	fun_torch: loss
Linear	[✓ Linear]	[✓ Linear]	Linear	[✓ Linear]	[✓ Linear]
[✓ Logarithmic]	Logarithmic	Logarithmic	[✓ Logarithmic]	Logarithmic	Logarithmic
Quantile	Quantile	Quantile	Quantile	Quantile	Quantile

Figure 3: Tensorboard

```
spot_tuner.plot_progress(log_y=False, filename="./figures/" + experiment_name+"_progress.p
```

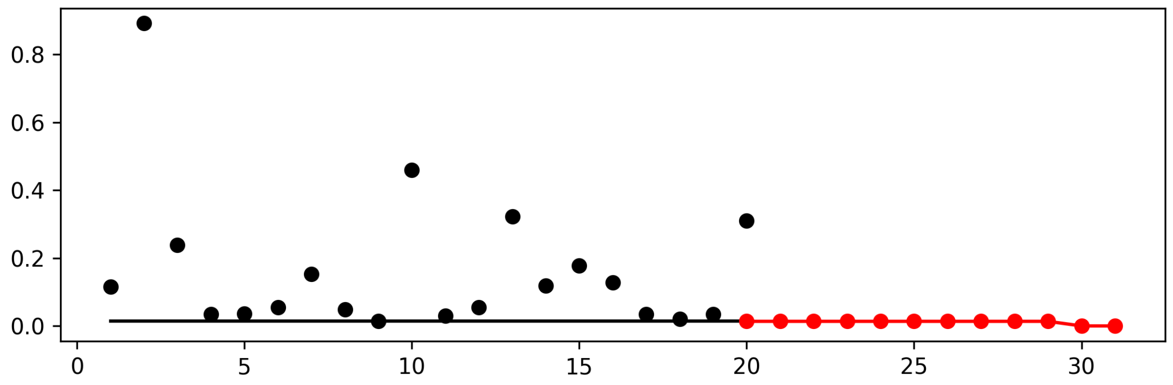


Figure 4: Progress plot. Black dots denote results from the initial design. Red dots illustrate the improvement found by the surrogate model based optimization (surrogate model based optimization).

Figure 4 shows a typical behaviour that can be observed in many hyperparameter studies (Bartz et al. 2022): the largest improvement is obtained during the evaluation of the initial design. The surrogate model based optimization-optimization with the surrogate refines the results. Figure 4 also illustrates one major difference between `ray[tune]` as used in PyTorch (2023) and `spotPython`: the `ray[tune]` uses a random search and will generate results similar to the *black* dots, whereas `spotPython` uses a surrogate model based optimization and presents results represented by *red* dots in Figure 4. The surrogate model based optimization is considered to be more efficient than a random search, because the surrogate model guides the search towards promising regions in the hyperparameter space.

In addition to the improved ("optimized") hyperparameter values, `spotPython` allows a statistical analysis, e.g., a sensitivity analysis, of the results. We can print the results of the hyperparameter tuning, see Table 4.

```
print(gen_design_table(fun_control=fun_control, spot=spot_tuner))
```

Table 4: Results of the hyperparameter tuning. The table shows the hyperparameters, their types, default values, lower and upper bounds, and the transformation function. The column “tuned” shows the tuned values. The column “importance” shows the importance of the hyperparameters. The column “stars” shows the importance of the hyperparameters in stars. The importance is computed by the SPOT software.

name	type	default	lower	upper	tuned	transform	importance	stars
_L_in	int	10	10.0	10.0	10.0	None	0.00	
_L_out	int	1	1.0	1.0	1.0	None	0.00	
l1	int	3	3.0	8.0	6.0	power_2_int	1.42	*
drop_p	float	0.01	0.0	0.9	0.0	None	0.00	
lr_mult	float	1.0	0.001	0.001	0.001	None	0.00	
batch_s	int	4	1.0	4.0	1.0	power_2_int	0.01	
epochs	int	4	2.0	16.0	13.0	power_2_int	100.00	***
k_folds	int	1	1.0	1.0	1.0	None	0.00	
patience	int	2	3.0	7.0	4.0	power_2_int	0.00	
optim	factor	SGD	0.0	6.0	4.0	None	0.00	
sgd_mom	float	0.0	0.9	0.9	0.9	None	0.00	

To visualize the most important hyperparameters, `spotPython` provides the function `plot_importance`. The following code generates the importance plot from Figure 5.

```
spot_tuner.plot_importance(threshold=0.025, filename="./figures/" + experiment_name+"_impo
```

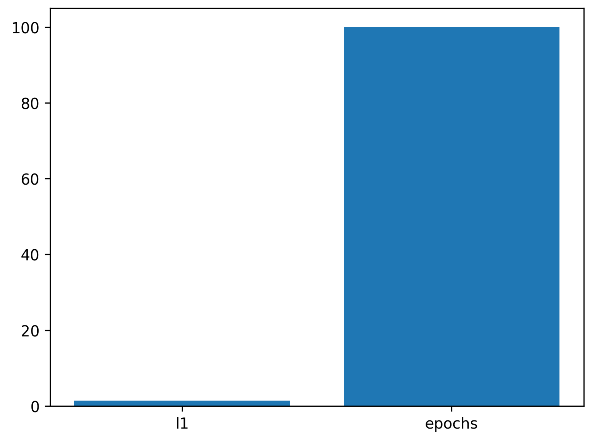


Figure 5: Variable importance

Get SPOT Results

The architecture of the `spotPython` model can be obtained by the following code:

```
from spotPython.hyperparameters.values import get_one_core_model_from_X
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
model_spot = get_one_core_model_from_X(X, fun_control)
model_spot
```

First, the numerical representation of the hyperparameters are obtained, i.e., the numpy array `X` is generated. This array is then used to generate the model `model_spot` by the function `get_one_core_model_from_X`. The model `model_spot` has the following architecture:

```
Net_lin_reg(
  (fc1): Linear(in_features=10, out_features=64, bias=True)
  (fc2): Linear(in_features=64, out_features=32, bias=True)
  (fc3): Linear(in_features=32, out_features=1, bias=True)
  (relu): ReLU()
  (softmax): Softmax(dim=1)
  (dropout1): Dropout(p=0.0, inplace=False)
  (dropout2): Dropout(p=0.0, inplace=False)
)
```

Evaluation of the Tuned Architecture

The method `train_tuned` takes a model architecture without trained weights and trains this model with the train data. The train data is split into train and validation data. The validation data is used for early stopping. The trained model weights are saved as a dictionary.

The following code trains the model `model_spot`. If `path` is set to a filename, e.g., `path = "model_spot_trained.pt"`, the weights of the trained model will be saved to this file.

```
from spotPython.torch.traintest import (
    train_tuned,
    test_tuned,
    )
train_tuned(net=model_spot, train_dataset=train,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        shuffle=True,
        device = DEVICE,
        path=None,
        task=fun_control["task"],)
```

```
Epoch: 1
Loss on hold-out set: 0.17853929138431945
MeanAbsoluteError value on hold-out data: 0.3907899856567383
Epoch: 2
Loss on hold-out set: 0.17439044278115035
MeanAbsoluteError value on hold-out data: 0.38570401072502136
```

If `path` is set to a filename, e.g., `path = "model_spot_trained.pt"`, the weights of the trained model will be loaded from this file.

```
test_tuned(net=model_spot, test_dataset=test,
            shuffle=False,
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            device = DEVICE,
            task=fun_control["task"],)
```

```
Loss on hold-out set: 1.85966069472272e-05
MeanAbsoluteError value on hold-out data: 0.0021022311411798
Final evaluation: Validation loss: 1.85966069472272e-05
Final evaluation: Validation metric: 0.0021022311411798
----------------------------------------------
(1.85966069472272e-05, nan, tensor(0.0021))
```

Cross-validated Evaluations

```
from spotPython.torch.traintest import evaluate_cv
# modify k-kolds:
setattr(model_spot, "k_folds",  10)
evaluate_cv(net=model_spot,
            dataset=fun_control["data"],
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            task=fun_control["task"],
            writer=fun_control["writer"],
            writerId="model_spot_cv", device=DEVICE)
```

```
Fold: 1
Epoch: 1
Loss on hold-out set: 0.36993918985128404
MeanAbsoluteError value on hold-out data: 0.5827060341835022
Epoch: 2
Loss on hold-out set: 0.3583159705996513

(0.0027241395250238156, nan, tensor(0.0147))
```

Table 5 shows the loss and meric value (MAE) of the model with the tuned hyperparameters from SPOT.

Table 5: Comparison of the loss and metric values.

Model	Loss	Metric (MAE)
`Validation`	1.8597e-05	0.0021
`10-fold CV`	0.00272	0.0147

Detailed Hyperparameter Plots

The contour plot in this section visualize the interactions of the two most important hyperparameters, `l1`, and `epochs` of the surrogate model used to optimize the hyperparameters. Since some of these hyperparameters take fatorial or integer values, sometimes step-like fitness landcapes (or response surfaces) are generated. SPOT draws the interactions of the main hyperparameters by default. It is also possible to visualize all interactions. For this, again refer to the notebook (Bartz-Beielstein 2023).

```
filename = "./figures/" + experiment_name
spot_tuner.plot_important_hyperparameter_contour(filename=filename)
```

Figure 6 shows a contour plot of the loss as a function of the hyperparameters. These plots are very helpful for benchmark studies and for understanding neural networks. `spotPython` provides additional tools for a visual inspection of the results and give valuable insights into the hyperparameter tuning process. This is especially useful for model explainability, transparency, and trustworthiness. In addition to the contour plots, Figure 7 shows the parallel plot of the hyperparameters.

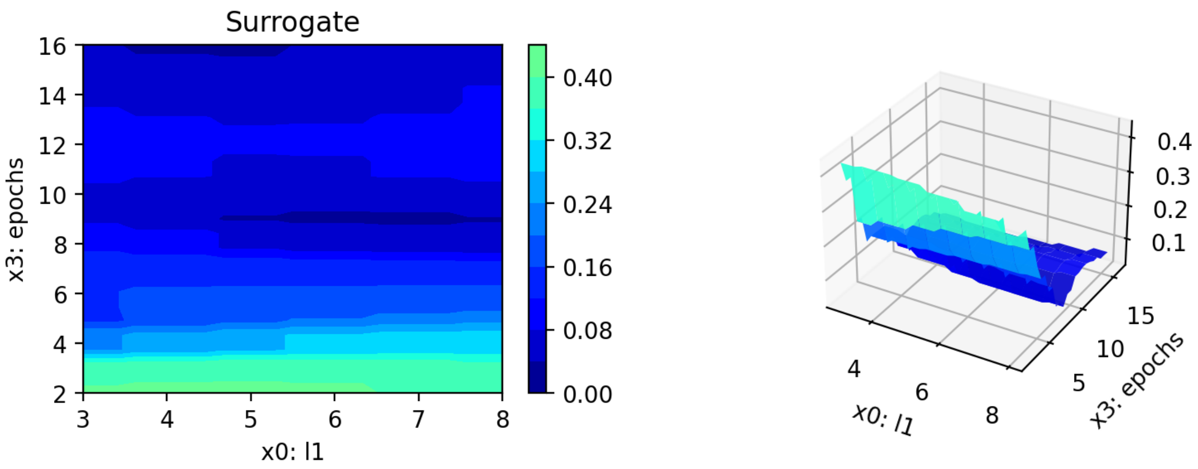


Figure 6: Contour plot of the loss as a function of `epochs` and `l1`, i.e., the number of neurons in the layers.

```
spot_tuner.parallel_plot()
```

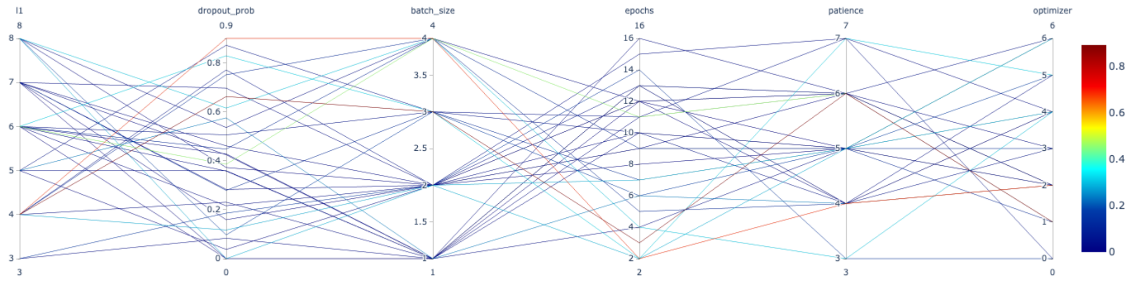


Figure 7: Parallel plot

Summary and Outlook

This tutorial presents the hyperparameter tuning open source software `spotPython` for `PyTorch`. Some of the advantages of `spotPython` are:

- Numerical and categorical hyperparameters.
- Powerful surrogate models.
- Flexible approach and easy to use.
- Simple JSON files for the specification of the hyperparameters.
- Extension of default and user specified network classes.
- Noise handling techniques.
- Online visualization of the hyperparameter tuning process with `tensorboard`.

Currently, only rudimentary parallel and distributed neural network training is possible, but these capabilities will be extended in the future. The next version of `spotPython` will also include a more detailed documentation and more examples.

! Important

Important: This tutorial does not present a complete benchmarking study (Bartz-Beielstein et al. 2020). The results are only preliminary and highly dependent on the local configuration (hard- and software). Our goal is to provide a first impression of the performance of the hyperparameter tuning package `spotPython`. The results should be interpreted with care.

Bartz, Eva, Thomas Bartz-Beielstein, Martin Zaefferer, and Olaf Mersmann, eds. 2022. *Hyperparameter Tuning for Machine and Deep Learning with R - A Practical Guide*. Springer.

Bartz-Beielstein, Thomas. 2023. "PyTorch Hyperparameter Tuning with SPOT: Comparison with Ray Tuner and Default Hyperparameters on CIFAR10." https://github.com/sequential-parameter-optimization/spotPython/blob/main/notebooks/14_spot_ray_hpt_torch_cifar10.ipynb.

Bartz-Beielstein, Thomas, Carola Doerr, Jakob Bossek, Sowmya Chandrasekaran, Tome Eftimov, Andreas Fischbach, Pascal Kerschke, et al. 2020. "Benchmarking in Optimization: Best Practice and Open Issues." arXiv. https://arxiv.org/abs/2007.03488.

Montiel, Jacob, Max Halford, Saulo Martiello Mastelini, Geoffrey Bolmier, Raphael Sourty, Robin Vaysse, Adil Zouitine, et al. 2021. "River: Machine Learning for Streaming Data in Python."

PyTorch. 2023. “Hyperparameter Tuning with Ray Tune.” https://pytorch.org/tutorials/beginner/hyperparameter_tuning_tutorial.html.