Hyperparameter Tuning Cookbook

A guide for scikit-learn, PyTorch, river, and spotPython

Thomas Bartz-Beielstein

Jul 16, 2023

Table of contents

Preface: Optimization and Hyperparameter Tuning

The goal of hyperparameter tuning is to optimize the hyperparameters in a way that improves the performance of the machine learning or deep learning model. Hyperparameters are parameters that are not learned during the training process, but are set before the training process begins. Hyperparameter tuning is an important, but often difficult and computationally intensive task. Changing the architecture of a neural network or the learning rate of an optimizer can have a significant impact on the performance.

Hyperparameter tuning is referred to as "hyperparameter optimization" (HPO) in the literature. However, since we do not consider the optimization, but also the understanding of the hyperparameters, we use the term "hyperparameter tuning" in this book. See also the discussion in Chapter 2 of (Bartz et al. 2022), which lays the groundwork and presents an introduction to the process of tuning Machine Learning and Deep Learning hyperparameters and the respective methodology. Since the key elements such as the hyperparameter tuning process and measures of tunability and performance are presented in (Bartz et al. 2022), we refer to this chapter for details.

The simplest, but also most computationally expensive, hyperparameter tuning approach uses manual search (or trial-and-error (Meignan et al. 2015)). Commonly encountered is simple random search, i.e., random and repeated selection of hyperparameters for evaluation, and lattice search ("grid search"). In addition, methods that perform directed search and other model-free algorithms, i.e., algorithms that do not explicitly rely on a model, e.g., evolution strategies (Bartz-Beielstein et al. 2014) or pattern search (Lewis, Torczon, and Trosset 2000) play an important role. Also, "hyperband", i.e., a multi-armed bandit strategy that dynamically allocates resources to a set of random configurations and uses successive bisections to stop configurations with poor performance (Li et al. 2016), is very common in hyperparameter tuning. The most sophisticated and efficient approaches are the Bayesian optimization and surrogate model based optimization methods, which are based on the optimization of cost functions determined by simulations or experiments.

We consider below a surrogate model based optimization-based hyperparameter tuning approach based on the Python version of the SPOT ("Sequential Parameter Optimization Toolbox") (Bartz-Beielstein, Lasarczyk, and Preuss 2005), which is suitable for situations where only limited resources are available. This may be due to limited availability and cost of hardware, or due to the fact that confidential data may only be processed locally, e.g., due to legal requirements. Furthermore, in our approach, the understanding of algorithms is seen as a key tool for enabling transparency and explainability. This can be enabled, for example, by quantifying the contribution of machine learning and deep learning components (nodes, layers, split decisions, activation functions, etc.). Understanding the importance of hyperparameters and the interactions between multiple hyperparameters plays a major role in the interpretability and explainability of machine learning models. SPOT provides statistical tools for understanding hyperparameters and their interactions. Last but not least, it should be noted that the SPOT software code is available in the open source `spotPython` package on github[1], allowing replicability of the results. This tutorial descries the Python variant of SPOT, which is called `spotPython`. The R implementation is described in Bartz et al. (2022). SPOT is an established open source software that has been maintained for more than 15 years (Bartz-Beielstein, Lasarczyk, and Preuss 2005) (Bartz et al. 2022).

> ❗ Important: This book is still under development.
>
> The most recent version of this book is available at https://sequential-parameter-optimization.github.io/Hyperparameter-Tuning-Cookbook/

Book Structure

This document is structured in two parts. The first part describes the surrogate model based optimization process and the second part describes the hyperparameter tuning. The first part is structured as follows:

The concept of the hyperparameter tuning software `spotPython` is described in Chapter **??**. This introduction is based on one-dimensional examples. Higher-dimensional examples are presented in Chapter **??**. Chapter **??** describes isotropic and anisotorpic kriging. How different surrogate models from `scikit-learn` can be used as surrogates in `spotPython` optimization runs is explained in Chapter **??**. Chapter **??** describes how different optimizers from the `scipy optimize` package can be used on the surrogate. The differences between the `Kriging` implementation in `spotPython` and the `GaussianProcessRegressor` in `scikit-learn` are explained in Chapter **??**. Chapter **??** describes the expected improvement approach. How noisy functions can be handled is described in Chapter **??**. Chapter **??** demonstrates how noisy functions can be handled with Optimal Computational Budget Allocation (OCBA) by `Spot`.

The second part is structured as follows:

Chapter **??** describes the hyperparameter tuning of a support vector classifier from `scikit-learn` [https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html#sklearn.svm.SVCriver python] with `spotPython`. Chapter **??** illustrates the hyperparameter tuning of a Hoeffding

[1] https://github.com/sequential-parameter-optimization

Adaptive Tree Regressor from river [https://riverml.xyz/0.18.0/api/tree/HoeffdingAdaptiveTreeRegressor/] with spotPython.

Chapter ?? describes the execution of the example from the tutorial "Hyperparameter Tuning with Ray Tune" (PyTorch 2023a). The integration of spotPython into the PyTorch training workflow is described in detail in the following sections. Section ?? describes the setup of the tuners. Section ?? describes the data loading. Section ?? describes the model to be tuned. The search space is introduced in Section ??. Optimizers are presented in Section ??. How to split the data in train, validation, and test sets is described in Section ??. The selection of the loss function and metrics is described in Section ??. Section ?? describes the preparation of the spotPython call. The objective function is described in Section ??. How to use results from previous runs and default hyperparameter configurations is described in Section ??. Starting the tuner is shown in Section ??. TensorBoard can be used to visualize the results as shown in Section ??. Results are discussed and explained in Section ??. Section ?? presents a summary and an outlook. Chapter ?? describes the hyperparameter tuning of a random forest classifier from scikit-learn [https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html] with spotPython. Chapter ?? describes the hyperparameter tuning of a XGBoost classifier from scikit-learn [https://scikit-learn.org/stable/modules/ensemble.html#histogram-based-gradient-boosting] with spotPython. Chapter ?? describes the hyperparameter tuning of a support vector classifier from scikit-learn [https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.htm with spotPython. Chapter ?? describes the hyperparameter tuning of a k-nearest neighbors classifier from scikit-learn [https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassi with spotPython. Chapter ?? shows the integration of spotPython into the PyTorch Lightning training workflow.

> **Hyperparameter Tuning Reference**
>
> - The open access book Bartz et al. (2022) provides a comprehensive overview of hyperparameter tuning. It can be downloaded from https://link.springer.com/book/10.1007/978-981-19-5170-1.

> **Note**
>
> The .ipynb notebook (Bartz-Beielstein 2023) is updated regularly and reflects updates and changes in the spotPython package. It can be downloaded from https://github.com/sequential-parameter-optimization/spotPython/blob/main/notebooks/14_spot_ray_hpt_torch_cifar10.ipynb.

Software Used in this Book

spotPython ("Sequential Parameter Optimization Toolbox in Python") is the Python version of the well-known hyperparameter tuner SPOT, which has been developed in the R programming environment for statistical analysis for over a decade. The related open-access book is available here: Hyperparameter Tuning for Machine and Deep Learning with R—A Practical Guide.

scikit-learn is a Python module for machine learning built on top of SciPy and is distributed under the 3-Clause BSD license. The project was started in 2007 by David Cournapeau as a Google Summer of Code project, and since then many volunteers have contributed.

PyTorch is an optimized tensor library for deep learning using GPUs and CPUs.

River is a Python library for online machine learning. It is designed to be used in real-world environments, where not all data is available at once, but streaming in.

spotRiver provides an interface between spotPython and River.

Part I

Spot as an Optimizer

1 Introduction to `spotPython`

Surrogate model based optimization methods are common approaches in simulation and optimization. SPOT was developed because there is a great need for sound statistical analysis of simulation and optimization algorithms. SPOT includes methods for tuning based on classical regression and analysis of variance techniques. It presents tree-based models such as classification and regression trees and random forests as well as Bayesian optimization (Gaussian process models, also known as Kriging). Combinations of different meta-modeling approaches are possible. SPOT comes with a sophisticated surrogate model based optimization method, that can handle discrete and continuous inputs. Furthermore, any model implemented in `scikit-learn` can be used out-of-the-box as a surrogate in `spotPython`.

SPOT implements key techniques such as exploratory fitness landscape analysis and sensitivity analysis. It can be used to understand the performance of various algorithms, while simultaneously giving insights into their algorithmic behavior.

The `spot` loop consists of the following steps:

1. Init: Build initial design X
2. Evaluate initial design on real objective f: $y = f(X)$
3. Build surrogate: $S = S(X, y)$
4. Optimize on surrogate: $X_0 = \text{optimize}(S)$
5. Evaluate on real objective: $y_0 = f(X_0)$
6. Impute (Infill) new points: $X = X \cup X_0$, $y = y \cup y_0$.
7. Got 3.

Central Idea: Evaluation of the surrogate model `S` is much cheaper (or / and much faster) than running the real-world experiment f. We start with a small example.

1.1 Example: `Spot` and the Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
```

```python
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
```

1.1.1 The Objective Function: Sphere

The `spotPython` package provides several classes of objective functions. We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x) = x^2$$

```python
fun = analytical().fun_sphere
```

We can apply the function `fun` to input values and plot the result:

```python
x = np.linspace(-1,1,100).reshape(-1,1)
y = fun(x)
plt.figure()
plt.plot(x, y, "k")
plt.show()
```

01_spot_intro_files/figure-pdf/cell-4-output-1.pdf

```python
spot_0 = spot.Spot(fun=fun,
                   lower = np.array([-1]),
                   upper = np.array([1]))
```

```python
spot_0.run()
```

```
spotPython tuning: 7.263311682641849e-09 [#######---] 73.33%

spotPython tuning: 7.263311682641849e-09 [########--] 80.00%

spotPython tuning: 7.263311682641849e-09 [#########-] 86.67%
```

```
spotPython tuning: 7.263311682641849e-09 [#########-] 93.33%
```

```
spotPython tuning: 3.696886711914087e-10 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x13889dea0>
```

```
spot_0.print_results()
```

```
min y: 3.696886711914087e-10
x0: 1.922728975158508e-05
```

```
[['x0', 1.922728975158508e-05]]
```

```
spot_0.plot_progress(log_y=True)
```

01_spot_intro_files/figure-pdf/cell-8-output-1.pdf

```
spot_0.plot_model()
```

01_spot_intro_files/figure-pdf/cell-9-output-1.pdf

1.2 `Spot` Parameters: `fun_evals`, `init_size` and `show_models`

We will modify three parameters:

1. The number of function evaluations (`fun_evals`)
2. The size of the initial design (`init_size`)
3. The parameter `show_models`, which visualizes the search process for 1-dim functions.

The full list of the Spot parameters is shown in the Help System and in the notebook spot_doc.ipynb.

```
spot_1 = spot.Spot(fun=fun,
                   lower = np.array([-1]),
                   upper = np.array([2]),
                   fun_evals= 10,
                   seed=123,
                   show_models=True,
                   design_control={"init_size": 9})
spot_1.run()
```

01_spot_intro_files/figure-pdf/cell-10-output-1.pdf

01_spot_intro_files/figure-pdf/cell-10-output-2.pdf

```
spotPython tuning: 3.6779240309761575e-07 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x1390a86d0>
```

1.3 Print the Results

```
spot_1.print_results()
```

```
min y: 3.6779240309761575e-07
x0: -0.0006064589047063418
```

```
[['x0', -0.0006064589047063418]]
```

1.4 Show the Progress

```
spot_1.plot_progress()
```

01_spot_intro_files/figure-pdf/cell-12-output-1.pdf

1.5 Visualizing the Optimization and Hyperparameter Tuning Process with TensorBoard

`spotPython` supports the visualization of the hyperparameter tuning process with TensorBoard. The following example shows how to use TensorBoard with `spotPython`.

First, we define an "experiment name" to identify the hyperparameter tuning process. The experiment name is used to create a directory for the TensorBoard files.

```
from spotPython.utils.file import get_experiment_name
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_spot_tensorboard_path

PREFIX = "01"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)

fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name))
```

```
01_bartz09_2023-07-16_14-12-37
```

Since the `spot_tensorboard_path` is defined, `spotPython` will log the optimization process in the TensorBoard files. The TensorBoard files are stored in the directory `spot_tensorboard_path`. We can pass the TensorBoard information to the `Spot` method via the `fun_control` dictionary.

```python
spot_tuner = spot.Spot(fun=fun,
                   lower = np.array([-1]),
                   upper = np.array([2]),
                   fun_evals= 10,
                   seed=123,
                   show_models=False,
                   design_control={"init_size": 5},
                   fun_control=fun_control,)
spot_tuner.run()
```

```
spotPython tuning: 2.7705924100183687e-05 [######----] 60.00%
```

```
spotPython tuning: 7.364661789374228e-07 [#######---] 70.00%
```

```
spotPython tuning: 7.364661789374228e-07 [########--] 80.00%
```

```
spotPython tuning: 3.5490065465299805e-07 [#########-] 90.00%
```

```
spotPython tuning: 7.234315072455918e-09 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x2b9d9f010>
```

Now we can start TensorBoard in the background. The TensorBoard process will read the TensorBoard files and visualize the hyperparameter tuning process. From the terminal, we can start TensorBoard with the following command:

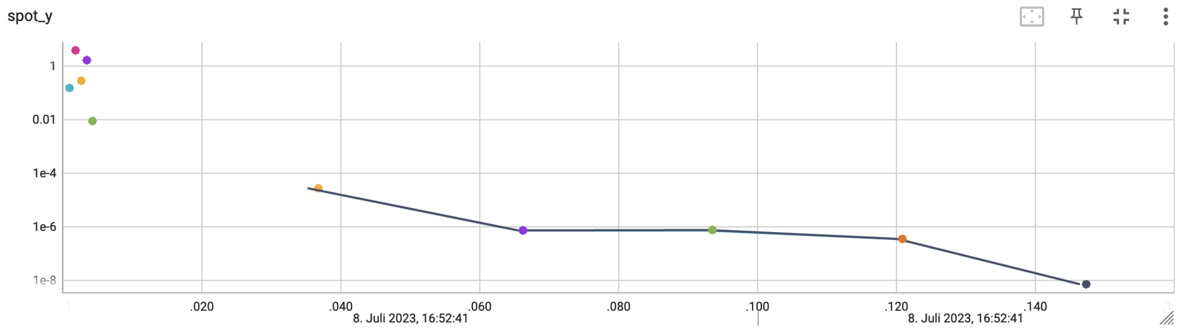
```
tensorboard --logdir="./runs"
```

`logdir` is the directory where the TensorBoard files are stored. In our case, the TensorBoard files are stored in the directory `./runs`.

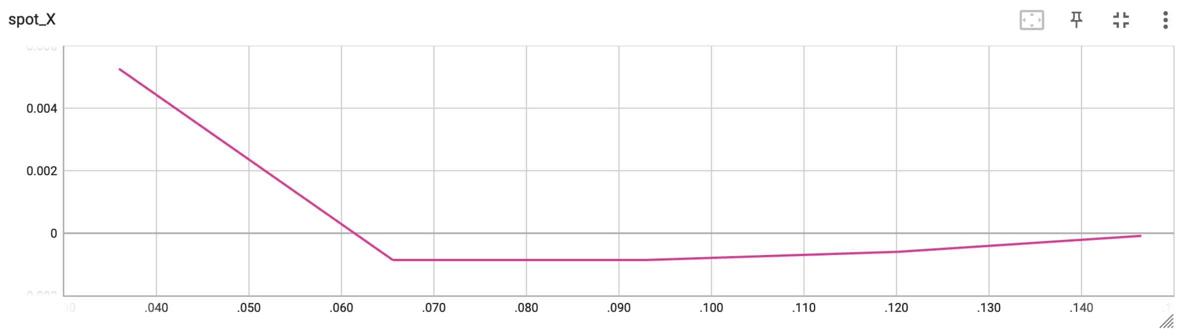
TensorBoard will start a web server on port 6006. We can access the TensorBoard web server with the following URL:

```
http://localhost:6006/
```

The first TensorBoard visualization shows the objective function values plotted against the wall time. The wall time is the time that has passed since the start of the hyperparameter tuning process. The five initial design points are shown in the upper left region of the plot. The line visualizes the optimization process.



The second TensorBoard visualization shows the input values, i.e., x_0, plotted against the wall



time.

The third TensorBoard plot illustrates how `spotPython` can be used as a microscope for the internal mechanisms of the surrogate-based optimization process. Here, one important parameter, the learning rate θ of the Kriging surrogate is plotted against the number of optimization steps.

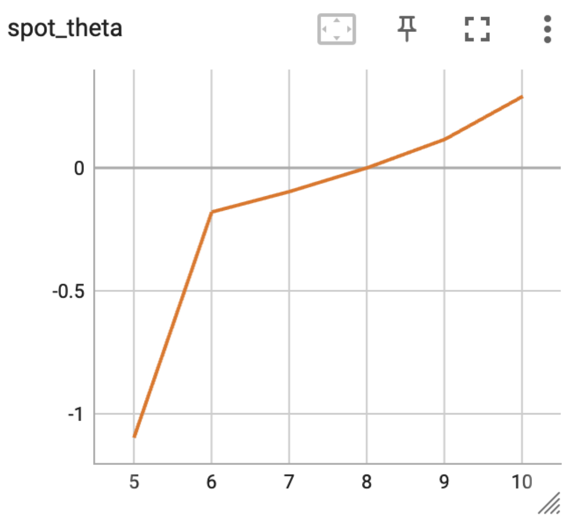


Figure 1.1: TensorBoard visualization of the spotPython process.

2 Multi-dimensional Functions

This text illustrates how high-dimensional functions can be analyzed.

2.1 Example: `Spot` and the 3-dim Sphere Function

```
import numpy as np
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
```

2.1.1 The Objective Function: 3-dim Sphere

- The `spotPython` package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x) = \sum_i^n x_i^2$$

- Here we will use $n = 3$.

```
fun = analytical().fun_sphere
```

- The size of the `lower` bound vector determines the problem dimension.
- Here we will use `-1.0 * np.ones(3)`, i.e., a three-dim function.
- We will use three different `theta` values (one for each dimension), i.e., we set `surrogate_control={"n_theta": 3}`.

> **TensorBoard**
>
> Similar to the one-dimensional case, which was introduced in Section Section **??**, we can use TensorBoard to monitor the progress of the optimization. We will use the same code,

only the prefix is different:

```
from spotPython.utils.file import get_experiment_name
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_spot_tensorboard_path

PREFIX = "02"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)

fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name))
```

```
02_bartz09_2023-07-16_14-12-51
```

```
spot_3 = spot.Spot(fun=fun,
                   lower = -1.0*np.ones(3),
                   upper = np.ones(3),
                   var_name=["Pressure", "Temp", "Lambda"],
                   show_progress=True,
                   surrogate_control={"n_theta": 3},
                   fun_control=fun_control,)

spot_3.run()
```

```
spotPython tuning: 0.03443344056467332 [#######---] 73.33%

spotPython tuning: 0.03134865993507926 [########--] 80.00%

spotPython tuning: 0.0009629342967936851 [#########-] 86.67%

spotPython tuning: 8.541951463966474e-05 [#########-] 93.33%

spotPython tuning: 6.285135731399678e-05 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x17cc6f8b0>
```

Now we can start TensorBoard in the background with the following command:

```
tensorboard --logdir="./runs"
```

We can access the TensorBoard web server with the following URL:

```
http://localhost:6006/
```

2.1.2 Results

```
spot_3.print_results()
```

```
min y: 6.285135731399678e-05
Pressure: 0.005236109709736696
Temp: 0.0019572552655686714
Lambda: 0.005621713639718905
```

```
[['Pressure', 0.005236109709736696],
 ['Temp', 0.0019572552655686714],
 ['Lambda', 0.005621713639718905]]
```

```
spot_3.plot_progress()
```

02_spot_multidim_files/figure-pdf/cell-7-output-1.pdf

2.1.3 A Contour Plot

- We can select two dimensions, say $i = 0$ and $j = 1$, and generate a contour plot as follows.
  - Note: We have specified identical `min_z` and `max_z` values to generate comparable plots!

```
spot_3.plot_contour(i=0, j=1, min_z=0, max_z=2.25)
```

02_spot_multidim_files/figure-pdf/cell-8-output-1.pdf

- In a similar manner, we can plot dimension $i = 0$ and $j = 2$:

```
spot_3.plot_contour(i=0, j=2, min_z=0, max_z=2.25)
```

02_spot_multidim_files/figure-pdf/cell-9-output-1.pdf

- The final combination is $i = 1$ and $j = 2$:

```
spot_3.plot_contour(i=1, j=2, min_z=0, max_z=2.25)
```

02_spot_multidim_files/figure-pdf/cell-10-output-1.pdf

- The three plots look very similar, because the `fun_sphere` is symmetric.
- This can also be seen from the variable importance:

```
spot_3.print_importance()
```

```
Pressure:  99.35185545837122
Temp:  99.99999999999999
Lambda:  94.31627052007231
```

```
[['Pressure', 99.35185545837122],
 ['Temp', 99.99999999999999],
 ['Lambda', 94.31627052007231]]
```

2.1.4 TensorBoard

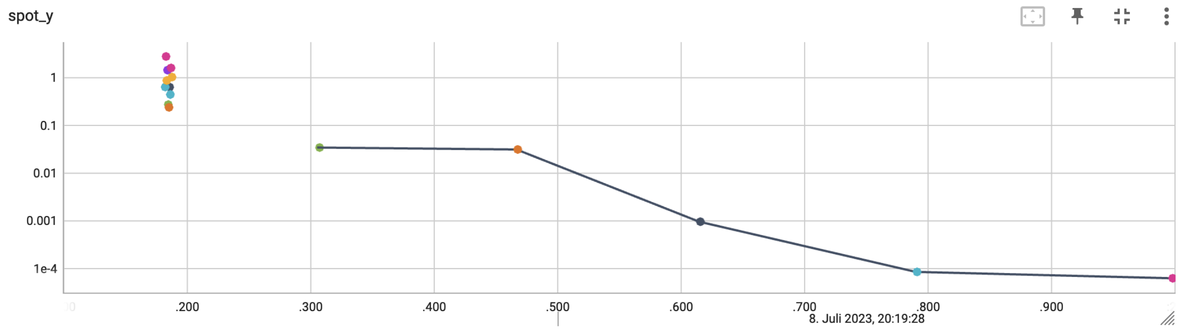
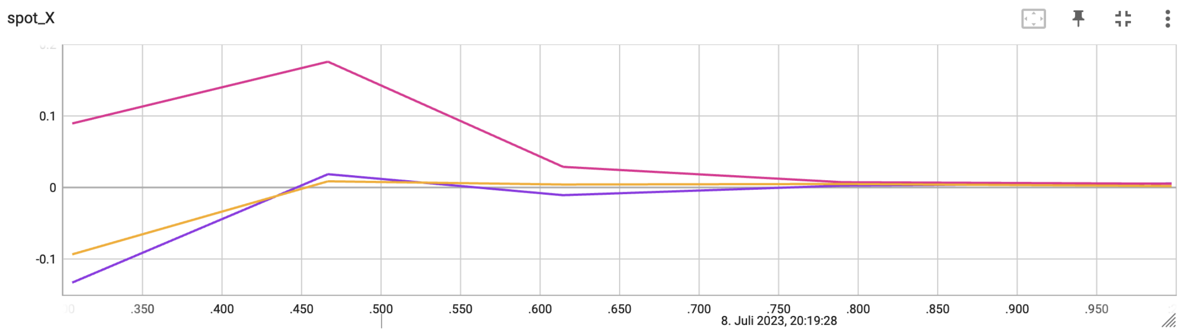


Figure 2.1: TensorBoard visualization of the spotPython process. Objective function values plotted against wall time.

The second TensorBoard visualization shows the input values, i.e., $x_0, \ldots, x_2$, plotted against the



wall time.

The third TensorBoard plot illustrates how `spotPython` can be used as a microscope for the internal mechanisms of the surrogate-based optimization process. Here, one important parameter, the learning rate θ of the Kriging surrogate is plotted against the number of optimization steps.

2.2 Conclusion

Based on this quick analysis, we can conclude that all three dimensions are equally important (as expected, because the analytical function is known).

2.3 Exercises

- Important:

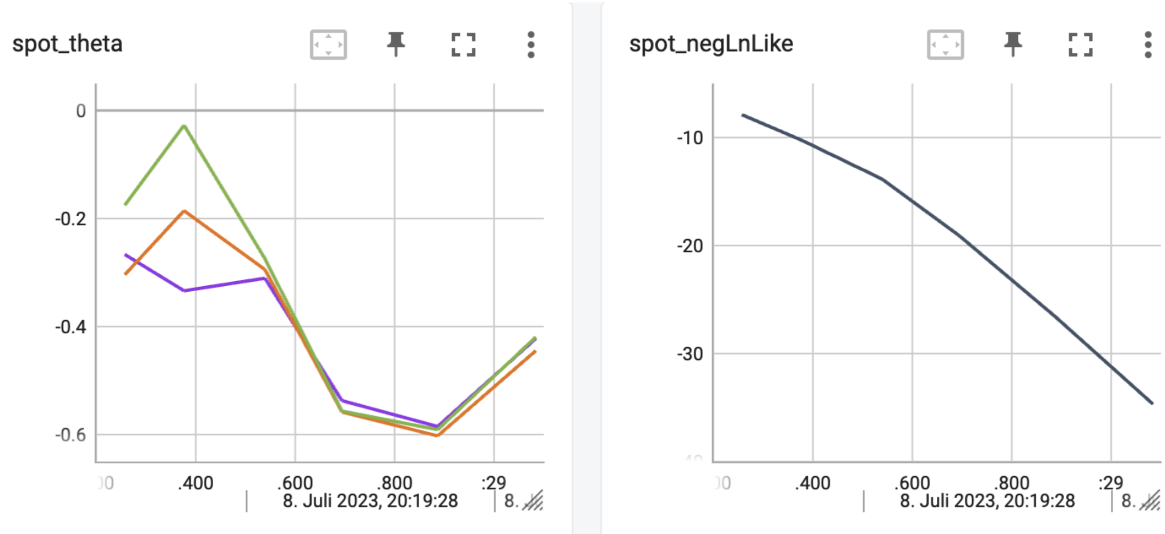


Figure 2.2: TensorBoard visualization of the spotPython surrogate model.

  - Results from these exercises should be added to this document, i.e., you should submit an updated version of this notebook.
  - Please combine your results using this notebook.
  - Only one notebook from each group!
  - Presentation is based on this notebook. No addtional slides are required!
  - spotPython version `0.16.11` (or greater) is required

2.3.1 The Three Dimensional `fun_cubed`

- The input dimension is `3`. The search range is $-1 \leq x \leq 1$ for all dimensions.
- Generate contour plots
- Calculate the variable importance.
- Discuss the variable importance:
  - Are all variables equally important?
  - If not:
    - Which is the most important variable?
    - Which is the least important variable?

2.3.2 The Ten Dimensional `fun_wing_wt`

- The input dimension is `10`. The search range is $0 \leq x \leq 1$ for all dimensions.
- Calculate the variable importance.

- Discuss the variable importance:
  - Are all variables equally important?
  - If not:
    - Which is the most important variable?
    - Which is the least important variable?
  - Generate contour plots for the three most important variables. Do they confirm your selection?

2.3.3 The Three Dimensional `fun_runge`

- The input dimension is `3`. The search range is $-5 \leq x \leq 5$ for all dimensions.
- Generate contour plots
- Calculate the variable importance.
- Discuss the variable importance:
  - Are all variables equally important?
  - If not:
    - Which is the most important variable?
    - Which is the least important variable?

2.3.4 The Three Dimensional `fun_linear`

- The input dimension is `3`. The search range is $-5 \leq x \leq 5$ for all dimensions.
- Generate contour plots
- Calculate the variable importance.
- Discuss the variable importance:
  - Are all variables equally important?
  - If not:
    - Which is the most important variable?
    - Which is the least important variable?

3 Isotropic and Anisotropic Kriging

3.1 Example: Isotropic Spot Surrogate and the 2-dim Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
```

3.1.1 The Objective Function: 2-dim Sphere

- The spotPython package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x, y) = x^2 + y^2$$

```
fun = analytical().fun_sphere
fun_control = {"sigma": 0,
               "seed": 123}
```

- The size of the lower bound vector determines the problem dimension.
- Here we will use np.array([-1, -1]), i.e., a two-dim function.

```
spot_2 = spot.Spot(fun=fun,
                   lower = np.array([-1, -1]),
                   upper = np.array([1, 1]))

spot_2.run()
```

```
spotPython tuning: 2.093282610941807e-05 [#######---] 73.33%
```

```
spotPython tuning: 2.093282610941807e-05 [########--] 80.00%
```

```
spotPython tuning: 2.093282610941807e-05 [#########-] 86.67%

spotPython tuning: 2.093282610941807e-05 [#########-] 93.33%

spotPython tuning: 2.093282610941807e-05 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x16469d330>
```

3.1.2 Results

```
spot_2.print_results()
```

```
min y: 2.093282610941807e-05
x0: 0.0016055267473267492
x1: 0.00428428640184529
```

```
[['x0', 0.0016055267473267492], ['x1', 0.00428428640184529]]
```

```
spot_2.plot_progress(log_y=True)
```

03_spot_anisotropic_files/figure-pdf/cell-6-output-1.pdf

3.2 Example With Anisotropic Kriging

- The default parameter setting of `spotPython`'s Kriging surrogate uses the same `theta` value for every dimension.
- This is referred to as "using an isotropic kernel".
- If different `theta` values are used for each dimension, then an anisotropic kernel is used
- To enable anisotropic models in `spotPython`, the number of `theta` values should be larger than one.
- We can use `surrogate_control={"n_theta": 2}` to enable this behavior (`2` is the problem dimension).

TensorBoard

Similar to the one-dimensional case, which was introduced in Section Section **??**, we can use TensorBoard to monitor the progress of the optimization. We will use the same code, only the prefix is different:

```
from spotPython.utils.file import get_experiment_name
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_spot_tensorboard_path

PREFIX = "03"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)

fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name))
```

```
03_bartz09_2023-07-16_14-13-08
```

```
spot_2_anisotropic = spot.Spot(fun=fun,
                    lower = np.array([-1, -1]),
                    upper = np.array([1, 1]),
                    surrogate_control={"n_theta": 2},
                    fun_control=fun_control)
spot_2_anisotropic.run()
```

```
spotPython tuning: 1.991152317760403e-05 [#######---] 73.33%

spotPython tuning: 1.991152317760403e-05 [########--] 80.00%

spotPython tuning: 1.991152317760403e-05 [#########-] 86.67%

spotPython tuning: 1.991152317760403e-05 [#########-] 93.33%

spotPython tuning: 7.77061191821505e-06 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x16469d930>
```

- The search progress of the optimization with the anisotropic model can be visualized:

```python
spot_2_anisotropic.plot_progress(log_y=True)
```

03_spot_anisotropic_files/figure-pdf/cell-9-output-1.pdf

```python
spot_2_anisotropic.print_results()
```

```
min y: 7.77061191821505e-06
x0: -0.0024488252797500764
x1: -0.0013318658594137815
```

```
[['x0', -0.0024488252797500764], ['x1', -0.0013318658594137815]]
```

```python
spot_2_anisotropic.surrogate.plot()
```

03_spot_anisotropic_files/figure-pdf/cell-11-output-1.pdf

3.2.1 Taking a Look at the `theta` Values

3.2.1.1 `theta` Values from the `spot` Model

- We can check, whether one or several `theta` values were used.
- The `theta` values from the surrogate can be printed as follows:

```python
spot_2_anisotropic.surrogate.theta
```

```
array([0.19447342, 0.30813872])
```

- Since the surrogate from the isotropic setting was stored as `spot_2`, we can also take a look at the `theta` value from this model:

```
spot_2.surrogate.theta
```

```
array([0.26287447])
```

3.2.1.2 TensorBoard

Now we can start TensorBoard in the background with the following command:

```
tensorboard --logdir="./runs"
```

We can access the TensorBoard web server with the following URL:

```
http://localhost:6006/
```

The TensorBoard plot illustrates how `spotPython` can be used as a microscope for the internal mechanisms of the surrogate-based optimization process. Here, one important parameter, the learning rate θ of the Kriging surrogate is plotted against the number of optimization steps.

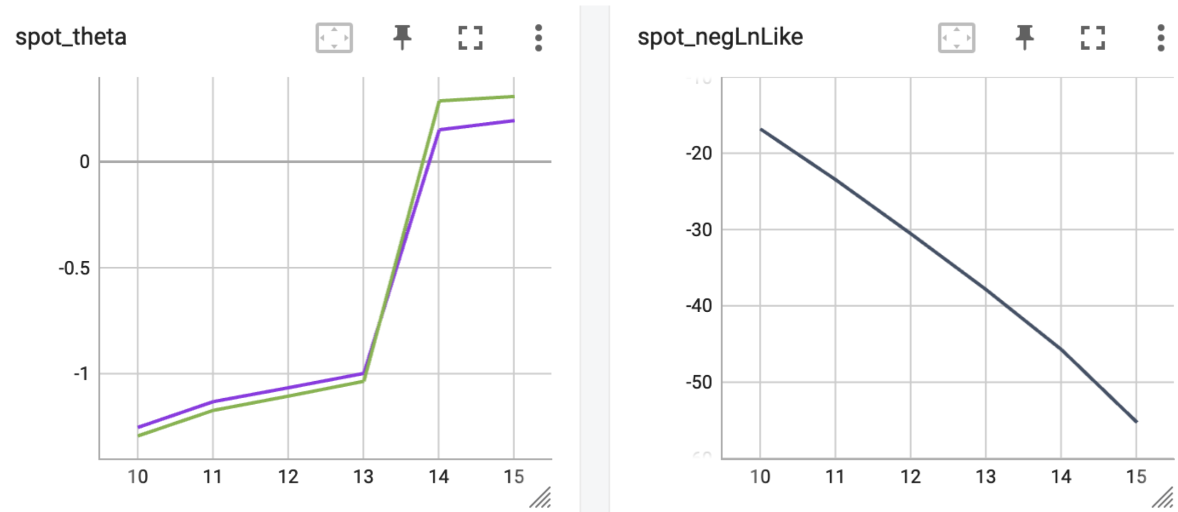


Figure 3.1: TensorBoard visualization of the spotPython surrogate model.

3.3 Exercises

3.3.1 `fun_branin`

- Describe the function.

– The input dimension is `2`. The search range is $-5 \leq x_1 \leq 10$ and $0 \leq x_2 \leq 15$.

- Compare the results from `spotPython` run a) with isotropic and b) anisotropic surrogate models.
- Modify the termination criterion: instead of the number of evaluations (which is specified via `fun_evals`), the time should be used as the termination criterion. This can be done as follows (`max_time=1` specifies a run time of one minute):

```
fun_evals=inf,
max_time=1,
```

3.3.2 `fun_sin_cos`

- Describe the function.
  – The input dimension is `2`. The search range is $-2\pi \leq x_1 \leq 2\pi$ and $-2\pi \leq x_2 \leq 2\pi$.
- Compare the results from `spotPython` run a) with isotropic and b) anisotropic surrogate models.
- Modify the termination criterion (`max_time` instead of `fun_evals`) as described for `fun_branin`.

3.3.3 `fun_runge`

- Describe the function.
  – The input dimension is `2`. The search range is $-5 \leq x_1 \leq 5$ and $-5 \leq x_2 \leq 5$.
- Compare the results from `spotPython` run a) with isotropic and b) anisotropic surrogate models.
- Modify the termination criterion (`max_time` instead of `fun_evals`) as described for `fun_branin`.

3.3.4 `fun_wingwt`

- Describe the function.
  – The input dimension is `10`. The search ranges are between 0 and 1 (values are mapped internally to their natural bounds).
- Compare the results from `spotPython` run a) with isotropic and b) anisotropic surrogate models.
- Modify the termination criterion (`max_time` instead of `fun_evals`) as described for `fun_branin`.

4 Using sklearn Surrogates in spotPython

This chapter explains how different surrogate models from scikit-learn can be used as surrogates in spotPython optimization runs.

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
```

4.1 Example: Branin Function with spotPython's Internal Kriging Surrogate

4.1.1 The Objective Function Branin

- The spotPython package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula.
- Here we will use the Branin function:

  ```
  y = a * (x2 - b * x1**2 + c * x1 - r) ** 2 + s * (1 - t) * np.cos(x1) + s,
  where values of a, b, c, r, s and t are: a = 1, b = 5.1 / (4*pi**2),
  c = 5 / pi, r = 6, s = 10 and t = 1 / (8*pi).
  ```

- It has three global minima:

  ```
  f(x) = 0.397887 at (-pi, 12.275), (pi, 2.275), and (9.42478, 2.475).
  ```

```
from spotPython.fun.objectivefunctions import analytical
lower = np.array([-5,-0])
upper = np.array([10,15])
```

```
fun = analytical().fun_branin
```

TensorBoard

Similar to the one-dimensional case, which was introduced in Section Section **??**, we can use TensorBoard to monitor the progress of the optimization. We will use the same code, only the prefix is different:

```
from spotPython.utils.file import get_experiment_name
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_spot_tensorboard_path

PREFIX = "04"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)

fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name))
```

```
04_bartz09_2023-07-16_14-13-35
```

4.1.2 Running the surrogate model based optimizer `Spot`:

```
spot_2 = spot.Spot(fun=fun,
                   lower = lower,
                   upper = upper,
                   fun_evals = 20,
                   max_time = inf,
                   seed=123,
                   design_control={"init_size": 10},
                   fun_control=fun_control)
```

```
spot_2.run()
```

```
spotPython tuning: 3.4474628349075243 [######----] 55.00%

spotPython tuning: 3.4474628349075243 [######----] 60.00%

spotPython tuning: 3.039485786016101 [######----] 65.00%

spotPython tuning: 3.039485786016101 [#######---] 70.00%
```

```
spotPython tuning: 1.1632959357427755 [########--] 75.00%

spotPython tuning: 0.6123887750698636 [########--] 80.00%

spotPython tuning: 0.4575920097730535 [########--] 85.00%

spotPython tuning: 0.3982295132785083 [#########-] 90.00%

spotPython tuning: 0.3982295132785083 [##########] 95.00%

spotPython tuning: 0.3982295132785083 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x17be6fc70>
```

4.1.3 TensorBoard

Now we can start TensorBoard in the background with the following command:

```
tensorboard --logdir="./runs"
```

We can access the TensorBoard web server with the following URL:

```
http://localhost:6006/
```

The TensorBoard plot illustrates how `spotPython` can be used as a microscope for the internal mechanisms of the surrogate-based optimization process. Here, one important parameter, the learning rate θ of the Kriging surrogate is plotted against the number of optimization steps.

4.1.4 Print the Results

```
spot_2.print_results()
```

```
min y: 0.3982295132785083
x0: 3.135528626303215
x1: 2.2926027772585886

[['x0', 3.135528626303215], ['x1', 2.2926027772585886]]
```

4.1.5 Show the Progress and the Surrogate

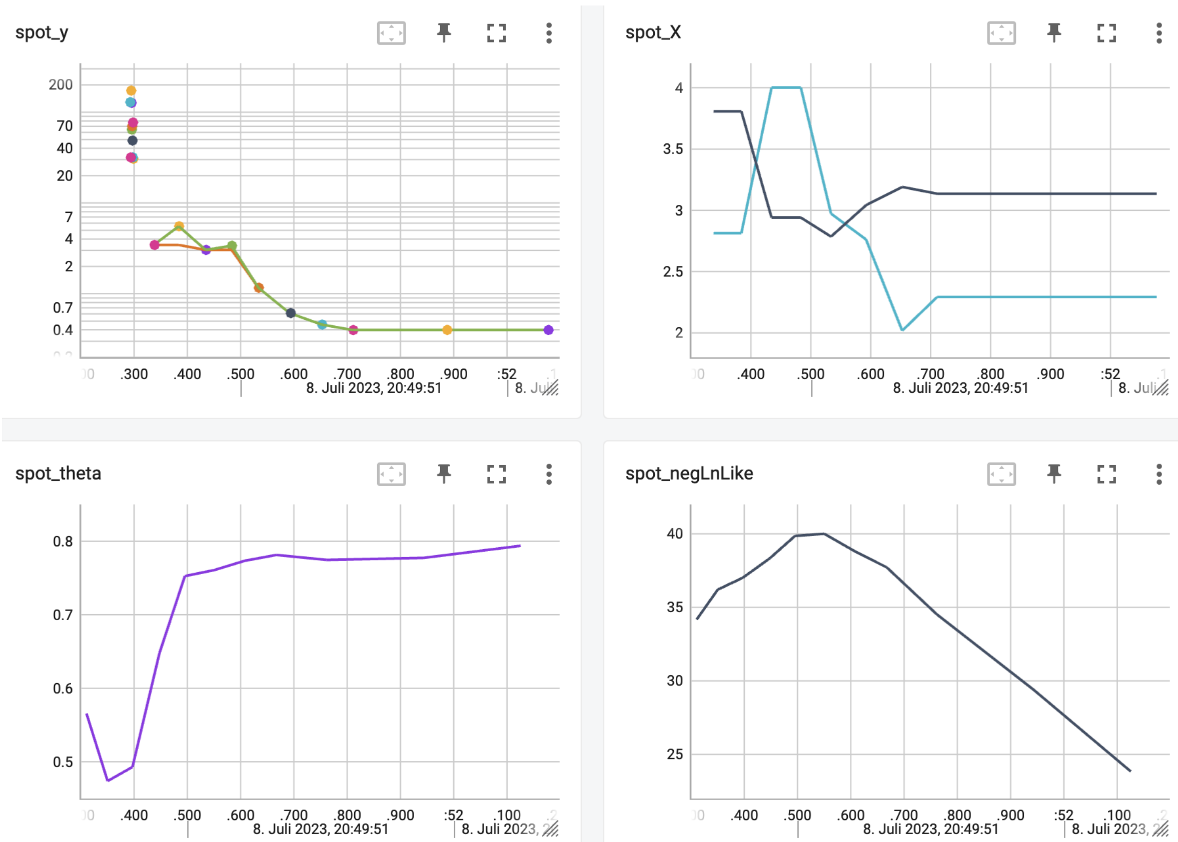


Figure 4.1: TensorBoard visualization of the spotPython optimization process and the surrogate model.

```
spot_2.plot_progress(log_y=True)
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-9-output-1.

```
spot_2.surrogate.plot()
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-10-output-1

4.2 Example: Using Surrogates From scikit-learn

- Default is the `spotPython` (i.e., the internal) `kriging` surrogate.
- It can be called explicitely and passed to `Spot`.

```
from spotPython.build.kriging import Kriging
S_0 = Kriging(name='kriging', seed=123)
```

- Alternatively, models from `scikit-learn` can be selected, e.g., Gaussian Process, RBFs, Regression Trees, etc.

```
# Needed for the sklearn surrogates:
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn import linear_model
from sklearn import tree
import pandas as pd
```

- Here are some additional models that might be useful later:

```python
S_Tree = DecisionTreeRegressor(random_state=0)
S_LM = linear_model.LinearRegression()
S_Ridge = linear_model.Ridge()
S_RF = RandomForestRegressor(max_depth=2, random_state=0)
```

4.2.1 GaussianProcessRegressor as a Surrogate

- To use a Gaussian Process model from `sklearn`, that is similar to `spotPython`'s `Kriging`, we can proceed as follows:

```python
kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
S_GP = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
```

- The scikit-learn GP model `S_GP` is selected for `Spot` as follows:

  `surrogate = S_GP`

- We can check the kind of surogate model with the command `isinstance`:

```python
isinstance(S_GP, GaussianProcessRegressor)
```

```
True
```

```python
isinstance(S_0, Kriging)
```

```
True
```

- Similar to the `Spot` run with the internal `Kriging` model, we can call the run with the `scikit-learn` surrogate:

```python
fun = analytical(seed=123).fun_branin
spot_2_GP = spot.Spot(fun=fun,
                     lower = lower,
                     upper = upper,
                     fun_evals = 20,
                     seed=123,
                     design_control={"init_size": 10},
                     surrogate = S_GP)
spot_2_GP.run()
```

```
spotPython tuning: 18.86511402323416 [######----] 55.00%

spotPython tuning: 4.0669082302178285 [######----] 60.00%

spotPython tuning: 3.4618162795514635 [######----] 65.00%

spotPython tuning: 3.4618162795514635 [#######---] 70.00%

spotPython tuning: 1.3283163482563598 [########--] 75.00%

spotPython tuning: 0.9542592376072765 [########--] 80.00%

spotPython tuning: 0.9289433893626615 [########--] 85.00%

spotPython tuning: 0.3981201359931852 [#########-] 90.00%

spotPython tuning: 0.39799355388506363 [##########] 95.00%

spotPython tuning: 0.39799355388506363 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x17f477610>
```

```
spot_2_GP.plot_progress()
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-18-output-1

```
spot_2_GP.print_results()
```

```
min y: 0.39799355388506363
x0: 3.1460470114516994
x1: 2.2748359190479013
```

```
[['x0', 3.1460470114516994], ['x1', 2.2748359190479013]]
```

4.3 Example: One-dimensional Sphere Function With `spotPython`'s Kriging

- In this example, we will use an one-dimensional function, which allows us to visualize the optimization process.
  - `show_models= True` is added to the argument list.

```
from spotPython.fun.objectivefunctions import analytical
lower = np.array([-1])
upper = np.array([1])
fun = analytical(seed=123).fun_sphere
```

```
spot_1 = spot.Spot(fun=fun,
                   lower = lower,
                   upper = upper,
                   fun_evals = 10,
                   max_time = inf,
                   seed=123,
                   show_models= True,
                   tolerance_x = np.sqrt(np.spacing(1)),
                   design_control={"init_size": 3},)
spot_1.run()
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-21-output-1

04_spot_sklearn_surrogate_files/figure-pdf/cell-21-output-2

```
spotPython tuning: 0.03475493366922229 [####------] 40.00%
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-21-output-4

```
spotPython tuning: 0.03475493366922229 [#####-----] 50.00%
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-21-output-6

```
spotPython tuning: 0.014958671130600643 [######----] 60.00%
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-21-output-8

```
spotPython tuning: 0.00021546330365371744 [#######---] 70.00%
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-21-output-1

```
spotPython tuning: 4.41925228274096e-08 [########--] 80.00%
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-21-output-1

```
spotPython tuning: 4.41925228274096e-08 [#########-] 90.00%
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-21-output-1

```
spotPython tuning: 4.41925228274096e-08 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x2b31fb8b0>
```

4.3.1 Results

```
spot_1.print_results()
```

```
min y: 4.41925228274096e-08
x0: -0.00021022017702259125
```

```
[['x0', -0.00021022017702259125]]
```

```
spot_1.plot_progress(log_y=True)
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-23-output-1

- The method `plot_model` plots the final surrogate:

```
spot_1.plot_model()
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-24-output-1

4.4 Example: `Sklearn` Model GaussianProcess

- This example visualizes the search process on the `GaussianProcessRegression` surrogate from `sklearn`.
- Therefore `surrogate = S_GP` is added to the argument list.

```
fun = analytical(seed=123).fun_sphere
spot_1_GP = spot.Spot(fun=fun,
                   lower = lower,
                   upper = upper,
                   fun_evals = 10,
                   max_time = inf,
                   seed=123,
                   show_models= True,
                   design_control={"init_size": 3},
                   surrogate = S_GP)
spot_1_GP.run()
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-25-output-1

04_spot_sklearn_surrogate_files/figure-pdf/cell-25-output-2

```
spotPython tuning: 0.004925761656816393 [####------] 40.00%
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-25-output-4

```
spotPython tuning: 0.0026120758453649505 [#####-----] 50.00%
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-25-output-6

spotPython tuning: 4.492968068412204e-07 [######----] 60.00%

04_spot_sklearn_surrogate_files/figure-pdf/cell-25-output-8

spotPython tuning: 5.520019085369139e-08 [#######---] 70.00%

04_spot_sklearn_surrogate_files/figure-pdf/cell-25-output-1

spotPython tuning: 1.8830522883506717e-08 [########--] 80.00%

04_spot_sklearn_surrogate_files/figure-pdf/cell-25-output-1

spotPython tuning: 1.2165253306918689e-08 [#########-] 90.00%

04_spot_sklearn_surrogate_files/figure-pdf/cell-25-output-1

```
spotPython tuning: 1.0471089618292772e-08 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x2b35f8b20>
```

```python
spot_1_GP.print_results()
```

```
min y: 1.0471089618292772e-08
x0: 0.00010232834220436082
```

```
[['x0', 0.00010232834220436082]]
```

```python
spot_1_GP.plot_progress(log_y=True)
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-27-output-1

```python
spot_1_GP.plot_model()
```

04_spot_sklearn_surrogate_files/figure-pdf/cell-28-output-1

4.5 Exercises

4.5.1 `DecisionTreeRegressor`

- Describe the surrogate model.
- Use the surrogate as the model for optimization.

4.5.2 `RandomForestRegressor`

- Describe the surrogate model.
- Use the surrogate as the model for optimization.

4.5.3 `linear_model.LinearRegression`

- Describe the surrogate model.
- Use the surrogate as the model for optimization.

4.5.4 `linear_model.Ridge`

- Describe the surrogate model.
- Use the surrogate as the model for optimization.

4.6 Exercise 2

- Compare the performance of the five different surrogates on both objective functions:
  - `spotPython`'s internal Kriging
  - `DecisionTreeRegressor`
  - `RandomForestRegressor`
  - `linear_model.LinearRegression`
  - `linear_model.Ridge`

5 Sequential Parameter Optimization: Using `scipy` Optimizers

This chapter describes how different optimizers from the `scipy optimize` package can be used on the surrogate. The optimization algorithms are available from https://docs.scipy.org/doc/scipy/reference/optimize.html

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
from scipy.optimize import dual_annealing
from scipy.optimize import basinhopping
```

5.1 The Objective Function Branin

- The `spotPython` package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula.
- Here we will use the Branin function. The 2-dim Branin function is

$$y = a * (x2 - b * x1 * *2 + c * x1 - r) * *2 + s * (1 - t) * cos(x1) + s,$$

  where values of a, b, c, r, s and t are: $a = 1, b = 5.1/(4 * pi * *2), c = 5/pi, r = 6, s = 10$ and $t = 1/(8 * pi)$.
- It has three global minima:

  $f(x) = 0.397887$ at $(-\pi, 12.275)$, $(\pi, 2.275)$, and $(9.42478, 2.475)$.
- Input Domain: This function is usually evaluated on the square x1 in [-5, 10] x x2 in [0, 15].

```python
from spotPython.fun.objectivefunctions import analytical
lower = np.array([-5,-0])
upper = np.array([10,15])
```

```python
fun = analytical(seed=123).fun_branin
```

5.2 The Optimizer

- Differential Evalution from the `scikit.optimize` package, see https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.differential_evolution.html#scipy.optimize.differential_evolution is the default optimizer for the search on the surrogate.
- Other optimiers that are available in `spotPython`:
  - `dual_annealing`
  - `direct`
  - `shgo`
  - `basinhopping`, see https://docs.scipy.org/doc/scipy/reference/optimize.html#global-optimization.
- These can be selected as follows:

  `surrogate_control = "model_optimizer": differential_evolution`
- We will use `differential_evolution`.
- The optimizer can use `1000` evaluations. This value will be passed to the `differential_evolution` method, which has the argument `maxiter` (int). It defines the maximum number of generations over which the entire differential evolution population is evolved, see https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.differential_evolution.html#scipy.optimize.differential_evolution

> **TensorBoard**
>
> Similar to the one-dimensional case, which was introduced in Section Section **??**, we can use TensorBoard to monitor the progress of the optimization. We will use the same code, only the prefix is different:

```python
from spotPython.utils.file import get_experiment_name
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_spot_tensorboard_path

PREFIX = "05_DE_"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)

fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name))
```

```
05_DE__bartz09_2023-07-16_14-14-03
```

```python
spot_de = spot.Spot(fun=fun,
                   lower = lower,
                   upper = upper,
                   fun_evals = 20,
                   max_time = inf,
                   seed=125,
                   noise=False,
                   show_models= False,
                   design_control={"init_size": 10},
                   surrogate_control={"n_theta": len(lower),
                                      "model_optimizer": differential_evolution,
                                      "model_fun_evals": 1000,
                                      },
                  fun_control=fun_control)
spot_de.run()
```

```
spotPython tuning: 5.213735995388665 [######----] 55.00%

spotPython tuning: 5.213735995388665 [######----] 60.00%

spotPython tuning: 2.5179080007735086 [######----] 65.00%

spotPython tuning: 1.0168713401682457 [#######---] 70.00%

spotPython tuning: 0.4160575412800043 [########--] 75.00%
```

```
spotPython tuning: 0.40966080781404557 [########--] 80.00%

spotPython tuning: 0.40966080781404557 [########--] 85.00%

spotPython tuning: 0.39989087044857285 [#########-] 90.00%

spotPython tuning: 0.3996741243343038 [##########] 95.00%

spotPython tuning: 0.39951958110619046 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2a1a2fd00>
```

5.2.1 TensorBoard

Now we can start TensorBoard in the background with the following command:

```
tensorboard --logdir="./runs"
```

We can access the TensorBoard web server with the following URL:

```
http://localhost:6006/
```

The TensorBoard plot illustrates how `spotPython` can be used as a microscope for the internal mechanisms of the surrogate-based optimization process. Here, one important parameter, the learning rate θ of the Kriging surrogate is plotted against the number of optimization steps.

5.3 Print the Results

```
spot_de.print_results()
```

```
min y: 0.39951958110619046
x0: -3.1570201165683587
x1: 12.289980569430284

[['x0', -3.1570201165683587], ['x1', 12.289980569430284]]
```

5.4 Show the Progress

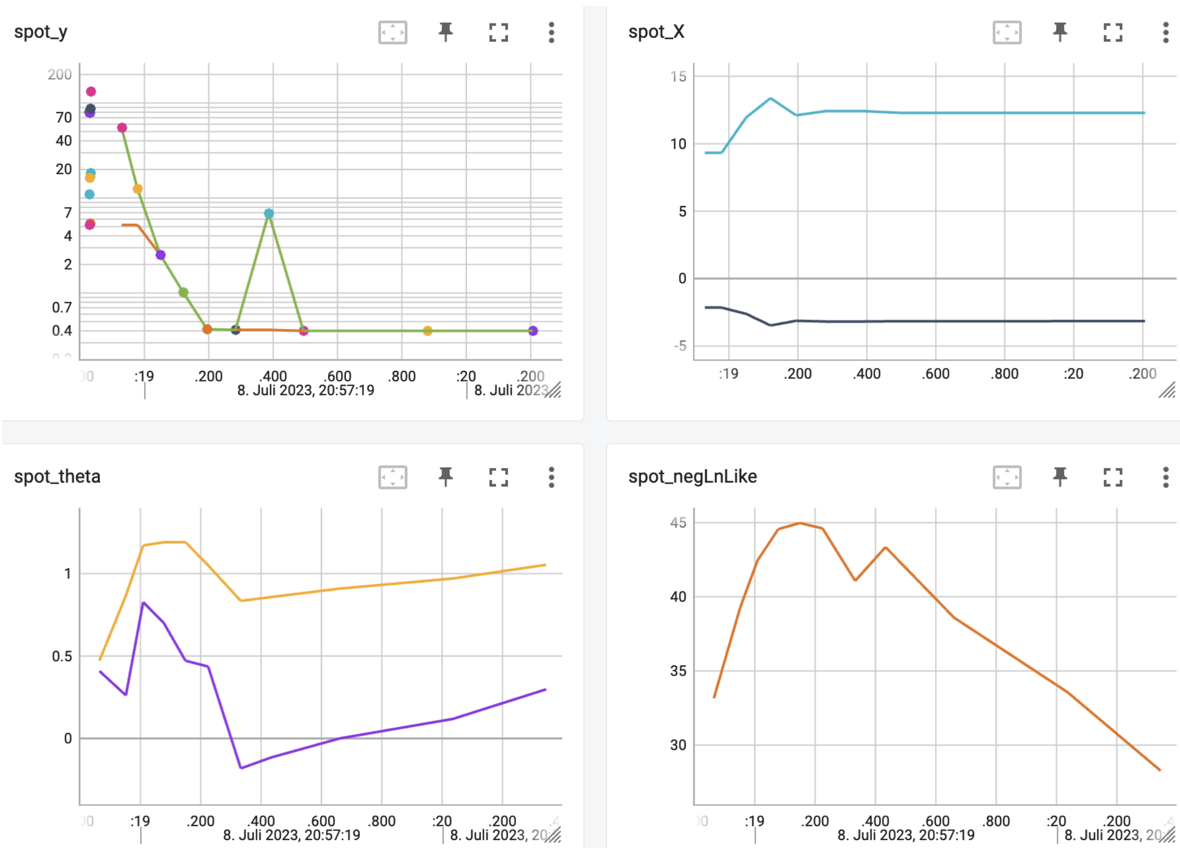


Figure 5.1: TensorBoard visualization of the spotPython optimization process and the surrogate model.

```
spot_de.plot_progress(log_y=True)
```

05_spot_sklearn_optimization_files/figure-pdf/cell-8-output

```
spot_de.surrogate.plot()
```

05_spot_sklearn_optimization_files/figure-pdf/cell-9-output

5.5 Exercises

5.5.1 `dual_annealing`

- Describe the optimization algorithm
- Use the algorithm as an optimizer on the surrogate

5.5.2 `direct`

- Describe the optimization algorithm
- Use the algorithm as an optimizer on the surrogate

5.5.3 `shgo`

- Describe the optimization algorithm
- Use the algorithm as an optimizer on the surrogate

5.5.4 `basinhopping`

- Describe the optimization algorithm
- Use the algorithm as an optimizer on the surrogate

5.5.5 Performance Comparison

Compare the performance and run time of the 5 different optimizers:

```
* `differential_evolution`
* `dual_annealing`
*  `direct`
* `shgo`
* `basinhopping`.
```

The Branin function has three global minima:

- $f(x) = 0.397887$ at
  - $(-\pi, 12.275)$,
  - $(\pi, 2.275)$, and
  - $(9.42478, 2.475)$.

- Which optima are found by the optimizers? Does the `seed` change this behavior?

6 Sequential Parameter Optimization: Gaussian Process Models

This Chapter analyzes differences between * the `Kriging` implementation in `spotPython` and * the `GaussianProcessRegressor` in `scikit-learn`.

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.design.spacefilling import spacefilling
from spotPython.spot import spot
from spotPython.build.kriging import Kriging
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
import math as m
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF
```

6.1 Gaussian Processes Regression: Basic Introductory `scikit-learn` Example

- This is the example from scikit-learn: https://scikit-learn.org/stable/auto_examples/gaussian_process/plot_
- After fitting our model, we see that the hyperparameters of the kernel have been optimized.
- Now, we will use our kernel to compute the mean prediction of the full dataset and plot the 95% confidence interval.

6.1.1 Train and Test Data

```
X = np.linspace(start=0, stop=10, num=1_000).reshape(-1, 1)
y = np.squeeze(X * np.sin(X))
rng = np.random.RandomState(1)
training_indices = rng.choice(np.arange(y.size), size=6, replace=False)
X_train, y_train = X[training_indices], y[training_indices]
```

6.1.2 Building the Surrogate With `Sklearn`

- The model building with `sklearn` consisits of three steps:
  1. Instantiating the model, then
  2. fitting the model (using `fit`), and
  3. making predictions (using `predict`)

```
kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
gaussian_process = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
gaussian_process.fit(X_train, y_train)
mean_prediction, std_prediction = gaussian_process.predict(X, return_std=True)
```

6.1.3 Plotting the `Sklearn`Model

```
plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
plt.fill_between(
    X.ravel(),
    mean_prediction - 1.96 * std_prediction,
    mean_prediction + 1.96 * std_prediction,
    alpha=0.5,
    label=r"95% confidence interval",
)
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("sk-learn Version: Gaussian process regression on noise-free dataset")
```

06_spot_gaussian_files/figure-pdf/cell-5-output-1.pdf

6.1.4 The spotPython Version

- The `spotPython` version is very similar:
    1. Instantiating the model, then
    2. fitting the model and
    3. making predictions (using `predict`).

```
S = Kriging(name='kriging',  seed=123, log_level=50, cod_type="norm")
S.fit(X_train, y_train)
S_mean_prediction, S_std_prediction, S_ei = S.predict(X, return_val="all")
```

```
plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, S_mean_prediction, label="Mean prediction")
plt.fill_between(
    X.ravel(),
    S_mean_prediction - 1.96 * S_std_prediction,
    S_mean_prediction + 1.96 * S_std_prediction,
    alpha=0.5,
    label=r"95% confidence interval",
)
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("spotPython Version: Gaussian process regression on noise-free dataset")
```

06_spot_gaussian_files/figure-pdf/cell-7-output-1.pdf

6.1.5 Visualizing the Differences Between the `spotPython` and the `sklearn` Model Fits

```
plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, S_mean_prediction, label="spotPython Mean prediction")
plt.plot(X, mean_prediction, label="Sklearn Mean Prediction")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Comparing Mean Predictions")
```

06_spot_gaussian_files/figure-pdf/cell-8-output-1.pdf

6.2 Exercises

6.2.1 `Schonlau Example Function`

- The Schonlau Example Function is based on sample points only (there is no analytical function description available):

```
X = np.linspace(start=0, stop=13, num=1_000).reshape(-1, 1)
X_train = np.array([1., 2., 3., 4., 12.]).reshape(-1,1)
y_train = np.array([0., -1.75, -2, -0.5, 5.])
```

- Describe the function.
- Compare the two models that were build using the `spotPython` and the `sklearn` surrogate.
- Note: Since there is no analytical function available, you might be interested in adding some points and describe the effects.

6.2.2 `Forrester Example Function`

- The Forrester Example Function is defined as follows:

  `f(x) = (6x- 2)^2 sin(12x-4) for x in [0,1].`

- Data points are generated as follows:

```
X = np.linspace(start=-0.5, stop=1.5, num=1_000).reshape(-1, 1)
X_train = np.array([0.0, 0.175, 0.225, 0.3, 0.35, 0.375, 0.5,1]).reshape(-1,1)
fun = analytical().fun_forrester
fun_control = {"sigma": 0.1,
               "seed": 123}
y = fun(X, fun_control=fun_control)
y_train = fun(X_train, fun_control=fun_control)
```

- Describe the function.
- Compare the two models that were build using the `spotPython` and the `sklearn` surrogate.
- Note: Modify the noise level (`"sigma"`), e.g., use a value of `0.2`, and compare the two models.

```
fun_control = {"sigma": 0.2}
```

6.2.3 `fun_runge` Function (1-dim)

- The Runge function is defined as follows:

  `f(x) = 1/ (1 + sum(x_i))^2`

- Data points are generated as follows:

```
gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_runge
fun_control = {"sigma": 0.025,
               "seed": 123}
X_train = gen.scipy_lhd(10, lower=lower, upper = upper).reshape(-1,1)
y_train = fun(X, fun_control=fun_control)
X = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
y = fun(X, fun_control=fun_control)
```

- Describe the function.
- Compare the two models that were build using the `spotPython` and the `sklearn` surrogate.
- Note: Modify the noise level (`"sigma"`), e.g., use a value of `0.05`, and compare the two models.

```
fun_control = {"sigma": 0.5}
```

6.2.4 `fun_cubed (1-dim)`

- The Cubed function is defined as follows:

  `np.sum(X[i]** 3)`

- Data points are generated as follows:

```
gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_cubed
fun_control = {"sigma": 0.025,
               "seed": 123}
X_train = gen.scipy_lhd(10, lower=lower, upper = upper).reshape(-1,1)
y_train = fun(X, fun_control=fun_control)
X = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
y = fun(X, fun_control=fun_control)
```

- Describe the function.
- Compare the two models that were build using the `spotPython` and the `sklearn` surrogate.
- Note: Modify the noise level (`"sigma"`), e.g., use a value of `0.05`, and compare the two models.

```
fun_control = {"sigma": 0.05}
```

6.2.5 The Effect of Noise

How does the behavior of the `spotPython` fit changes when the argument `noise` is set to `True`, i.e.,

`S = Kriging(name='kriging',  seed=123, n_theta=1, noise=True)`

is used?

7 Expected Improvement

7.1 Example: `Spot` and the 1-dim Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
import matplotlib.pyplot as plt
```

7.1.1 The Objective Function: 1-dim Sphere

- The `spotPython` package provides several classes of objective functions.
- We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x) = x^2$$

```
fun = analytical().fun_sphere
```

```
fun = analytical().fun_sphere
```

- The size of the `lower` bound vector determines the problem dimension.
- Here we will use `np.array([-1])`, i.e., a one-dim function.

> **TensorBoard**
>
> Similar to the one-dimensional case, which was introduced in Section Section **??**, we can use TensorBoard to monitor the progress of the optimization. We will use the same code, only the prefix is different:

```python
from spotPython.utils.file import get_experiment_name
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_spot_tensorboard_path

PREFIX = "07_Y"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)

fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    sigma=0,
    seed=123,)
```

```
07_Y_bartz09_2023-07-16_14-14-52
```

```python
spot_1 = spot.Spot(fun=fun,
                   fun_evals = 25,
                   lower = np.array([-1]),
                   upper = np.array([1]),
                   design_control={"init_size": 10},
                   tolerance_x = np.sqrt(np.spacing(1)),
                   fun_control = fun_control,)

spot_1.run()
```

```
spotPython tuning: 7.263311682641849e-09 [####------] 44.00%

spotPython tuning: 7.263311682641849e-09 [#####-----] 48.00%

spotPython tuning: 7.263311682641849e-09 [#####-----] 52.00%

spotPython tuning: 7.263311682641849e-09 [######----] 56.00%

spotPython tuning: 3.696886711914087e-10 [######----] 60.00%

spotPython tuning: 3.696886711914087e-10 [######----] 64.00%

spotPython tuning: 3.696886711914087e-10 [#######---] 68.00%
```

```
spotPython tuning: 3.696886711914087e-10 [#######---] 72.00%

spotPython tuning: 3.696886711914087e-10 [########--] 76.00%

spotPython tuning: 3.696886711914087e-10 [########--] 80.00%

spotPython tuning: 3.696886711914087e-10 [########--] 84.00%

spotPython tuning: 3.696886711914087e-10 [#########-] 88.00%

spotPython tuning: 1.3792745942664307e-11 [#########-] 92.00%

spotPython tuning: 1.3792745942664307e-11 [##########] 96.00%

spotPython tuning: 1.3792745942664307e-11 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x10335f8b0>
```

7.1.2 Results

```python
spot_1.print_results()
```

```
min y: 1.3792745942664307e-11
x0: 3.7138586325632142e-06

[['x0', 3.7138586325632142e-06]]
```

```python
spot_1.plot_progress(log_y=True)
```

07_spot_ei_files/figure-pdf/cell-8-output-1.pdf

7.2 Same, but with EI as infill_criterion

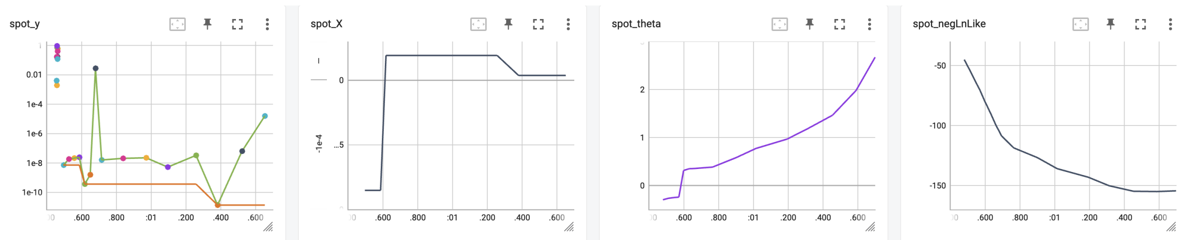


Figure 7.1: TensorBoard visualization of the spotPython optimization process and the surrogate model.

```
PREFIX = "07_EI_ISO"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    sigma=0,
    seed=123,)
```

```
07_EI_ISO_bartz09_2023-07-16_14-14-53
```

```
spot_1_ei = spot.Spot(fun=fun,
                   lower = np.array([-1]),
                   upper = np.array([1]),
                   fun_evals = 25,
                   tolerance_x = np.sqrt(np.spacing(1)),
                   infill_criterion = "ei",
                   design_control={"init_size": 10},
                   fun_control = fun_control,)
spot_1_ei.run()
```

```
spotPython tuning: 1.1630341306771934e-08 [####------] 44.00%

spotPython tuning: 1.1630341306771934e-08 [#####-----] 48.00%

spotPython tuning: 1.1630341306771934e-08 [#####-----] 52.00%

spotPython tuning: 1.1630341306771934e-08 [######----] 56.00%

spotPython tuning: 2.207887258868953e-10 [######----] 60.00%
```

```
spotPython tuning: 2.207887258868953e-10 [######----] 64.00%

spotPython tuning: 2.207887258868953e-10 [#######---] 68.00%

spotPython tuning: 2.207887258868953e-10 [#######---] 72.00%

spotPython tuning: 2.207887258868953e-10 [########--] 76.00%

spotPython tuning: 2.207887258868953e-10 [########--] 80.00%

spotPython tuning: 2.207887258868953e-10 [########--] 84.00%

spotPython tuning: 2.207887258868953e-10 [#########-] 88.00%

spotPython tuning: 1.3536080613078865e-10 [#########-] 92.00%

spotPython tuning: 1.3536080613078865e-10 [##########] 96.00%

spotPython tuning: 1.3536080613078865e-10 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2b202d900>
```

```
spot_1_ei.plot_progress(log_y=True)
```

07_spot_ei_files/figure-pdf/cell-11-output-1.pdf

```
spot_1_ei.print_results()
```

```
min y: 1.3536080613078865e-10
x0: 1.1634466301931888e-05

[['x0', 1.1634466301931888e-05]]
```

7.3 Non-isotropic Kriging

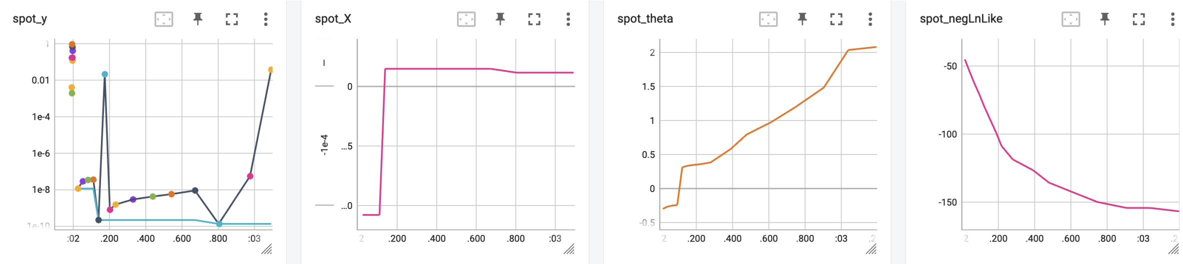


Figure 7.2: TensorBoard visualization of the spotPython optimization process and the surrogate model. Expected improvement, isotropic Kriging.

```
PREFIX = "07_EI_NONISO"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    sigma=0,
    seed=123,)
```

```
07_EI_NONISO_bartz09_2023-07-16_14-14-55
```

```
spot_2_ei_noniso = spot.Spot(fun=fun,
                   lower = np.array([-1, -1]),
                   upper = np.array([1, 1]),
                   fun_evals = 25,
                   tolerance_x = np.sqrt(np.spacing(1)),
                   infill_criterion = "ei",
                   show_models=True,
                   design_control={"init_size": 10},
                   surrogate_control={"noise": False,
                                      "cod_type": "norm",
                                      "min_theta": -4,
                                      "max_theta": 3,
                                      "n_theta": 2,
                                      "model_fun_evals": 1000,
                                      },
                    fun_control=fun_control,)
spot_2_ei_noniso.run()
```

```
spotPython tuning: 1.754686753274553e-05 [####------] 44.00%
```

```
spotPython tuning: 1.754686753274553e-05 [#####-----] 48.00%

spotPython tuning: 1.754686753274553e-05 [#####-----] 52.00%

spotPython tuning: 1.0120806700557811e-05 [######----] 56.00%

spotPython tuning: 1.0120806700557811e-05 [######----] 60.00%

spotPython tuning: 1.8779971830281702e-07 [######----] 64.00%

spotPython tuning: 1.8779971830281702e-07 [#######---] 68.00%

spotPython tuning: 1.8779971830281702e-07 [#######---] 72.00%

spotPython tuning: 1.8779971830281702e-07 [########--] 76.00%

spotPython tuning: 1.8779971830281702e-07 [########--] 80.00%

spotPython tuning: 1.8779971830281702e-07 [########--] 84.00%

spotPython tuning: 1.8779971830281702e-07 [#########-] 88.00%

spotPython tuning: 1.8779971830281702e-07 [#########-] 92.00%

spotPython tuning: 1.8779971830281702e-07 [##########] 96.00%

spotPython tuning: 1.8779971830281702e-07 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2b6611db0>
```

```python
spot_2_ei_noniso.plot_progress(log_y=True)
```

07_spot_ei_files/figure-pdf/cell-15-output-1.pdf

```
spot_2_ei_noniso.print_results()
```

```
min y: 1.8779971830281702e-07
x0: -0.0002783721390529846
x1: 0.0003321274913371111
```

```
[['x0', -0.0002783721390529846], ['x1', 0.0003321274913371111]]
```

```
spot_2_ei_noniso.surrogate.plot()
```

07_spot_ei_files/figure-pdf/cell-17-output-1.pdf

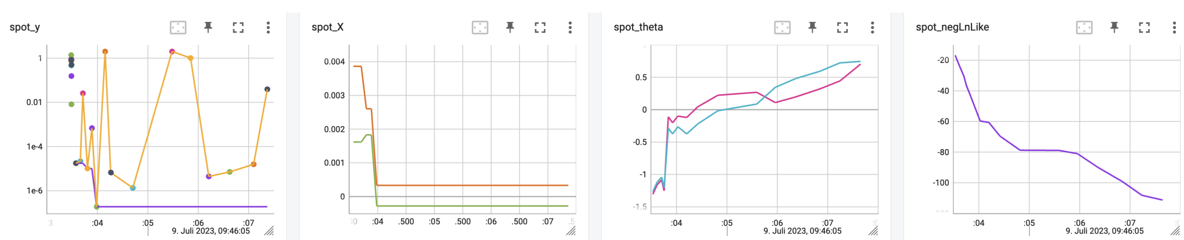


Figure 7.3: TensorBoard visualization of the spotPython optimization process and the surrogate model. Expected improvement, isotropic Kriging.

7.4 Using `sklearn` Surrogates

7.4.1 The spot Loop

The `spot` loop consists of the following steps:

1. Init: Build initial design X
2. Evaluate initial design on real objective f: $y = f(X)$
3. Build surrogate: $S = S(X, y)$
4. Optimize on surrogate: $X_0 = \text{optimize}(S)$
5. Evaluate on real objective: $y_0 = f(X_0)$

6. Impute (Infill) new points: $X = X \cup X_0$, $y = y \cup y_0$.
7. Got 3.

The `spot` loop is implemented in `R` as follows:

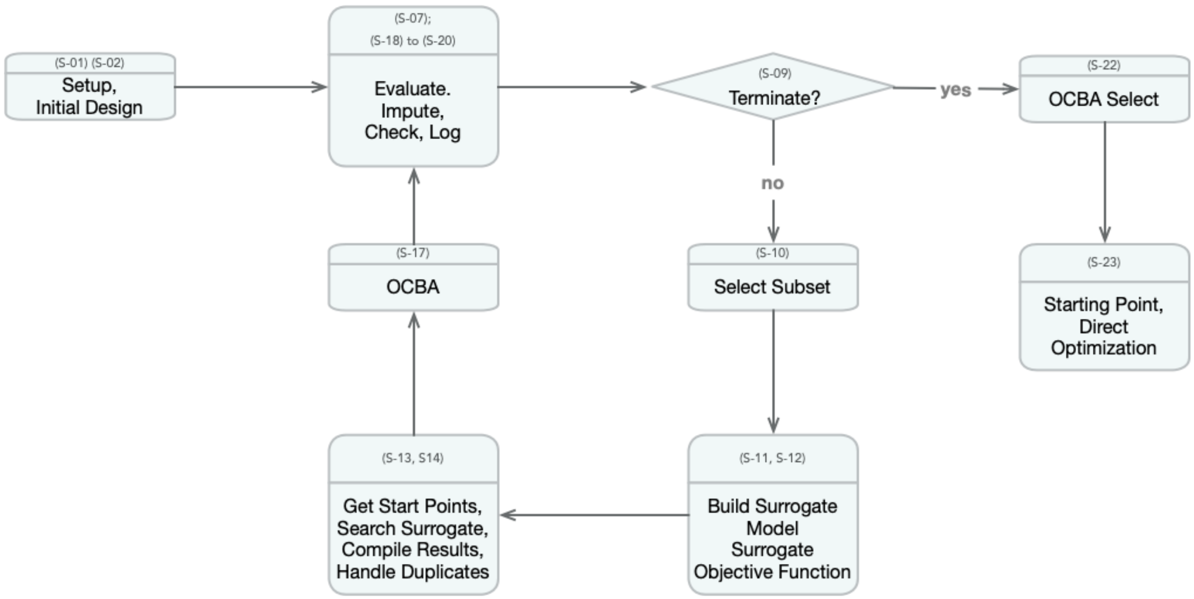


Figure 7.4: Visual representation of the model based search with SPOT. Taken from: Bartz-Beielstein, T., and Zaefferer, M. Hyperparameter tuning approaches. In Hyperparameter Tuning for Machine and Deep Learning with R - A Practical Guide, E. Bartz, T. Bartz-Beielstein, M. Zaefferer, and O. Mersmann, Eds. Springer, 2022, ch. 4, pp. 67–114.

7.4.2 spot: The Initial Model

7.4.2.1 Example: Modifying the initial design size

This is the "Example: Modifying the initial design size" from Chapter 4.5.1 in [bart21i].

```
spot_ei = spot.Spot(fun=fun,
                    lower = np.array([-1,-1]),
                    upper= np.array([1,1]),
                    design_control={"init_size": 5})
spot_ei.run()
```

```
spotPython tuning: 0.13881986540743513 [####------] 40.00%
```

```
spotPython tuning: 0.0111581443080968 [#####-----] 46.67%

spotPython tuning: 0.0010079970679825743 [#####-----] 53.33%

spotPython tuning: 0.000631621365403864 [######----] 60.00%

spotPython tuning: 0.0005883893741686826 [#######---] 66.67%

spotPython tuning: 0.00058412889636168 [#######---] 73.33%

spotPython tuning: 0.0005539414734082665 [########--] 80.00%

spotPython tuning: 0.0004401288692983916 [#########-] 86.67%

spotPython tuning: 5.8179647898944394e-05 [#########-] 93.33%

spotPython tuning: 1.7928640814182596e-05 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2b511f5b0>
```

```
spot_ei.plot_progress()
```

07_spot_ei_files/figure-pdf/cell-19-output-1.pdf

```
np.min(spot_1.y), np.min(spot_ei.y)
```

```
(1.3792745942664307e-11, 1.7928640814182596e-05)
```

7.4.3 Init: Build Initial Design

```python
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
from spotPython.fun.objectivefunctions import analytical
gen = spacefilling(2)
rng = np.random.RandomState(1)
lower = np.array([-5,-0])
upper = np.array([10,15])
fun = analytical().fun_branin

X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
print(y)
```

```
[[ 8.97647221 13.41926847]
 [ 0.66946019  1.22344228]
 [ 5.23614115 13.78185824]
 [ 5.6149825  11.5851384 ]
 [-1.72963184  1.66516096]
 [-4.26945568  7.1325531 ]
 [ 1.26363761 10.17935555]
 [ 2.88779942  8.05508969]
 [-3.39111089  4.15213772]
 [ 7.30131231  5.22275244]]
[128.95676449  31.73474356 172.89678121 126.71295908  64.34349975
  70.16178611  48.71407916  31.77322887  76.91788181  30.69410529]
```

```python
S = Kriging(name='kriging',  seed=123)
S.fit(X, y)
S.plot()
```

07_spot_ei_files/figure-pdf/cell-22-output-1.pdf

```python
gen = spacefilling(2, seed=123)
X0 = gen.scipy_lhd(3)
```

```
gen = spacefilling(2, seed=345)
X1 = gen.scipy_lhd(3)
X2 = gen.scipy_lhd(3)
gen = spacefilling(2, seed=123)
X3 = gen.scipy_lhd(3)
X0, X1, X2, X3
```

```
(array([[0.77254938, 0.31539299],
        [0.59321338, 0.93854273],
        [0.27469803, 0.3959685 ]]),
 array([[0.78373509, 0.86811887],
        [0.06692621, 0.6058029 ],
        [0.41374778, 0.00525456]]),
 array([[0.121357  , 0.69043832],
        [0.41906219, 0.32838498],
        [0.86742658, 0.52910374]]),
 array([[0.77254938, 0.31539299],
        [0.59321338, 0.93854273],
        [0.27469803, 0.3959685 ]]))
```

7.4.4 Evaluate

7.4.5 Build Surrogate

7.4.6 A Simple Predictor

The code below shows how to use a simple model for prediction.

- Assume that only two (very costly) measurements are available:

  1. f(0) = 0.5
  2. f(2) = 2.5

- We are interested in the value at $x_0 = 1$, i.e., $f(x_0 = 1)$, but cannot run an additional, third experiment.

```
from sklearn import linear_model
X = np.array([[0], [2]])
y = np.array([0.5, 2.5])
S_lm = linear_model.LinearRegression()
S_lm = S_lm.fit(X, y)
```

```
X0 = np.array([[1]])
y0 = S_lm.predict(X0)
print(y0)
```

```
[1.5]
```

- Central Idea:
  - Evaluation of the surrogate model `S_lm` is much cheaper (or / and much faster) than running the real-world experiment f.

7.5 Gaussian Processes regression: basic introductory example

This example was taken from scikit-learn. After fitting our model, we see that the hyperparameters of the kernel have been optimized. Now, we will use our kernel to compute the mean prediction of the full dataset and plot the 95% confidence interval.

```
import numpy as np
import matplotlib.pyplot as plt
import math as m
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF

X = np.linspace(start=0, stop=10, num=1_000).reshape(-1, 1)
y = np.squeeze(X * np.sin(X))
rng = np.random.RandomState(1)
training_indices = rng.choice(np.arange(y.size), size=6, replace=False)
X_train, y_train = X[training_indices], y[training_indices]

kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
gaussian_process = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
gaussian_process.fit(X_train, y_train)
gaussian_process.kernel_

mean_prediction, std_prediction = gaussian_process.predict(X, return_std=True)

plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
plt.fill_between(
    X.ravel(),
```

```
    mean_prediction - 1.96 * std_prediction,
    mean_prediction + 1.96 * std_prediction,
    alpha=0.5,
    label=r"95% confidence interval",
)
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("sk-learn Version: Gaussian process regression on noise-free dataset")
```

07_spot_ei_files/figure-pdf/cell-25-output-1.pdf

```
from spotPython.build.kriging import Kriging
import numpy as np
import matplotlib.pyplot as plt
rng = np.random.RandomState(1)
X = np.linspace(start=0, stop=10, num=1_000).reshape(-1, 1)
y = np.squeeze(X * np.sin(X))
training_indices = rng.choice(np.arange(y.size), size=6, replace=False)
X_train, y_train = X[training_indices], y[training_indices]


S = Kriging(name='kriging',  seed=123, log_level=50, cod_type="norm")
S.fit(X_train, y_train)

mean_prediction, std_prediction, ei = S.predict(X, return_val="all")

std_prediction

plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
plt.fill_between(
    X.ravel(),
    mean_prediction - 1.96 * std_prediction,
    mean_prediction + 1.96 * std_prediction,
```

```
    alpha=0.5,
    label=r"95% confidence interval",
)
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("spotPython Version: Gaussian process regression on noise-free dataset")
```

07_spot_ei_files/figure-pdf/cell-26-output-1.pdf

7.6 The Surrogate: Using scikit-learn models

Default is the internal `kriging` surrogate.

```
S_0 = Kriging(name='kriging', seed=123)
```

Models from `scikit-learn` can be selected, e.g., Gaussian Process:

```
# Needed for the sklearn surrogates:
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn import linear_model
from sklearn import tree
import pandas as pd
```

```
kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
S_GP = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
```

- and many more:

```
S_Tree = DecisionTreeRegressor(random_state=0)
S_LM = linear_model.LinearRegression()
S_Ridge = linear_model.Ridge()
```

```
S_RF = RandomForestRegressor(max_depth=2, random_state=0)
```

- The scikit-learn GP model `S_GP` is selected.

```
S = S_GP
```

```
isinstance(S, GaussianProcessRegressor)
```

```
True
```

```
from spotPython.fun.objectivefunctions import analytical
fun = analytical().fun_branin
lower = np.array([-5,-0])
upper = np.array([10,15])
design_control={"init_size": 5}
surrogate_control={
            "infill_criterion": None,
            "n_points": 1,
        }
spot_GP = spot.Spot(fun=fun, lower = lower, upper= upper, surrogate=S,
                    fun_evals = 15, noise = False, log_level = 50,
                    design_control=design_control,
                    surrogate_control=surrogate_control)

spot_GP.run()
```

```
spotPython tuning: 24.51465459019188 [####------] 40.00%

spotPython tuning: 11.003073503598229 [#####-----] 46.67%

spotPython tuning: 10.960665185123245 [#####-----] 53.33%

spotPython tuning: 10.960665185123245 [######----] 60.00%

spotPython tuning: 10.960665185123245 [#######---] 66.67%

spotPython tuning: 4.089511646427124 [#######---] 73.33%
```

```
spotPython tuning: 1.4230307255030858 [########--] 80.00%
```

```
spotPython tuning: 1.4230307255030858 [#########-] 86.67%
```

```
spotPython tuning: 1.4230307255030858 [#########-] 93.33%
```

```
spotPython tuning: 0.6949448160267053 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x2c86285b0>
```

```
spot_GP.y
```

```
array([ 69.32459936, 152.38491454, 107.92560483,  24.51465459,
        76.73500031,  86.30425659,  11.0030735 ,  10.96066519,
        16.06666933,  24.08428925,   4.08951165,   1.42303073,
         1.4736037 ,  16.03577039,   0.69494482])
```

```
spot_GP.plot_progress()
```

07_spot_ei_files/figure-pdf/cell-35-output-1.pdf

```
spot_GP.print_results()
```

```
min y: 0.6949448160267053
x0: 3.3575232000433637
x1: 2.3847893450472464
```

```
[['x0', 3.3575232000433637], ['x1', 2.3847893450472464]]
```

7.7 Additional Examples

```python
# Needed for the sklearn surrogates:
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn import linear_model
from sklearn import tree
import pandas as pd
```

```python
kernel = 1 * RBF(length_scale=1.0, length_scale_bounds=(1e-2, 1e2))
S_GP = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
```

```python
from spotPython.build.kriging import Kriging
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot

S_K = Kriging(name='kriging',
              seed=123,
              log_level=50,
              infill_criterion = "y",
              n_theta=1,
              noise=False,
              cod_type="norm")
fun = analytical().fun_sphere
lower = np.array([-1,-1])
upper = np.array([1,1])

design_control={"init_size": 10}
surrogate_control={
            "n_points": 1,
        }
spot_S_K = spot.Spot(fun=fun,
                     lower = lower,
                     upper= upper,
                     surrogate=S_K,
                     fun_evals = 25,
                     noise = False,
                     log_level = 50,
```

```
                             design_control=design_control,
                             surrogate_control=surrogate_control)

spot_S_K.run()
```

```
spotPython tuning: 2.0398360048852566e-05 [####------] 44.00%

spotPython tuning: 2.0398360048852566e-05 [#####-----] 48.00%

spotPython tuning: 2.0398360048852566e-05 [#####-----] 52.00%

spotPython tuning: 2.0398360048852566e-05 [######----] 56.00%

spotPython tuning: 2.0398360048852566e-05 [######----] 60.00%

spotPython tuning: 1.0937897482978201e-05 [######----] 64.00%

spotPython tuning: 3.950539536972047e-06 [#######---] 68.00%

spotPython tuning: 3.2602730419203698e-06 [#######---] 72.00%

spotPython tuning: 2.4704028732017656e-06 [########--] 76.00%

spotPython tuning: 1.7687713431606244e-06 [########--] 80.00%

spotPython tuning: 1.7395335905335862e-06 [########--] 84.00%

spotPython tuning: 1.7395335905335862e-06 [#########-] 88.00%

spotPython tuning: 1.7395335905335862e-06 [#########-] 92.00%

spotPython tuning: 1.7395335905335862e-06 [##########] 96.00%

spotPython tuning: 1.7395335905335862e-06 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2c8d26dd0>
```

```
spot_S_K.plot_progress(log_y=True)
```

07_spot_ei_files/figure-pdf/cell-40-output-1.pdf

```
spot_S_K.surrogate.plot()
```

07_spot_ei_files/figure-pdf/cell-41-output-1.pdf

```
spot_S_K.print_results()
```

```
min y: 1.7395335905335862e-06
x0: -0.0013044072412622557
x1: 0.0001950777780173277
```

```
[['x0', -0.0013044072412622557], ['x1', 0.0001950777780173277]]
```

7.7.1 Optimize on Surrogate

7.7.2 Evaluate on Real Objective

7.7.3 Impute / Infill new Points

7.8 Tests

```
import numpy as np
from spotPython.spot import spot
from spotPython.fun.objectivefunctions import analytical
```

```python
fun_sphere = analytical().fun_sphere
spot_1 = spot.Spot(
    fun=fun_sphere,
    lower=np.array([-1, -1]),
    upper=np.array([1, 1]),
    n_points = 2
)

# (S-2) Initial Design:
spot_1.X = spot_1.design.scipy_lhd(
    spot_1.design_control["init_size"], lower=spot_1.lower, upper=spot_1.upper
)
print(spot_1.X)

# (S-3): Eval initial design:
spot_1.y = spot_1.fun(spot_1.X)
print(spot_1.y)

spot_1.surrogate.fit(spot_1.X, spot_1.y)
X0 = spot_1.suggest_new_X()
print(X0)
assert X0.size == spot_1.n_points * spot_1.k
```

```
[[ 0.86352963  0.7892358 ]
 [-0.24407197 -0.83687436]
 [ 0.36481882  0.8375811 ]
 [ 0.415331    0.54468512]
 [-0.56395091 -0.77797854]
 [-0.90259409 -0.04899292]
 [-0.16484832  0.35724741]
 [ 0.05170659  0.07401196]
 [-0.78548145 -0.44638164]
 [ 0.64017497 -0.30363301]]
[1.36857656 0.75992983 0.83463487 0.46918172 0.92329124 0.8170764
 0.15480068 0.00815134 0.81623768 0.502017  ]
[[0.00160553 0.00428429]
 [0.00160553 0.00428429]]
```

7.9 EI: The Famous Schonlau Example

```
X_train0 = np.array([1, 2, 3, 4, 12]).reshape(-1,1)
X_train = np.linspace(start=0, stop=10, num=5).reshape(-1, 1)
```

```
from spotPython.build.kriging import Kriging
import numpy as np
import matplotlib.pyplot as plt

X_train = np.array([1., 2., 3., 4., 12.]).reshape(-1,1)
y_train = np.array([0., -1.75, -2, -0.5, 5.])

S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=1, noise=False, cod_type="nor
S.fit(X_train, y_train)

X = np.linspace(start=0, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
if True:
    plt.fill_between(
        X.ravel(),
        mean_prediction - 2 * std_prediction,
        mean_prediction + 2 * std_prediction,
        alpha=0.5,
        label=r"95% confidence interval",
    )
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noise-free dataset")
```

07_spot_ei_files/figure-pdf/cell-45-output-1.pdf

```python
#plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
# plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, -ei, label="Expected Improvement")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noise-free dataset")
```

07_spot_ei_files/figure-pdf/cell-46-output-1.pdf

```python
S.log
```

```
{'negLnLike': array([1.20788205]),
 'theta': array([1.09276]),
 'p': [],
 'Lambda': []}
```

7.10 EI: The Forrester Example

```python
from spotPython.build.kriging import Kriging
import numpy as np
import matplotlib.pyplot as plt
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot

# exact x locations are unknown:
X_train = np.array([0.0, 0.175, 0.225, 0.3, 0.35, 0.375, 0.5,1]).reshape(-1,1)

fun = analytical().fun_forrester
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    sigma=1.0,
    seed=123,)
```

```python
y_train = fun(X_train, fun_control=fun_control)

S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=1, noise=False, cod_type="nor
S.fit(X_train, y_train)

X = np.linspace(start=0, stop=1, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, mean_prediction, label="Mean prediction")
if True:
    plt.fill_between(
        X.ravel(),
        mean_prediction - 2 * std_prediction,
        mean_prediction + 2 * std_prediction,
        alpha=0.5,
        label=r"95% confidence interval",
    )
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noise-free dataset")
```

07_spot_ei_files/figure-pdf/cell-48-output-1.pdf

```python
#plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
# plt.scatter(X_train, y_train, label="Observations")
plt.plot(X, -ei, label="Expected Improvement")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noise-free dataset")
```

07_spot_ei_files/figure-pdf/cell-49-output-1.pdf

7.11 Noise

```python
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_sphere
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    sigma=2.0,
    seed=123,)
X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
print(y)
y.shape
X_train = X.reshape(-1,1)
y_train = y

S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=False)
S.fit(X_train, y_train)
```

```python
X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

#plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression on noisy dataset")
```

```
[[ 0.63529627]
 [-4.10764204]
 [-0.44071975]
 [ 9.63125638]
 [-8.3518118 ]
 [-3.62418901]
 [ 4.15331   ]
 [ 3.4468512 ]
 [ 6.36049088]
 [-7.77978539]]
[-1.57464135 16.13714981  2.77008442 93.14904827 71.59322218 14.28895359
 15.9770567  12.96468767 39.82265329 59.88028242]
```

07_spot_ei_files/figure-pdf/cell-50-output-2.pdf

```python
S.log
```

```
{'negLnLike': array([25.26601605]),
 'theta': array([-1.98024488]),
 'p': [],
 'Lambda': []}
```

```python
S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=True)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

#plt.plot(X, y, label=r"$f(x) = x \sin(x)$", linestyle="dotted")
plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression with nugget on noisy dataset")
```

07_spot_ei_files/figure-pdf/cell-52-output-1.pdf

```python
S.log
```

```
{'negLnLike': array([21.82530943]),
 'theta': array([-0.41935831]),
 'p': [],
 'Lambda': array([5.20850907e-05])}
```

7.12 Cubic Function

```python
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
```

```python
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_cubed
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    sigma=10.0,
    seed=123,)

X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
print(y)
y.shape
X_train = X.reshape(-1,1)
y_train = y

S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=1, noise=False)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Cubed: Gaussian process regression on noisy dataset")
```

```
[[ 0.63529627]
 [-4.10764204]
 [-0.44071975]
 [ 9.63125638]
 [-8.3518118 ]
 [-3.62418901]
```

```
 [ 4.15331   ]
 [ 3.4468512 ]
 [ 6.36049088]
 [-7.77978539]]
[  -9.63480707  -72.98497325   12.7936499   895.34567477 -573.35961837
  -41.83176425   65.27989461   46.37081417  254.1530734  -474.09587355]
```

07_spot_ei_files/figure-pdf/cell-54-output-2.pdf

```python
S = Kriging(name='kriging',  seed=123, log_level=0, n_theta=1, noise=True)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Cubed: Gaussian process with nugget regression on noisy dataset")
```

07_spot_ei_files/figure-pdf/cell-55-output-1.pdf

```python
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
```

```python
import matplotlib.pyplot as plt

gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_runge
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    sigma=0.25,
    seed=123,)

X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
print(y)
y.shape
X_train = X.reshape(-1,1)
y_train = y

S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=1, noise=False)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression on noisy dataset")
```

```
[[ 0.63529627]
 [-4.10764204]
 [-0.44071975]
 [ 9.63125638]
 [-8.3518118 ]
 [-3.62418901]
 [ 4.15331   ]
 [ 3.4468512 ]
```

```
 [ 6.36049088]
 [-7.77978539]]
[0.712453   0.05595118 0.83735691 0.0106654  0.01413372 0.07074765
 0.05479457 0.07763503 0.02412205 0.01625354]
```

07_spot_ei_files/figure-pdf/cell-56-output-2.pdf

```python
S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=True)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
#plt.plot(X, ei, label="Expected Improvement")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Gaussian process regression with nugget on noisy dataset")
```

07_spot_ei_files/figure-pdf/cell-57-output-1.pdf

7.13 Factors

```
["num"] * 3
```

```
['num', 'num', 'num']
```

```
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
from spotPython.fun.objectivefunctions import analytical
import numpy as np
```

```
gen = spacefilling(2)
n = 30
rng = np.random.RandomState(1)
lower = np.array([-5,-0])
upper = np.array([10,15])
fun = analytical().fun_branin_factor
#fun = analytical(sigma=0).fun_sphere

X0 = gen.scipy_lhd(n, lower=lower, upper = upper)
X1 = np.random.randint(low=1, high=3, size=(n,))
X = np.c_[X0, X1]
y = fun(X)
S = Kriging(name='kriging',  seed=123, log_level=50, n_theta=3, noise=False, var_type=["nu
S.fit(X, y)
Sf = Kriging(name='kriging',  seed=123, log_level=50, n_theta=3, noise=False, var_type=["n
Sf.fit(X, y)
n = 50
X0 = gen.scipy_lhd(n, lower=lower, upper = upper)
X1 = np.random.randint(low=1, high=3, size=(n,))
X = np.c_[X0, X1]
y = fun(X)
s=np.sum(np.abs(S.predict(X)[0] - y))
sf=np.sum(np.abs(Sf.predict(X)[0] - y))
sf - s
```

```
-40.48225931963543
```

```
# vars(S)
```

```
# vars(Sf)
```

8 Hyperparameter Tuning and Noise

This chapter demonstrates how noisy functions can be handled by `Spot`.

8.1 Example: `Spot` and the Noisy Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
import matplotlib.pyplot as plt
from spotPython.utils.file import get_experiment_name
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_spot_tensorboard_path

PREFIX = "08"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)
```

```
08_bartz09_2023-07-16_14-15-32
```

8.1.1 The Objective Function: Noisy Sphere

- The `spotPython` package provides several classes of objective functions.
- We will use an analytical objective function with noise, i.e., a function that can be described by a (closed) formula:
$$f(x) = x^2 + \epsilon$$
- Since `sigma` is set to `0.1`, noise is added to the function:

```
fun = analytical().fun_sphere
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
```

```
    sigma=0.02,
    seed=123,)
```

- A plot illustrates the noise:

```
x = np.linspace(-1,1,100).reshape(-1,1)
y = fun(x, fun_control=fun_control)
plt.figure()
plt.plot(x,y, "k")
plt.show()
```

08_spot_noisy_files/figure-pdf/cell-4-output-1.pdf

`Spot` is adopted as follows to cope with noisy functions:

1. `fun_repeats` is set to a value larger than 1 (here: 2)
2. `noise` is set to `true`. Therefore, a nugget (`Lambda`) term is added to the correlation matrix
3. `init size` (of the `design_control` dictionary) is set to a value larger than 1 (here: 2)

```
spot_1_noisy = spot.Spot(fun=fun,
                   lower = np.array([-1]),
                   upper = np.array([1]),
                   fun_evals = 20,
                   fun_repeats = 2,
                   noise = True,
                   seed=123,
                   show_models=True,
                   design_control={"init_size": 3,
                                   "repeats": 2},
                   surrogate_control={"noise": True},
                   fun_control=fun_control,)
```

```
spot_1_noisy.run()
```

08_spot_noisy_files/figure-pdf/cell-6-output-1.pdf

08_spot_noisy_files/figure-pdf/cell-6-output-2.pdf

```
spotPython tuning: 0.01497250376669991 [####------] 40.00%
```

08_spot_noisy_files/figure-pdf/cell-6-output-4.pdf

```
spotPython tuning: 0.01497226931667417 [#####-----] 50.00%
```

08_spot_noisy_files/figure-pdf/cell-6-output-6.pdf

```
spotPython tuning: 0.01496618769080537 [######----] 60.00%
```

08_spot_noisy_files/figure-pdf/cell-6-output-8.pdf

```
spotPython tuning: 0.014808104491512888 [#######---] 70.00%
```

08_spot_noisy_files/figure-pdf/cell-6-output-10.pdf

```
spotPython tuning: 0.011631261600357518 [########--] 80.00%
```

08_spot_noisy_files/figure-pdf/cell-6-output-12.pdf

```
spotPython tuning: -0.012946672238374722 [#########-] 90.00%
```

08_spot_noisy_files/figure-pdf/cell-6-output-14.pdf

```
spotPython tuning: -0.015070457665271902 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x2a880cdf0>
```

8.2 Print the Results

```
spot_1_noisy.print_results()
```

```
min y: -0.015070457665271902
x0: 0.06864378589271657
min mean y: -0.008857110676472227
x0: 0.06864378589271657
```

```
[['x0', 0.06864378589271657], ['x0', 0.06864378589271657]]
```

```
spot_1_noisy.plot_progress(log_y=False,
    filename="./figures/" + experiment_name+"_progress.png")
```

08_spot_noisy_files/figure-pdf/cell-8-output-1.pdf

Figure 8.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

8.3 Noise and Surrogates: The Nugget Effect

8.3.1 The Noisy Sphere

8.3.1.1 The Data

- We prepare some data first:

```
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_sphere
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    sigma=2,
    seed=123,)
X = gen.scipy_lhd(10, lower=lower, upper = upper)
y = fun(X, fun_control=fun_control)
```

```python
X_train = X.reshape(-1,1)
y_train = y
```

- A surrogate without nugget is fitted to these data:

```python
S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=False)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")

plt.scatter(X_train, y_train, label="Observations")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression on noisy dataset")
```

08_spot_noisy_files/figure-pdf/cell-10-output-1.pdf

- In comparison to the surrogate without nugget, we fit a surrogate with nugget to the data:

```python
S_nug = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=True)
S_nug.fit(X_train, y_train)
X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S_nug.predict(X_axis, return_val="all")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X_axis, mean_prediction, label="mue")
```

```
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression with nugget on noisy dataset")
```

08_spot_noisy_files/figure-pdf/cell-11-output-1.pdf

- The value of the nugget term can be extracted from the model as follows:

```
S.Lambda
```

```
S_nug.Lambda
```

```
5.2085090734655785e-05
```

- We see:
  - the first model `S` has no nugget,
  - whereas the second model has a nugget value (`Lambda`) larger than zero.

8.4 Exercises

8.4.1 Noisy `fun_cubed`

- Analyse the effect of noise on the `fun_cubed` function with the following settings:

```
fun = analytical().fun_cubed
fun_control = fun_control_init(
    sigma=10,
    seed=123,)
lower = np.array([-10])
upper = np.array([10])
```

8.4.2 fun_runge

- Analyse the effect of noise on the `fun_runge` function with the following settings:

```
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_runge
fun_control = fun_control_init(
    sigma=0.25,
    seed=123,)
```

8.4.3 fun_forrester

- Analyse the effect of noise on the `fun_forrester` function with the following settings:

```
lower = np.array([0])
upper = np.array([1])
fun = analytical().fun_forrester
fun_control = fun_control_init(
    sigma=5,
    seed=123,)
```

8.4.4 fun_xsin

- Analyse the effect of noise on the `fun_xsin` function with the following settings:

```
lower = np.array([-1.])
upper = np.array([1.])
fun = analytical().fun_xsin
fun_control = fun_control_init(
    sigma=0.5,
    seed=123,)
```

9 Handling Noise: Optimal Computational Budget Allocation in `Spot`

This chapter demonstrates how noisy functions can be handled with Optimal Computational Budget Allocation (OCBA) by `Spot`.

9.1 Example: `Spot`, OCBA, and the Noisy Sphere Function

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
import matplotlib.pyplot as plt
from spotPython.utils.file import get_experiment_name
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_spot_tensorboard_path

PREFIX = "09"
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)
```

```
09_bartz09_2023-07-16_14-15-49
```

9.1.1 The Objective Function: Noisy Sphere

The `spotPython` package provides several classes of objective functions. We will use an analytical objective function with noise, i.e., a function that can be described by a (closed) formula:

$$f(x) = x^2 + \epsilon$$

Since `sigma` is set to `0.1`, noise is added to the function:

```
fun = analytical().fun_sphere
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    sigma=0.1,
    seed=123,)
```

A plot illustrates the noise:

```
x = np.linspace(-1,1,100).reshape(-1,1)
y = fun(x, fun_control=fun_control)
plt.figure()
plt.plot(x,y, "k")
plt.show()
```

09_spot_ocba_files/figure-pdf/cell-4-output-1.pdf

`Spot` is adopted as follows to cope with noisy functions:

1. `fun_repeats` is set to a value larger than 1 (here: 2)
2. `noise` is set to `true`. Therefore, a nugget (`Lambda`) term is added to the correlation matrix
3. `init size` (of the `design_control` dictionary) is set to a value larger than 1 (here: 2)

```
spot_1_noisy = spot.Spot(fun=fun,
                   lower = np.array([-1]),
                   upper = np.array([1]),
                   fun_evals = 20,
                   fun_repeats = 2,
                   infill_criterion="ei",
                   noise = True,
                   tolerance_x=0.0,
                   ocba_delta = 1,
                   seed=123,
                   show_models=True,
                   fun_control = fun_control,
                   design_control={"init_size": 3,
                                   "repeats": 2},
```

```
                        surrogate_control={"noise": True})
```

```
spot_1_noisy.run()
```

09_spot_ocba_files/figure-pdf/cell-6-output-1.pdf

09_spot_ocba_files/figure-pdf/cell-6-output-2.pdf

```
spotPython tuning: -0.0641572013655628 [####------] 45.00%
```

09_spot_ocba_files/figure-pdf/cell-6-output-4.pdf

```
spotPython tuning: -0.08106318979661208 [######----] 60.00%
```

09_spot_ocba_files/figure-pdf/cell-6-output-6.pdf

```
spotPython tuning: -0.08106318979661208 [########--] 75.00%
```

09_spot_ocba_files/figure-pdf/cell-6-output-8.pdf

```
spotPython tuning: -0.08106318979661208 [#########-] 90.00%
```

09_spot_ocba_files/figure-pdf/cell-6-output-10.pdf

```
spotPython tuning: -0.08106318979661208 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x2abb04e20>
```

9.2 Print the Results

```
spot_1_noisy.print_results()
```

```
min y: -0.08106318979661208
x0: 0.1335999447536301
min mean y: -0.03275683462132762
x0: 0.1335999447536301
```

```
[['x0', 0.1335999447536301], ['x0', 0.1335999447536301]]
```

```
spot_1_noisy.plot_progress(log_y=False)
```

09_spot_ocba_files/figure-pdf/cell-8-output-1.pdf

9.3 Noise and Surrogates: The Nugget Effect

9.3.1 The Noisy Sphere

9.3.1.1 The Data

We prepare some data first:

```
import numpy as np
import spotPython
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
import matplotlib.pyplot as plt

gen = spacefilling(1)
rng = np.random.RandomState(1)
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_sphere
fun_control = fun_control_init(
    sigma=2,
    seed=125)
X = gen.scipy_lhd(10, lower=lower, upper = upper)
y = fun(X, fun_control=fun_control)
X_train = X.reshape(-1,1)
y_train = y
```

A surrogate without nugget is fitted to these data:

```
S = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=False)
S.fit(X_train, y_train)

X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S.predict(X_axis, return_val="all")
```

```python
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression on noisy dataset")
```

09_spot_ocba_files/figure-pdf/cell-10-output-1.pdf

In comparison to the surrogate without nugget, we fit a surrogate with nugget to the data:

```python
S_nug = Kriging(name='kriging',
            seed=123,
            log_level=50,
            n_theta=1,
            noise=True)
S_nug.fit(X_train, y_train)
X_axis = np.linspace(start=-13, stop=13, num=1000).reshape(-1, 1)
mean_prediction, std_prediction, ei = S_nug.predict(X_axis, return_val="all")
plt.scatter(X_train, y_train, label="Observations")
plt.plot(X_axis, mean_prediction, label="mue")
plt.legend()
plt.xlabel("$x$")
plt.ylabel("$f(x)$")
_ = plt.title("Sphere: Gaussian process regression with nugget on noisy dataset")
```

09_spot_ocba_files/figure-pdf/cell-11-output-1.pdf

The value of the nugget term can be extracted from the model as follows:

```python
S.Lambda
```

```
S_nug.Lambda
```

```
9.088150066416743e-05
```

We see:

- the first model `S` has no nugget,
- whereas the second model has a nugget value (`Lambda`) larger than zero.

9.4 Exercises

9.4.1 Noisy `fun_cubed`

Analyse the effect of noise on the `fun_cubed` function with the following settings:

```
fun = analytical().fun_cubed
fun_control = fun_control_init(
    sigma=10,
    seed=123)
lower = np.array([-10])
upper = np.array([10])
```

9.4.2 `fun_runge`

Analyse the effect of noise on the `fun_runge` function with the following settings:

```
lower = np.array([-10])
upper = np.array([10])
fun = analytical().fun_runge
fun_control = fun_control_init(
    sigma=0.25,
    seed=123)
```

9.4.3 `fun_forrester`

Analyse the effect of noise on the `fun_forrester` function with the following settings:

```
lower = np.array([0])
upper = np.array([1])
fun = analytical().fun_forrester
fun_control = {"sigma": 5,
               "seed": 123}
```

9.4.4 `fun_xsin`

Analyse the effect of noise on the `fun_xsin` function with the following settings:

```
lower = np.array([-1.])
upper = np.array([1.])
fun = analytical().fun_xsin
fun_control = fun_control_init(
    sigma=0.5,
    seed=123)
```

Part II

Hyperparameter Tuning

10 HPT: sklearn SVC on Moons Data

`spotPython` can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

10.1 Step 1: 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.

> Caution: Run time and initial design size should be increased for real experiments
>
> - MAX_TIME is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
> - INIT_SIZE is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.

```
MAX_TIME = 1
INIT_SIZE = 10
PREFIX = "10"
```

10.2 Step 2: Initialization of the Empty `fun_control` Dictionary

The `fun_control` dictionary is the central data structure that is used to control the optimization process. It is initialized as follows:

```
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_experiment_name, get_spot_tensorboard_path
from spotPython.utils.device import getDevice

experiment_name = get_experiment_name(prefix=PREFIX)
```

```
fun_control = fun_control_init(
    task="classification",
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    TENSORBOARD_CLEAN=True)
```

10.3 Step 3: SKlearn Load Data (Classification)

Randomly generate classification data.

```
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.datasets import make_moons, make_circles, make_classification
n_features = 2
n_samples = 500
target_column = "y"
ds =  make_moons(n_samples, noise=0.5, random_state=0)
X, y = ds
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.3, random_state=42
)
train = pd.DataFrame(np.hstack((X_train, y_train.reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, y_test.reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
train.head()
```

	x1	x2	y
0	1.960101	0.383172	0.0
1	2.354420	-0.536942	1.0
2	1.682186	-0.332108	0.0
3	1.856507	0.687220	1.0
4	1.925524	0.427413	1.0

```
import matplotlib.pyplot as plt
from matplotlib.colors import ListedColormap

x_min, x_max = X[:, 0].min() - 0.5, X[:, 0].max() + 0.5
```

```python
y_min, y_max = X[:, 1].min() - 0.5, X[:, 1].max() + 0.5
cm = plt.cm.RdBu
cm_bright = ListedColormap(["#FF0000", "#0000FF"])
ax = plt.subplot(1, 1, 1)
ax.set_title("Input data")
# Plot the training points
ax.scatter(X_train[:, 0], X_train[:, 1], c=y_train, cmap=cm_bright, edgecolors="k")
# Plot the testing points
ax.scatter(
    X_test[:, 0], X_test[:, 1], c=y_test, cmap=cm_bright, alpha=0.6, edgecolors="k"
)
ax.set_xlim(x_min, x_max)
ax.set_ylim(y_min, y_max)
ax.set_xticks(())
ax.set_yticks(())
plt.tight_layout()
plt.show()
```

10_spot_hpt_sklearn_classification_files/figure-pdf/cell-5-

```python
n_samples = len(train)
# add the dataset to the fun_control
fun_control.update({"data": None, # dataset,
               "train": train,
               "test": test,
               "n_samples": n_samples,
               "target_column": target_column})
```

10.4 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

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

A default approach for numerical data is the StandardScaler (mean 0, variance 1). This can be selected as follows:

```
from sklearn.preprocessing import StandardScaler
prep_model = StandardScaler()
fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

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

10.5 Step 5: Select Model (algorithm) and core_model_hyper_dict

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the sklearn implementation. For example, the SVC support vector machine classifier is selected as follows:

```
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from sklearn.svm import SVC
add_core_model_to_fun_control(core_model=SVC,
                              fun_control=fun_control,
                              hyper_dict=SklearnHyperDict,
                              filename=None)
```

Now fun_control has the information from the JSON file. The corresponding entries for the core_model class are shown below.

```
fun_control['core_model_hyper_dict']
```

```
{'C': {'type': 'float',
  'default': 1.0,
  'transform': 'None',
  'lower': 0.1,
  'upper': 10.0},
 'kernel': {'levels': ['linear', 'poly', 'rbf', 'sigmoid'],
  'type': 'factor',
  'default': 'rbf',
  'transform': 'None',
  'core_model_parameter_type': 'str',
  'lower': 0,
  'upper': 3},
 'degree': {'type': 'int',
  'default': 3,
  'transform': 'None',
  'lower': 3,
  'upper': 3},
 'gamma': {'levels': ['scale', 'auto'],
  'type': 'factor',
  'default': 'scale',
  'transform': 'None',
  'core_model_parameter_type': 'str',
  'lower': 0,
  'upper': 1},
 'coef0': {'type': 'float',
  'default': 0.0,
  'transform': 'None',
  'lower': 0.0,
  'upper': 0.0},
 'shrinking': {'levels': [0, 1],
  'type': 'factor',
  'default': 0,
  'transform': 'None',
  'core_model_parameter_type': 'bool',
  'lower': 0,
  'upper': 1},
 'probability': {'levels': [0, 1],
  'type': 'factor',
  'default': 0,
  'transform': 'None',
  'core_model_parameter_type': 'bool',
  'lower': 0,
  'upper': 1},
```

```
'tol': {'type': 'float',
 'default': 0.001,
 'transform': 'None',
 'lower': 0.0001,
 'upper': 0.01},
'cache_size': {'type': 'float',
 'default': 200,
 'transform': 'None',
 'lower': 100,
 'upper': 400},
'break_ties': {'levels': [0, 1],
 'type': 'factor',
 'default': 0,
 'transform': 'None',
 'core_model_parameter_type': 'bool',
 'lower': 0,
 'upper': 1}}
```

`sklearn` Model Selection

The following `sklearn` models are supported by default:

- RidgeCV
- RandomForestClassifier
- SVC
- LogisticRegression
- KNeighborsClassifier
- GradientBoostingClassifier
- GradientBoostingRegressor
- ElasticNet

They can be imported as follows:

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.linear_model import ElasticNet
```

10.6 Step 6: Modify hyper_dict Hyperparameters for the Selected Algorithm aka core_model

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 were described in Section ??.

10.6.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the modify_hyper_parameter_bounds method.

> **sklearn Model Hyperparameters**
>
> The hyperparameters of the sklearn SVC model are described in the sklearn documentation.

- For example, to change the tol hyperparameter of the SVC model to the interval [1e-5, 1e-3], the following code can be used:

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-5, 1e-3])
modify_hyper_parameter_bounds(fun_control, "probability", bounds=[0, 0])
fun_control["core_model_hyper_dict"]["tol"]
```

```
{'type': 'float',
 'default': 0.001,
 'transform': 'None',
 'lower': 1e-05,
 'upper': 0.001}
```

10.6.2 Modify hyperparameter of type factor

Factors can be modified with the modify_hyper_parameter_levels function. For example, to exclude the sigmoid kernel from the tuning, the kernel hyperparameter of the SVC model can be modified as follows:

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
modify_hyper_parameter_levels(fun_control, "kernel", ["poly", "rbf"])
fun_control["core_model_hyper_dict"]["kernel"]
```

```
{'levels': ['poly', 'rbf'],
 'type': 'factor',
 'default': 'rbf',
 'transform': 'None',
 'core_model_parameter_type': 'str',
 'lower': 0,
 'upper': 1}
```

10.6.3 Optimizers

Optimizers are described in Section **??**.

10.7 Step 7: Selection of the Objective (Loss) Function

There are two metrics:

1. `metric_river` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `metric_sklearn` is used for the sklearn based evaluation.

```python
from sklearn.metrics import mean_absolute_error, accuracy_score, roc_curve, roc_auc_score,
fun_control.update({
               "metric_sklearn": log_loss,
               "weights": 1.0,
               })
```

`metric_sklearn`: Minimization and Maximization

- Because the `metric_sklearn` is used for the sklearn based evaluation, it is important to know whether the metric should be minimized or maximized.
- The `weights` parameter is used to indicate whether the metric should be minimized or maximized.
- If `weights` is set to `-1.0`, the metric is maximized.
- If `weights` is set to `1.0`, the metric is minimized, e.g., `weights = 1.0` for `mean_absolute_error`, or `weights = -1.0` for `roc_auc_score`.

10.7.1 Predict Classes or Class Probabilities

If the key `"predict_proba"` is set to `True`, the class probabilities are predicted. `False` is the default, i.e., the classes are predicted.

```
fun_control.update({
               "predict_proba": False,
               })
```

10.8 Step 8: Calling the SPOT Function

10.8.1 Preparing the SPOT Call

The following code passes the information about the parameter ranges and bounds to `spot`.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (
    get_var_name,
    get_var_type,
    get_bound_values
    )
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

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

```
| name         | type   | default   |   lower |   upper | transform   |
|-------------|--------|-----------|---------|---------|-------------|
| C            | float  | 1.0       |   0.1   |  10     | None        |
| kernel       | factor | rbf       |   0     |   1     | None        |
| degree       | int    | 3         |   3     |   3     | None        |
| gamma        | factor | scale     |   0     |   1     | None        |
| coef0        | float  | 0.0       |   0     |   0     | None        |
| shrinking    | factor | 0         |   0     |   1     | None        |
| probability  | factor | 0         |   0     |   0     | None        |
| tol          | float  | 0.001     |   1e-05 |   0.001 | None        |
| cache_size   | float  | 200.0     | 100     | 400     | None        |
| break_ties   | factor | 0         |   0     |   1     | None        |
```

10.8.2 The Objective Function

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

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
# X_start = get_default_hyperparameters_as_array(fun_control)
```

10.8.3 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

10.8.4 Starting the Hyperparameter Tuning

```
import numpy as np
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,
```

```python
                        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()
```

```
spotPython tuning: 5.734217584632275 [----------] 1.53%

spotPython tuning: 5.734217584632275 [----------] 3.49%

spotPython tuning: 5.734217584632275 [#---------] 5.60%

spotPython tuning: 5.734217584632275 [#---------] 7.55%

spotPython tuning: 5.734217584632275 [#---------] 9.31%

spotPython tuning: 5.734217584632275 [#---------] 11.16%

spotPython tuning: 5.734217584632275 [#---------] 13.14%

spotPython tuning: 5.734217584632275 [##--------] 21.20%

spotPython tuning: 5.734217584632275 [###-------] 28.86%

spotPython tuning: 5.734217584632275 [####------] 37.71%

spotPython tuning: 5.734217584632275 [#####-----] 45.91%

spotPython tuning: 5.734217584632275 [######----] 55.29%

spotPython tuning: 5.734217584632275 [######----] 64.90%
```

```
spotPython tuning: 5.734217584632275 [#######---] 72.95%

spotPython tuning: 5.734217584632275 [########--] 84.60%

spotPython tuning: 5.734217584632275 [#########-] 92.46%

spotPython tuning: 5.734217584632275 [##########] 98.51%

spotPython tuning: 5.734217584632275 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x29bd5fe80>
```

10.9 Step 9: Results

```python
from spotPython.utils.file import save_pickle
save_pickle(spot_tuner, experiment_name)
```

```python
from spotPython.utils.file import load_pickle
spot_tuner = load_pickle(experiment_name)
```

- Show the Progress of the hyperparameter tuning:

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized.

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

10_spot_hpt_sklearn_classification_files/figure-pdf/cell-22

Figure 10.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

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

```
| name        | type   | default   |   lower |   upper |                tuned | transform
|-------------|--------|-----------|---------|---------|----------------------|-------------
| C           | float  | 1.0       |     0.1 |    10.0 |    2.394471655384338 | None
| kernel      | factor | rbf       |     0.0 |     1.0 |                  1.0 | None
| degree      | int    | 3         |     3.0 |     3.0 |                  3.0 | None
| gamma       | factor | scale     |     0.0 |     1.0 |                  0.0 | None
| coef0       | float  | 0.0       |     0.0 |     0.0 |                  0.0 | None
| shrinking   | factor | 0         |     0.0 |     1.0 |                  0.0 | None
| probability | factor | 0         |     0.0 |     0.0 |                  0.0 | None
| tol         | float  | 0.001     |   1e-05 |   0.001 | 0.000982585315792582 | None
| cache_size  | float  | 200.0     |   100.0 |   400.0 |    375.6371648003268 | None
| break_ties  | factor | 0         |     0.0 |     1.0 |                  0.0 | None
```

10.9.1 Show variable importance

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

10_spot_hpt_sklearn_classification_files/figure-pdf/cell-24

Figure 10.2: Variable importance plot, threshold 0.025.

10.9.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'C': 1.0,
 'kernel': 'rbf',
 'degree': 3,
```

```
 'gamma': 'scale',
 'coef0': 0.0,
 'shrinking': 0,
 'probability': 0,
 'tol': 0.001,
 'cache_size': 200.0,
 'break_ties': 0}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('standardscaler', StandardScaler()),
                ('svc',
                 SVC(break_ties=0, cache_size=200.0, probability=0,
                     shrinking=0))])
```

10.9.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[2.39447166e+00 1.00000000e+00 3.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00 9.82585316e-04
  3.75637165e+02 0.00000000e+00]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
[{'C': 2.394471655384338,
  'kernel': 'rbf',
  'degree': 3,
  'gamma': 'scale',
  'coef0': 0.0,
  'shrinking': 0,
  'probability': 0,
  'tol': 0.000982585315792582,
  'cache_size': 375.6371648003268,
  'break_ties': 0}]
```

```python
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

```
Pipeline(steps=[('standardscaler', StandardScaler()),
                ('svc',
                 SVC(C=2.394471655384338, break_ties=0,
                     cache_size=375.6371648003268, probability=0, shrinking=0,
                     tol=0.000982585315792582))])
```

10.9.4 Plot: Compare Predictions

```python
from spotPython.plot.validation import plot_roc
plot_roc([model_default, model_spot], fun_control, model_names=["Default", "Spot"])
```

10_spot_hpt_sklearn_classification_files/figure-pdf/cell-30

```python
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```

10_spot_hpt_sklearn_classification_files/figure-pdf/cell-31

```python
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```

10_spot_hpt_sklearn_classification_files/figure-pdf/cell-32

```
min(spot_tuner.y), max(spot_tuner.y)
```

```
(5.734217584632275, 7.782152436286657)
```

10.9.5 Detailed Hyperparameter Plots

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

```
C:  6.78742297418671
kernel:  100.0
```

10_spot_hpt_sklearn_classification_files/figure-pdf/cell-34

10.9.6 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

10.9.7 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
```

```
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

11 `river` Hyperparameter Tuning: Hoeffding Adaptive Tree Regressor with Friedman Drift Data

11.1 Setup

Before we consider the detailed experimental setup, we select the parameters that affect run time, initial design size, size of the data set, and the experiment name.

- `MAX_TIME`: The maximum run time in seconds for the hyperparameter tuning process.
- `INIT_SIZE`: The initial design size for the hyperparameter tuning process.
- `PREFIX`: The prefix for the experiment name.
- `K`: The factor that determines the number of samples in the data set.

Caution: Run time and initial design size should be increased for real experiments

- `MAX_TIME` is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
- `INIT_SIZE` is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.
- `K` is the multiplier for the number of samples. If it is set to 1, then `100_000`samples are taken. It is set to 0.1 for demonstration purposes. For real experiments, this should be increased to at least 1.

```
MAX_TIME = 1
INIT_SIZE = 5
PREFIX="10-river"
K = .1
```

```
import os
from spotPython.utils.file import get_experiment_name
experiment_name = get_experiment_name(prefix=PREFIX)
print(experiment_name)
```

10-river_bartz09_2023-07-16_14-21-16

- This notebook exemplifies hyperparameter tuning with SPOT (spotPython and spotRiver).
- The hyperparameter software SPOT was developed in R (statistical programming language), see Open Access book "Hyperparameter Tuning for Machine and Deep Learning with R - A Practical Guide", available here: https://link.springer.com/book/10.1007/978-981-19-5170-1.
- This notebook demonstrates hyperparameter tuning for `river`. It is based on the notebook "Incremental decision trees in river: the Hoeffding Tree case", see: https://riverml.xyz/0.15.0/recipes/on-hoeffding-trees/#42-regression-tree-splitters.
- Here we will use the river `HTR` and `HATR` functions as in "Incremental decision trees in river: the Hoeffding Tree case", see: https://riverml.xyz/0.15.0/recipes/on-hoeffding-trees/#42-regression-tree-splitters.

11.2 Initialization of the `fun_control` Dictionary

`spotPython` supports the visualization of the hyperparameter tuning process with TensorBoard. The following example shows how to use TensorBoard with `spotPython`.

First, we define an "experiment name" to identify the hyperparameter tuning process. The experiment name is also used to create a directory for the TensorBoard files.

```
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_spot_tensorboard_path

experiment_name = get_experiment_name(prefix=PREFIX)
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    TENSORBOARD_CLEAN=True)
```

Tip: TensorBoard

- Since the `spot_tensorboard_path` argument is not `None`, which is the default, `spotPython` will log the optimization process in the TensorBoard folder.
- Section **??** describes how to start TensorBoard and access the TensorBoard dashboard.
- The `TENSORBOARD_CLEAN` argument is set to `True` to archive the TensorBoard folder if it already exists. This is useful if you want to start a hyperparameter tuning process from scratch. If you want to continue a hyperparameter tuning process, set `TENSORBOARD_CLEAN` to `False`. Then the TensorBoard folder will not be archived and the old and new TensorBoard files will shown in the TensorBoard dashboard.

11.3 Load Data: The Friedman Drift Data

We will use the Friedman synthetic dataset with concept drifts [SOURCE]. Each observation is composed of ten features. Each feature value is sampled uniformly in [0, 1]. Only the first five features are relevant. The target is defined by different functions depending on the type of the drift. Global Recurring Abrupt drift will be used, i.e., the concept drift appears over the whole instance space. There are two points of concept drift. At the second point of drift the old concept reoccurs.

The following parameters are used to generate and handle the data set:

- horizon: The prediction horizon in hours.
- n_samples: The number of samples in the data set.
- p_1: The position of the first concept drift.
- p_2: The position of the second concept drift.
- position: The position of the concept drifts.
- n_train: The number of samples used for training.

```
horizon = 7*24
n_samples = int(K*100_000)
p_1 = int(K*25_000)
p_2 = int(K*50_000)
position=(p_1, p_2)
n_train = 1_000
```

```
from river.datasets import synth
import pandas as pd
dataset = synth.FriedmanDrift(
   drift_type='gra',
   position=position,
   seed=123
)
```

- We will use `spotRiver`'s `convert_to_df` function [SOURCE] to convert the `river` data set to a `pandas` data frame.

```
from spotRiver.utils.data_conversion import convert_to_df
target_column = "y"
df = convert_to_df(dataset, target_column=target_column, n_total=n_samples)
```

- Add column names x1 until x10 to the first 10 columns of the dataframe and the column name y to the last column of the dataframe.

- Then split the data frame into a training and test data set. The train and test data sets are stored in the `fun_control` dictionary.

```
df.columns = [f"x{i}" for i in range(1, 11)] + ["y"]
fun_control.update({"train":  df[:n_train],
                    "test":  df[n_train:],
                    "n_samples": n_samples,
                    "target_column": target_column})
```

11.4 Specification of the Preprocessing Model

- We use the `StandardScaler` [SOURCE] from `river` as the preprocessing model. The `StandardScaler` is used to standardize the data set, i.e., it has zero mean and unit variance.

```
from river import preprocessing
prep_model = preprocessing.StandardScaler()
fun_control.update({"prep_model": prep_model})
```

11.5 SelectSelect Model (`algorithm`) and `core_model_hyper_dict`

`spotPython` hyperparameter tuning approach uses two components:

1. a model (class) and
2. an associated hyperparameter dictionary.

Here, the `river` model class `HoeffdingAdaptiveTreeRegressor` [SOURCE] is selected.

The corresponding hyperparameters are loaded from the associated dictionary, which is stored as a JSON file [SOURCE]. The JSON file contains hyperparameter type information, names, and bounds.

The method `add_core_model_to_fun_control` adds the model and the hyperparameter dictionary to the `fun_control` dictionary.

Alternatively, you can load a local hyper_dict. Simply set `river_hyper_dict.json` as the filename. If `filename`is set to `None`, which is the default, the hyper_dict [SOURCE] is loaded from the `spotRiver` package.

```python
from river.tree import HoeffdingAdaptiveTreeRegressor
from spotRiver.data.river_hyper_dict import RiverHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
add_core_model_to_fun_control(core_model=HoeffdingAdaptiveTreeRegressor,
                              fun_control=fun_control,
                              hyper_dict=RiverHyperDict,
                              filename=None)
```

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

After the `core_model` and the `core_model_hyper_dict` are added to the `fun_control` dictionary, the hyperparameter tuning can be started. However, in some settings, the user wants to modify the hyperparameters of the `core_model_hyper_dict`. This can be done with the `modify_hyper_parameter_bounds` and `modify_hyper_parameter_levels` functions [SOURCE].

The following code shows how hyperparameter of type numeric and integer (boolean) can be modified. The `modify_hyper_parameter_bounds` function is used to modify the bounds of the hyperparameter `delta` and `merit_preprune`. Similar option exists for the `modify_hyper_parameter_levels` function to modify the levels of categorical hyperparameters.

```python
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
modify_hyper_parameter_bounds(fun_control, "delta", bounds=[1e-10, 1e-6])
modify_hyper_parameter_bounds(fun_control, "merit_preprune", [0, 0])
```

> **Note: Active and Inactive Hyperparameters**
>
> Hyperparameters can be excluded from the tuning procedure by selecting identical values for the lower and upper bounds. For example, the hyperparameter `merit_preprune` is excluded from the tuning procedure by setting the bounds to `[0, 0]`.

`spotPython`'s method `gen_design_table` summarizes the experimental design that is used for the hyperparameter tuning:

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

```
| name                     | type   | default          |       lower |     upper | transform
```

```
|------------------------|--------|------------------|------------|----------|---------------
| grace_period           | int    | 200              |     10     | 1000     | None
| max_depth              | int    | 20               |      2     |   20     | transform_powe
| delta                  | float  | 1e-07            |      1e-10 |    1e-06 | None
| tau                    | float  | 0.05             |      0.01  |    0.1   | None
| leaf_prediction        | factor | mean             |      0     |    2     | None
| leaf_model             | factor | LinearRegression |      0     |    2     | None
| model_selector_decay   | float  | 0.95             |      0.9   |    0.99  | None
| splitter               | factor | EBSTSplitter     |      0     |    2     | None
| min_samples_split      | int    | 5                |      2     |   10     | None
| bootstrap_sampling     | factor | 0                |      0     |    1     | None
| drift_window_threshold | int    | 300              |    100     |  500     | None
| switch_significance    | float  | 0.05             |      0.01  |    0.1   | None
| binary_split           | factor | 0                |      0     |    1     | None
| max_size               | float  | 500.0            |    100     | 1000     | None
| memory_estimate_period | int    | 1000000          | 100000     |    1e+06 | None
| stop_mem_management    | factor | 0                |      0     |    1     | None
| remove_poor_attrs      | factor | 0                |      0     |    1     | None
| merit_preprune         | factor | 0                |      0     |    0     | None
```

11.7 Selection of the Objective Function

The `metric_sklearn` is used for the sklearn based evaluation via `eval_oml_horizon` [SOURCE]. Here we use the `mean_absolute_error` [SOURCE] as the objective function.

> **Note: Additional metrics**
>
> `spotRiver` also supports additional metrics. For example, the `metric_river` is used for the river based evaluation via `eval_oml_iter_progressive` [SOURCE]. The `metric_river` is implemented to simulate the behaviour of the "original" `river` metrics.

`spotRiver` provides information about the model' s score (metric), memory, and time. The hyperparamter tuner requires a single objective. Therefore, a weighted sum of the metric, memory, and time is computed. The weights are defined in the `weights` array.

> **Note: Weights**
>
> The `weights` provide a flexible way to define specific requirements, e.g., if the memory is more important than the time, the weight for the memory can be increased.

The `oml_grace_period` defines the number of observations that are used for the initial training of the model. The `step` defines the iteration number at which to yield results. This only takes into account the predictions, and not the training steps. The `weight_coeff` defines a multiplier for the results: results are multiplied by (step/n_steps)**weight_coeff, where n_steps is the total number of iterations. Results from the beginning have a lower weight than results from the end if weight_coeff > 1. If weight_coeff == 0, all results have equal weight. Note, that the `weight_coeff` is only used internally for the tuner and does not affect the results that are used for the evaluation or comparisons.

```
import numpy as np
from sklearn.metrics import mean_absolute_error

weights = np.array([1, 1/1000, 1/1000])*10_000.0
oml_grace_period = 2
step = 100
weight_coeff = 1.0

fun_control.update({
               "horizon": horizon,
               "oml_grace_period": oml_grace_period,
               "weights": weights,
               "step": step,
               "weight_coeff": weight_coeff,
               "metric_sklearn": mean_absolute_error
               })
```

11.8 Calling the SPOT Function

11.8.1 Prepare the SPOT Parameters

The hyperparameter tuning configuration is stored in the `fun_control` dictionary. Since `Spot` can be used as an optimization algorithm with a similar interface as optimization algorithms from `scipy.optimize` [LINK], the bounds and variable types have to be specified explicitely. The `get_var_type`, `get_var_name`, and `get_bound_values` functions [SOURCE] implement the required functionality.

- Get types and variable names as well as lower and upper bounds for the hyperparameters, so that they can be passed to the `Spot` function.

```
from spotPython.hyperparameters.values import (
    get_var_type,
    get_var_name,
```

```
    get_bound_values
    )
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

11.8.2 The Objective Function

The objective function `fun_oml_horizon` [SOURCE] is selected next.

```
from spotRiver.fun.hyperriver import HyperRiver
fun = HyperRiver().fun_oml_horizon
```

The following code snippet shows how to get the default hyperparameters as an array, so that they can be passed to the `Spot` function.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
X_start = get_default_hyperparameters_as_array(fun_control)
```

11.8.3 Run the `Spot` Optimizer

The class `Spot` [SOURCE] is the hyperparameter tuning workhorse. It is initialized with the following parameters:

- `fun`: the objective function
- `lower`: lower bounds of the hyperparameters
- `upper`: upper bounds of the hyperparameters
- `fun_evals`: number of function evaluations
- `max_time`: maximum time in seconds
- `tolerance_x`: tolerance for the hyperparameters
- `var_type`: variable types of the hyperparameters
- `var_name`: variable names of the hyperparameters
- `show_progress`: show progress bar
- `fun_control`: dictionary with control parameters for the objective function
- `design_control`: dictionary with control parameters for the initial design
- `surrogate_control`: dictionary with control parameters for the surrogate model

Note: Total run time

The total run time may exceed the specified `max_time`, because the initial design (here: `init_size` = INIT_SIZE as specified above) is always evaluated, even if this takes longer than `max_time`.

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

```
spotPython tuning: 2.1993773044234755 [####------] 40.20%

spotPython tuning: 2.026725388455467 [#######---] 69.98%

spotPython tuning: 2.026725388455467 [#########-] 91.73%

spotPython tuning: 2.026725388455467 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2b1fcafe0>
```

11.8.4 TensorBoard

Now we can start TensorBoard in the background with the following command, where `./runs` is the default directory for the TensorBoard log files:

```
tensorboard --logdir="./runs"
```

> **Tip: TENSORBOARD_PATH**
>
> The TensorBoard path can be printed with the following command:
>
> ```
> from spotPython.utils.file import get_tensorboard_path
> get_tensorboard_path(fun_control)
> ```
>
> ```
> 'runs/'
> ```

We can access the TensorBoard web server with the following URL:

```
http://localhost:6006/
```

The TensorBoard plot illustrates how **spotPython** can be used as a microscope for the internal mechanisms of the surrogate-based optimization process. Here, one important parameter, the learning rate θ of the Kriging surrogate [SOURCE] is plotted against the number of optimization steps.

11.8.5 Results

After the hyperparameter tuning run is finished, the results can be saved and reloaded with the following commands:

```
from spotPython.utils.file import save_pickle
save_pickle(spot_tuner, experiment_name)
```

```
from spotPython.utils.file import load_pickle
spot_tuner = load_pickle(experiment_name)
```

After the hyperparameter tuning run is finished, the progress of the hyperparameter tuning can be visualized. The black points represent the performace values (score or metric) of hyperparameter configurations from the initial design, whereas the red points represents the hyperparameter configurations found by the surrogate model based optimization.

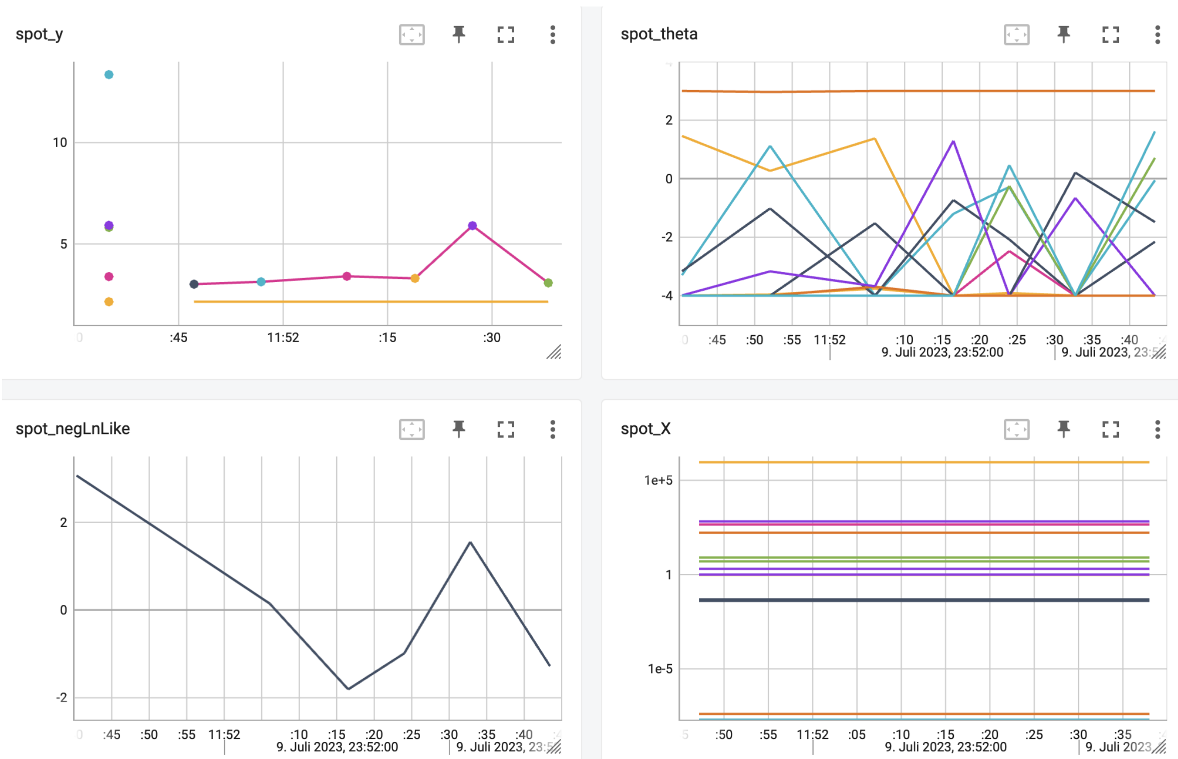


Figure 11.1: TensorBoard visualization of the spotPython optimization process and the surrogate model.

```
spot_tuner.plot_progress(log_y=True, filename="./figures/" + experiment_name+"_progress.pd
```

13_spot_hpt_river_files/figure-pdf/cell-21-output-1.pdf

Results can also be printed in tabular form.

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

```
| name                   | type   | default          |    lower |     upper |             tune
|------------------------|--------|------------------|----------|-----------|-----------------
| grace_period           | int    | 200              |     10.0 |    1000.0 |              218
| max_depth              | int    | 20               |      2.0 |      20.0 |               10
| delta                  | float  | 1e-07            |    1e-10 |     1e-06 |             1e-0
| tau                    | float  | 0.05             |     0.01 |       0.1 |                0
| leaf_prediction        | factor | mean             |      0.0 |       2.0 |                2
| leaf_model             | factor | LinearRegression |      0.0 |       2.0 |                0
| model_selector_decay   | float  | 0.95             |      0.9 |      0.99 |              0.9
| splitter               | factor | EBSTSplitter     |      0.0 |       2.0 |                2
| min_samples_split      | int    | 5                |      2.0 |      10.0 |                9
| bootstrap_sampling     | factor | 0                |      0.0 |       1.0 |                0
| drift_window_threshold | int    | 300              |    100.0 |     500.0 |              105
| switch_significance    | float  | 0.05             |     0.01 |       0.1 |              0.0
| binary_split           | factor | 0                |      0.0 |       1.0 |                0
| max_size               | float  | 500.0            |    100.0 |    1000.0 | 236.44742355804
| memory_estimate_period | int    | 1000000          | 100000.0 | 1000000.0 |           983671
| stop_mem_management    | factor | 0                |      0.0 |       1.0 |                0
| remove_poor_attrs      | factor | 0                |      0.0 |       1.0 |                1
| merit_preprune         | factor | 0                |      0.0 |       0.0 |                0
```

A histogram can be used to visualize the most important hyperparameters.

```
spot_tuner.plot_importance(threshold=0.0025, filename="./figures/" + experiment_name+"_imp
```

13_spot_hpt_river_files/figure-pdf/cell-23-output-1.pdf

11.9 The Larger Data Set

After the hyperparamter were tuned on a small data set, we can now apply the hyperparameter configuration to a larger data set. The following code snippet shows how to generate the larger data set.

> Caution: Increased Friedman-Drift Data Set
>
> - The Friedman-Drift Data Set is increased by a factor of two to show the transferability of the hyperparameter tuning results.
> - Larger values of `K` lead to a longer run time.

```
K = 0.2
n_samples = int(K*100_000)
p_1 = int(K*25_000)
p_2 = int(K*50_000)
position=(p_1, p_2)
```

```
dataset = synth.FriedmanDrift(
   drift_type='gra',
   position=position,
   seed=123
)
```

The larger data set is converted to a Pandas data frame and passed to the `fun_control` dictionary.

```
df = convert_to_df(dataset, target_column=target_column, n_total=n_samples)
df.columns = [f"x{i}" for i in range(1, 11)] + ["y"]
fun_control.update({"train": df[:n_train],
                    "test": df[n_train:],
                    "n_samples": n_samples,
                    "target_column": target_column})
```

11.10 Get Default Hyperparameters

The default hyperparameters, whihc will be used for a comparion with the tuned hyperparameters, can be obtained with the following commands:

```
from spotPython.hyperparameters.values import get_one_core_model_from_X
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
X_start = get_default_hyperparameters_as_array(fun_control)
model_default = get_one_core_model_from_X(X_start, fun_control)
```

> **Note: `spotPython` tunes numpy arrays**
>
> - `spotPython` tunes numpy arrays, i.e., the hyperparameters are stored in a numpy array.

The model with the default hyperparameters can be trained and evaluated with the following commands:

```
from spotRiver.evaluation.eval_bml import eval_oml_horizon

df_eval_default, df_true_default = eval_oml_horizon(
                    model=model_default,
                    train=fun_control["train"],
                    test=fun_control["test"],
                    target_column=fun_control["target_column"],
                    horizon=fun_control["horizon"],
                    oml_grace_period=fun_control["oml_grace_period"],
                    metric=fun_control["metric_sklearn"],
                )
```

The three performance criteria, i.e., scaoe (metric), runtime, and memory consumption, can be visualized with the following commands:

```
from spotRiver.evaluation.eval_bml import plot_bml_oml_horizon_metrics, plot_bml_oml_horiz
df_labels=["default"]
plot_bml_oml_horizon_metrics(df_eval = [df_eval_default], log_y=False, df_labels=df_labels
```

13_spot_hpt_river_files/figure-pdf/cell-29-output-1.pdf

11.10.1 Show Predictions

- Select a subset of the data set for the visualization of the predictions:
  - We use the mean, m, of the data set as the center of the visualization.
  - We use 100 data points, i.e., $m \pm 50$ as the visualization window.

```
m = fun_control["test"].shape[0]
a = int(m/2)-50
b = int(m/2)
```

```
plot_bml_oml_horizon_predictions(df_true = [df_true_default[a:b]], target_column=target_co
```

13_spot_hpt_river_files/figure-pdf/cell-31-output-1.pdf

11.11 Get SPOT Results

In a similar way, we can obtain the hyperparameters found by `spotPython`.

```
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)
```

```
df_eval_spot, df_true_spot = eval_oml_horizon(
                    model=model_spot,
                    train=fun_control["train"],
                    test=fun_control["test"],
                    target_column=fun_control["target_column"],
```

```
                          horizon=fun_control["horizon"],
                          oml_grace_period=fun_control["oml_grace_period"],
                          metric=fun_control["metric_sklearn"],
                      )
```

```
df_labels=["default", "spot"]
plot_bml_oml_horizon_metrics(df_eval = [df_eval_default, df_eval_spot], log_y=False, df_la
```

13_spot_hpt_river_files/figure-pdf/cell-34-output-1.pdf

```
plot_bml_oml_horizon_predictions(df_true = [df_true_default[a:b], df_true_spot[a:b]], targ
```

13_spot_hpt_river_files/figure-pdf/cell-35-output-1.pdf

```
from spotPython.plot.validation import plot_actual_vs_predicted
plot_actual_vs_predicted(y_test=df_true_default["y"], y_pred=df_true_default["Prediction"]
plot_actual_vs_predicted(y_test=df_true_spot["y"], y_pred=df_true_spot["Prediction"], titl
```

13_spot_hpt_river_files/figure-pdf/cell-36-output-1.pdf

13_spot_hpt_river_files/figure-pdf/cell-36-output-2.pdf

11.12 Visualize Regression Trees

```
dataset_f = dataset.take(n_samples)
for x, y in dataset_f:
    model_default.learn_one(x, y)
```

Caution: Large Trees

- Since the trees are large, the visualization is suppressed by default.
- To visualize the trees, uncomment the following line.

```
# model_default.draw()
```

```
model_default.summary
```

```
{'n_nodes': 35,
 'n_branches': 17,
 'n_leaves': 18,
 'n_active_leaves': 96,
 'n_inactive_leaves': 0,
 'height': 6,
 'total_observed_weight': 39002.0,
 'n_alternate_trees': 21,
 'n_pruned_alternate_trees': 6,
 'n_switch_alternate_trees': 2}
```

11.12.1 Spot Model

```
dataset_f = dataset.take(n_samples)
for x, y in dataset_f:
    model_spot.learn_one(x, y)
```

Caution: Large Trees

- Since the trees are large, the visualization is suppressed by default.
- To visualize the trees, uncomment the following line.

```python
# model_spot.draw()
```

```python
model_spot.summary
```

```
{'n_nodes': 173,
 'n_branches': 86,
 'n_leaves': 87,
 'n_active_leaves': 101,
 'n_inactive_leaves': 0,
 'height': 18,
 'total_observed_weight': 39002.0,
 'n_alternate_trees': 43,
 'n_pruned_alternate_trees': 40,
 'n_switch_alternate_trees': 0}
```

```python
from spotPython.utils.eda import compare_two_tree_models
print(compare_two_tree_models(model_default, model_spot))
```

```
| Parameter                 |    Default |    Spot |
|---------------------------|------------|---------|
| n_nodes                   |         35 |     173 |
| n_branches                |         17 |      86 |
| n_leaves                  |         18 |      87 |
| n_active_leaves           |         96 |     101 |
| n_inactive_leaves         |          0 |       0 |
| height                    |          6 |      18 |
| total_observed_weight     |      39002 |   39002 |
| n_alternate_trees         |         21 |      43 |
| n_pruned_alternate_trees  |          6 |      40 |
| n_switch_alternate_trees  |          2 |       0 |
```

11.13 Detailed Hyperparameter Plots

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

```
leaf_prediction:  0.03488006319675041
```

```
leaf_model:  2.581352361510414
splitter:  100.0
```

13_spot_hpt_river_files/figure-pdf/cell-44-output-2.pdf

13_spot_hpt_river_files/figure-pdf/cell-44-output-3.pdf

13_spot_hpt_river_files/figure-pdf/cell-44-output-4.pdf

11.14 Parallel Coordinates Plots

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

11.15 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

12 HPT: PyTorch With spotPython and Ray Tune on CIFAR10

In this tutorial, we will show how spotPython can be integrated into the PyTorch training workflow. It is based on the tutorial "Hyperparameter Tuning with Ray Tune" from the PyTorch documentation (PyTorch 2023a), which is an extension of the tutorial "Training a Classifier" (PyTorch 2023b) for training a CIFAR10 image classifier.

A typical hyperparameter tuning process with spotPython consists of the following steps:

1. Loading the data (training and test datasets), see Section ??.
2. Specification of the preprocessing model, see Section ??. This model is called prep_model ("preparation" or pre-processing). The information required for the hyperparameter tuning is stored in the dictionary fun_control. Thus, the information needed for the execution of the hyperparameter tuning is available in a readable form.
3. Selection of the machine learning or deep learning model to be tuned, see Section ??. This is called the core_model. Once the core_model is defined, then the associated hyperparameters are stored in the fun_control dictionary. First, the hyperparameters of the core_model are initialized with the default values of the core_model. As default values we use the default values contained in the spotPython package for the algorithms of the torch package.
4. Modification of the default values for the hyperparameters used in core_model, see Section ??. This step is optional.

    1. numeric parameters are modified by changing the bounds.
    2. categorical parameters are modified by changing the categories ("levels").

5. Selection of target function (loss function) for the optimizer, see Section ??.
6. Calling SPOT with the corresponding parameters, see Section ??. The results are stored in a dictionary and are available for further analysis.
7. Presentation, visualization and interpretation of the results, see Section ??.

spotPython can be installed via pip[1].

```
!pip install spotPython
```

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

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

Results that refer to the `Ray Tune` package are taken from https://PyTorch.org/tutorials/beginner/hyperparameter_tuning_tutorial.html[2].

12.1 Step 1: 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.

> Caution: Run time and initial design size should be increased for real experiments
>
> - MAX_TIME is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
> - INIT_SIZE is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.

> Note: Device selection
>
> - The device can be selected by setting the variable `DEVICE`.
> - Since we are using a simple neural net, the setting `"cpu"` is preferred (on Mac).
> - If you have a GPU, you can use `"cuda:0"` instead.
> - If DEVICE is set to `"auto"` or `None`, `spotPython` will automatically select the device.
>   - This might result in `"mps"` on Macs, which is not the best choice for simple neural nets.

```
MAX_TIME = 1
INIT_SIZE = 5
DEVICE = "auto" # "cpu"
PREFIX = "14-torch"
```

[2] We were not able to install `Ray Tune` on our system. Therefore, we used the results from the `PyTorch` tutorial.

```python
from spotPython.utils.device import getDevice
DEVICE = getDevice(DEVICE)
print(DEVICE)
```

```
mps
```

```python
import warnings
warnings.filterwarnings("ignore")
```

12.2 Step 2: 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.

```python
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_experiment_name, get_spot_tensorboard_path
from spotPython.utils.device import getDevice

experiment_name = get_experiment_name(prefix=PREFIX)

fun_control = fun_control_init(
    task="classification",
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    device=DEVICE,)
```

12.3 Step 3: PyTorch Data Loading

The data loading process is implemented in the same manner as described in the Section "Data loaders" in PyTorch (2023a). The data loaders are wrapped into the function `load_data_cifar10` which is identical to the function `load_data` in PyTorch (2023a). A global data directory is used, which allows sharing the data directory between different trials. The method `load_data_cifar10` is part of the `spotPython` package and can be imported from `spotPython.data.torchdata`.

In the following step, the test and train data are added to the dictionary `fun_control`.

```
from spotPython.data.torchdata import load_data_cifar10
train, test = load_data_cifar10()
n_samples = len(train)
# add the dataset to the fun_control
fun_control.update({
    "train": train,
    "test": test,
    "n_samples": n_samples})
```

```
Files already downloaded and verified
```

```
Files already downloaded and verified
```

12.4 Step 4: 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(),
     )
```

Because the Ray Tune (`ray[tune]`) hyperparameter tuning as described in PyTorch (2023a) does not use a preprocessing model, the preprocessing model is set to `None` here.

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

12.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The same neural network model as implemented in the section "Configurable neural network" of the `PyTorch` tutorial (PyTorch 2023a) is used here. We will show the implementation from PyTorch (2023a) in Section **??** first, before the extended implementation with `spotPython` is shown in Section **??**.

12.5.0.1 Implementing a Configurable Neural Network With Ray Tune

We used the same hyperparameters that are implemented as configurable in the `PyTorch` tutorial. We specify the layer sizes, namely `l1` and `l2`, of the fully connected layers:

```
class Net(nn.Module):
    def __init__(self, l1=120, l2=84):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(3, 6, 5)
        self.pool = nn.MaxPool2d(2, 2)
        self.conv2 = nn.Conv2d(6, 16, 5)
        self.fc1 = nn.Linear(16 * 5 * 5, l1)
        self.fc2 = nn.Linear(l1, l2)
        self.fc3 = nn.Linear(l2, 10)

    def forward(self, x):
        x = self.pool(F.relu(self.conv1(x)))
        x = self.pool(F.relu(self.conv2(x)))
        x = x.view(-1, 16 * 5 * 5)
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```

The learning rate, i.e., `lr`, of the optimizer is made configurable, too:

```
optimizer = optim.SGD(net.parameters(), lr=config["lr"], momentum=0.9)
```

12.5.0.2 Implementing a Configurable Neural Network With spotPython

`spotPython` implements a class which is similar to the class described in the `PyTorch` tutorial. The class is called `Net_CIFAR10` and is implemented in the file `netcifar10.py`.

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


class Net_CIFAR10(netcore.Net_Core):
    def __init__(self, l1, l2, lr_mult, batch_size, epochs, k_folds, patience,
    optimizer, sgd_momentum):
        super(Net_CIFAR10, self).__init__(
            lr_mult=lr_mult,
            batch_size=batch_size,
            epochs=epochs,
            k_folds=k_folds,
            patience=patience,
            optimizer=optimizer,
            sgd_momentum=sgd_momentum,
        )
        self.conv1 = nn.Conv2d(3, 6, 5)
        self.pool = nn.MaxPool2d(2, 2)
        self.conv2 = nn.Conv2d(6, 16, 5)
        self.fc1 = nn.Linear(16 * 5 * 5, l1)
        self.fc2 = nn.Linear(l1, l2)
        self.fc3 = nn.Linear(l2, 10)

    def forward(self, x):
        x = self.pool(F.relu(self.conv1(x)))
        x = self.pool(F.relu(self.conv2(x)))
        x = x.view(-1, 16 * 5 * 5)
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```

12.5.1 The `Net_Core` class

`Net_CIFAR10` 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
```

12.5.2 Comparison of the Approach Described in the PyTorch Tutorial With spotPython

Comparing the class Net from the PyTorch tutorial and the class Net_CIFAR10 from spotPython, we see that the class Net_CIFAR10 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_CIFAR10 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 hyperparameters and additional attributes to the fun_control dictionary. The method is shown below.

```
from spotPython.torch.netcifar10 import Net_CIFAR10
from spotPython.data.torch_hyper_dict import TorchHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
core_model = Net_CIFAR10
add_core_model_to_fun_control(core_model=core_model,
```

```
                                        fun_control=fun_control,
                                        hyper_dict=TorchHyperDict,
                                        filename=None)
```

12.5.3 The Search Space: Hyperparameters

In Section **??**, we first describe how to configure the search space with `ray[tune]` (as shown in PyTorch (2023a)) and then how to configure the search space with `spotPython` in -14.

12.5.4 Configuring the Search Space With Ray Tune

Ray Tune's search space can be configured as follows (PyTorch 2023a):

```
config = {
    "l1": tune.sample_from(lambda _: 2**np.random.randint(2, 9)),
    "l2": tune.sample_from(lambda _: 2**np.random.randint(2, 9)),
    "lr": tune.loguniform(1e-4, 1e-1),
    "batch_size": tune.choice([2, 4, 8, 16])
}
```

The `tune.sample_from()` function enables the user to define sample methods to obtain hyperparameters. In this example, the `l1` and `l2` parameters should be powers of 2 between 4 and 256, so either 4, 8, 16, 32, 64, 128, or 256. The `lr` (learning rate) should be uniformly sampled between 0.0001 and 0.1. Lastly, the batch size is a choice between 2, 4, 8, and 16.

At each trial, `ray[tune]` will 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. `ray[tune]` uses the `ASHAScheduler` which will terminate bad performing trials early.

12.5.5 Configuring the Search Space With spotPython

12.5.5.1 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`.

In contrast to `ray[tune]`, `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 core_model‘ class are shown below.

```
fun_control['core_model_hyper_dict']
```

```
{'l1': {'type': 'int',
  'default': 5,
  'transform': 'transform_power_2_int',
  'lower': 2,
  'upper': 9},
 'l2': {'type': 'int',
  'default': 5,
  'transform': 'transform_power_2_int',
  'lower': 2,
  'upper': 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': 3,
  'transform': 'transform_power_2_int',
  'lower': 3,
  'upper': 4},
 'k_folds': {'type': 'int',
```

```
  'default': 1,
  'transform': 'None',
  'lower': 1,
  'upper': 1},
 'patience': {'type': 'int',
  'default': 5,
  'transform': 'None',
  'lower': 2,
  'upper': 10},
 '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}}
```

12.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

Ray tune (PyTorch 2023a) does not provide a way to change the specified hyperparameters without re-compilation. However, `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.

12.6.0.1 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.

12.6.0.2 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".

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
modify_hyper_parameter_bounds(fun_control,
    "batch_size", bounds=[1, 5])
modify_hyper_parameter_bounds(fun_control,
    "k_folds", bounds=[0, 0])
modify_hyper_parameter_bounds(fun_control,
    "patience", bounds=[3, 3])
```

12.6.0.3 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.

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

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

```
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:

```
modify_hyper_parameter_levels(fun_control, "optimizer",
    ["Adadelta", "Adagrad", "Adam", "AdamW", "Adamax", "ASGD",
    "NAdam", "RAdam", "RMSprop", "SGD"])
```

12.6.1 Optimizers

Table **??** shows some of the optimizers available in `PyTorch`:

a denotes (0.9,0.999), b (0.5,1.2), and c (1e-6, 50), respectively. R denotes `required, but unspecified`. "m" denotes `momentum`, "w_d" `weight_decay`, "d" `dampening`, "n" `nesterov`, "r" `rho`, "l_s" `learning rate for scaling delta`, "l_d" `lr_decay`, "b" `betas`, "l" `lambd`, "a" `alpha`, "m_d" for `momentum_decay`, "e" `etas`, and "s_s" for `step_sizes`.

Table 12.1: Optimizers available in PyTorch (selection). The default values are shown in the table.

Optimizer	lr	m	w_d	d	n	r	l_s	l_d	b	l	a	m_d	e	s_s
Adadelta	-	-	0.	-	-	0.9	1.	-	-	-	-	-	-	-
Adagrad	1e-2	-	0.	-	-	-	-	0.	-	-	-	-	-	-
Adam	1e-3	-	0.	-	-	-	-	-	a	-	-	-	-	-
AdamW	1e-3	-	1e-2	-	-	-	-	-	a	-	-	-	-	-
SparseAdam	1e-3	-	-	-	-	-	-	-	a	-	-	-	-	-
Adamax	2e-3	-	0.	-	-	-	-	-	a	-	-	-	-	-
ASGD	1e-2	.9	0.	-	F	-	-	-	-	1e-4	.75	-	-	-
LBFGS	1.	-	-	-	-	-	-	-	-	-	-	-	-	-
NAdam	2e-3	-	0.	-	-	-	-	-	a	-	-	0	-	-
RAdam	1e-3	-	0.	-	-	-	-	-	a	-	-	-	-	-
RMSprop	1e-2	0.	0.	-	-	-	-	-	a	-	-	-	-	-
Rprop	1e-2	-	-	-	-	-	-	-	-	-	b	c	-	-
SGD	R	0.	0.	0.	F	-	-	-	-	-	-	-	-	-

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 ten 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`.

```
modify_hyper_parameter_bounds(fun_control,
    "lr_mult", bounds=[1.0, 1.0])
modify_hyper_parameter_bounds(fun_control,
    "sgd_momentum", bounds=[0.9, 0.9])
```

12.7 Step 7: Selection of the Objective (Loss) Function

12.7.1 Evaluation: Data Splitting

The evaluation procedure requires the specification of the way how the data is split into a train and a test set and the loss function (and a metric). As a default, `spotPython` provides a standard hold-out data split and cross validation.

12.7.2 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.

> **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).

12.7.3 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 2023a), it is not considered further here.

12.7.4 Overview of the Evaluation Settings

12.7.4.1 Settings for the Hyperparameter Tuning

An overview of the training evaluations is shown in Table **??**. `"train_cv"` and `"test_cv"` use `sklearn.model_selection.KFold()` internally. More details on the data splitting are provided in Section **??** (in the Appendix).

Table 12.2: 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
`"test_cv"`		✓	`evaluate_cv(net, test)`	CV using the `test` data set . Identical to `"train_cv"`, uses only test data.

12.7.4.2 Settings for the Final Evaluation of the Tuned Architecture

12.7.4.2.1 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 `train`data 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_hold_out()`. The `validation` data is used for early stopping using `validate_fold_or_hold_out()` on the `validation` data set.

12.7.4.2.2 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_fold_or_hold_out()` function. Note: During training, `"shuffle"` is set to `True`, whereas during testing, `"shuffle"` is set to `False`.

Section **??** describes the final evaluation of the tuned architecture.

```
fun_control.update({
    "eval": "train_hold_out",
    "path": "torch_model.pt",
    "shuffle": True})
```

12.7.5 Evaluation: 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.

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

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, see https://torchmetrics.readthedocs.io/en/latest/. Because the PyTorch tutorial uses the accuracy as metric, we use the same metric here. Currently, accuracy is computed in the tutorial's example code. We will use TorchMetrics instead, because it offers more flexibilty, e.g., it can be used for regression and classification. Furthermore, TorchMetrics offers the following advantages:

```
* A standardized interface to increase reproducibility
* Reduces Boilerplate
* Distributed-training compatible
* Rigorously tested
* Automatic accumulation over batches
* Automatic synchronization between multiple devices
```

Therefore, we set

```
import torchmetrics
metric_torch = torchmetrics.Accuracy(task="multiclass", num_classes=10).to(fun_control["de
fun_control.update({"metric_torch": metric_torch})
```

12.8 Step 8: Calling the SPOT Function

12.8.1 Preparing the SPOT Call

The following code passes the information about the parameter ranges and bounds to spot.

```
from spotPython.hyperparameters.values import (
    get_var_type,
    get_var_name,
    get_bound_values
    )
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)

lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

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))
```

```
| name         | type   | default   |    lower |    upper | transform             |
|--------------|--------|-----------|----------|----------|-----------------------|
| l1           | int    | 5         |      2   |      9   | transform_power_2_int |
| l2           | int    | 5         |      2   |      9   | transform_power_2_int |
| lr_mult      | float  | 1.0       |      1   |      1   | None                  |
| batch_size   | int    | 4         |      1   |      5   | transform_power_2_int |
| epochs       | int    | 3         |      3   |      4   | transform_power_2_int |
| k_folds      | int    | 1         |      0   |      0   | None                  |
| patience     | int    | 5         |      3   |      3   | None                  |
| optimizer    | factor | SGD       |      0   |      9   | None                  |
| sgd_momentum | float  | 0.0       |      0.9 |      0.9 | None                  |
```

This allows to check if all information is available and if the information is correct. **?@tbl-design** shows the 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. 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 $2^4 = 16$.

12.8.2 The Objective Function `fun_torch`

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
```

12.8.3 Using Default Hyperparameters or Results from Previous Runs

We add the default setting to the initial design:

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
X_start = get_default_hyperparameters_as_array(fun_control)
```

12.8.4 Starting the Hyperparameter Tuning

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`. During the run, results from the training is shown. These results can be visualized with Tensorboard as will be shown in Section **??**.

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

```
config: {'l1': 128, 'l2': 8, 'lr_mult': 1.0, 'batch_size': 32, 'epochs': 16, 'k_folds': 0, '
Epoch: 1 |

MulticlassAccuracy: 0.3889499902725220 | Loss: 1.6403590366363525 | Acc: 0.3889500000000000.
Epoch: 2 |
```

```
MulticlassAccuracy: 0.4578999876976013 | Loss: 1.4816969134330749 | Acc: 0.4579000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.4945999979972839 | Loss: 1.3767625138282775 | Acc: 0.4946000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.5118499994277954 | Loss: 1.3446329971313478 | Acc: 0.5118500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5447499752044678 | Loss: 1.2767737101554870 | Acc: 0.5447500000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5664499998092651 | Loss: 1.2234437763214112 | Acc: 0.5664500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5648499727249146 | Loss: 1.2325385323524476 | Acc: 0.5648500000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5896499752998352 | Loss: 1.1611093239784240 | Acc: 0.5896500000000000.
Epoch: 9 |

MulticlassAccuracy: 0.6015999913215637 | Loss: 1.1370150957107543 | Acc: 0.6016000000000000.
Epoch: 10 |

MulticlassAccuracy: 0.6074000000953674 | Loss: 1.1378371593475343 | Acc: 0.6074000000000001.
Epoch: 11 |

MulticlassAccuracy: 0.6036999821662903 | Loss: 1.1592556796073914 | Acc: 0.6037000000000000.
Epoch: 12 |

MulticlassAccuracy: 0.5997499823570251 | Loss: 1.1987680685997009 | Acc: 0.5997500000000000.
Early stopping at epoch 11
Returned to Spot: Validation loss: 1.1987680685997009

config: {'l1': 16, 'l2': 16, 'lr_mult': 1.0, 'batch_size': 8, 'epochs': 8, 'k_folds': 0, 'pa
Epoch: 1 |

MulticlassAccuracy: 0.3920499980449677 | Loss: 1.6102165319681168 | Acc: 0.3920500000000000.
Epoch: 2 |
```

```
MulticlassAccuracy: 0.4390000104904175 | Loss: 1.5077767979741097 | Acc: 0.4390000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.4700999855995178 | Loss: 1.4581756867766380 | Acc: 0.4701000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.4981499910354614 | Loss: 1.3969129746913911 | Acc: 0.4981500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5059000253677368 | Loss: 1.3693460956692696 | Acc: 0.5059000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5133500099182129 | Loss: 1.3540988440275192 | Acc: 0.5133500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5081499814987183 | Loss: 1.3817692994177342 | Acc: 0.5081500000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5159500241279602 | Loss: 1.3653468480706215 | Acc: 0.5159500000000000.
Returned to Spot: Validation loss: 1.3653468480706215

config: {'l1': 256, 'l2': 128, 'lr_mult': 1.0, 'batch_size': 2, 'epochs': 16, 'k_folds': 0,
Epoch: 1 |

MulticlassAccuracy: 0.0958499982953072 | Loss: 2.3086834851264952 | Acc: 0.0958500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.0987000018358231 | Loss: 2.3107500833988190 | Acc: 0.0987000000000000.
Epoch: 3 |

MulticlassAccuracy: 0.0958499982953072 | Loss: 2.3054559610605239 | Acc: 0.0958500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.1013000011444092 | Loss: 2.3091404678583145 | Acc: 0.1013000000000000.
Epoch: 5 |

MulticlassAccuracy: 0.0958499982953072 | Loss: 2.3109533527135850 | Acc: 0.0958500000000000.
Epoch: 6 |
```

```
MulticlassAccuracy: 0.0987000018358231 | Loss: 2.3080133529186249 | Acc: 0.0987000000000000.
Early stopping at epoch 5
Returned to Spot: Validation loss: 2.308013352918625

config: {'l1': 8, 'l2': 32, 'lr_mult': 1.0, 'batch_size': 4, 'epochs': 8, 'k_folds': 0, 'pat
Epoch: 1 |

MulticlassAccuracy: 0.3910000026226044 | Loss: 1.6194829273104667 | Acc: 0.3910000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.4532499909400940 | Loss: 1.5181912495672703 | Acc: 0.4532500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.5023999810218811 | Loss: 1.3594324642419815 | Acc: 0.5024000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.5066999793052673 | Loss: 1.3639220094040037 | Acc: 0.5067000000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5313000082969666 | Loss: 1.3084210138827563 | Acc: 0.5313000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5376499891281128 | Loss: 1.3020537653062492 | Acc: 0.5376500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5404999852180481 | Loss: 1.2979997927054763 | Acc: 0.5405000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5505999922752380 | Loss: 1.2794678398683668 | Acc: 0.5506000000000000.
Returned to Spot: Validation loss: 1.2794678398683668

config: {'l1': 64, 'l2': 512, 'lr_mult': 1.0, 'batch_size': 16, 'epochs': 16, 'k_folds': 0,
Epoch: 1 |

MulticlassAccuracy: 0.4688499867916107 | Loss: 1.4396714681148528 | Acc: 0.4688500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.4978500008583069 | Loss: 1.3743870592117309 | Acc: 0.4978500000000000.
Epoch: 3 |
```

```
MulticlassAccuracy: 0.5149000287055969 | Loss: 1.3301207626819611 | Acc: 0.5149000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.5352500081062317 | Loss: 1.2803554334163665 | Acc: 0.5352500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5407999753952026 | Loss: 1.2673199267387389 | Acc: 0.5407999999999999.
Epoch: 6 |

MulticlassAccuracy: 0.5474500060081482 | Loss: 1.2426155496835709 | Acc: 0.5474500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5532000064849854 | Loss: 1.2252585200309754 | Acc: 0.5532000000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5598499774932861 | Loss: 1.2217366221427917 | Acc: 0.5598500000000000.
Epoch: 9 |

MulticlassAccuracy: 0.5702000260353088 | Loss: 1.2027698907375335 | Acc: 0.5702000000000000.
Epoch: 10 |

MulticlassAccuracy: 0.5695499777793884 | Loss: 1.1946598905563355 | Acc: 0.5695500000000000.
Epoch: 11 |

MulticlassAccuracy: 0.5720999836921692 | Loss: 1.1931119963169099 | Acc: 0.5721000000000001.
Epoch: 12 |

MulticlassAccuracy: 0.5777500271797180 | Loss: 1.1757407437086105 | Acc: 0.5777500000000000.
Epoch: 13 |

MulticlassAccuracy: 0.5833500027656555 | Loss: 1.1655059050798415 | Acc: 0.5833500000000000.
Epoch: 14 |

MulticlassAccuracy: 0.5854499936103821 | Loss: 1.1665637883186339 | Acc: 0.5854500000000000.
Epoch: 15 |

MulticlassAccuracy: 0.5885499715805054 | Loss: 1.1581050729990006 | Acc: 0.5885500000000000.
Epoch: 16 |
```

```
MulticlassAccuracy: 0.5877500176429749 | Loss: 1.1598053013563157 | Acc: 0.5877500000000000.
Returned to Spot: Validation loss: 1.1598053013563157

config: {'l1': 64, 'l2': 256, 'lr_mult': 1.0, 'batch_size': 16, 'epochs': 16, 'k_folds': 0,

Epoch: 1 |

MulticlassAccuracy: 0.4435999989509583 | Loss: 1.5161994444847107 | Acc: 0.4436000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.4676499962806702 | Loss: 1.4507200250148773 | Acc: 0.4676500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.4885500073432922 | Loss: 1.4064176963806152 | Acc: 0.4885500000000000.
Epoch: 4 |

MulticlassAccuracy: 0.4984500110149384 | Loss: 1.3765785826206207 | Acc: 0.4984500000000000.
Epoch: 5 |

MulticlassAccuracy: 0.5091999769210815 | Loss: 1.3492139563083649 | Acc: 0.5092000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5235000252723694 | Loss: 1.3260424315452575 | Acc: 0.5235000000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5347999930381775 | Loss: 1.2992566047668457 | Acc: 0.5348000000000001.
Epoch: 8 |

MulticlassAccuracy: 0.5384500026702881 | Loss: 1.2924042490005494 | Acc: 0.5384500000000000.
Epoch: 9 |

MulticlassAccuracy: 0.5433999896049500 | Loss: 1.2770100817918777 | Acc: 0.5434000000000000.
Epoch: 10 |

MulticlassAccuracy: 0.5457999706268311 | Loss: 1.2646812784671784 | Acc: 0.5458000000000000.
Epoch: 11 |

MulticlassAccuracy: 0.5486000180244446 | Loss: 1.2627830792903900 | Acc: 0.5486000000000000.
Epoch: 12 |
```

```
MulticlassAccuracy: 0.5608000159263611 | Loss: 1.2396654787063599 | Acc: 0.5608000000000000.
Epoch: 13 |

MulticlassAccuracy: 0.5554000139236450 | Loss: 1.2407209475994110 | Acc: 0.5554000000000000.
Epoch: 14 |

MulticlassAccuracy: 0.5677000284194946 | Loss: 1.2263578844547272 | Acc: 0.5677000000000000.
Epoch: 15 |

MulticlassAccuracy: 0.5665000081062317 | Loss: 1.2272662802696228 | Acc: 0.5665000000000000.
Epoch: 16 |

MulticlassAccuracy: 0.5688999891281128 | Loss: 1.2138021411895752 | Acc: 0.5689000000000000.
Returned to Spot: Validation loss: 1.2138021411895752
spotPython tuning: 1.1598053013563157 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x16a83cac0>
```

12.9 Step 9: Tensorboard

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

12.9.1 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.

12.9.2 Saving the State of the Notebook

The state of the notebook can be saved and reloaded as follows:

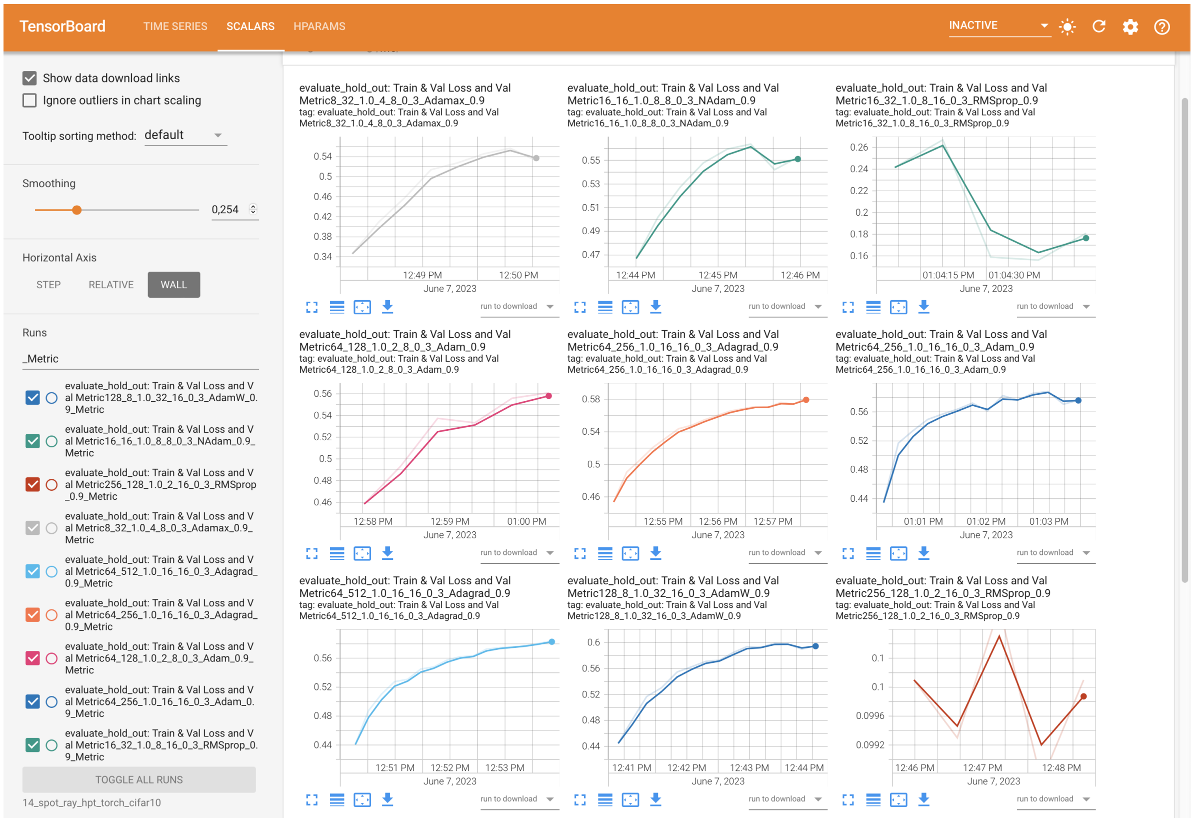


Figure 12.1: Tensorboard

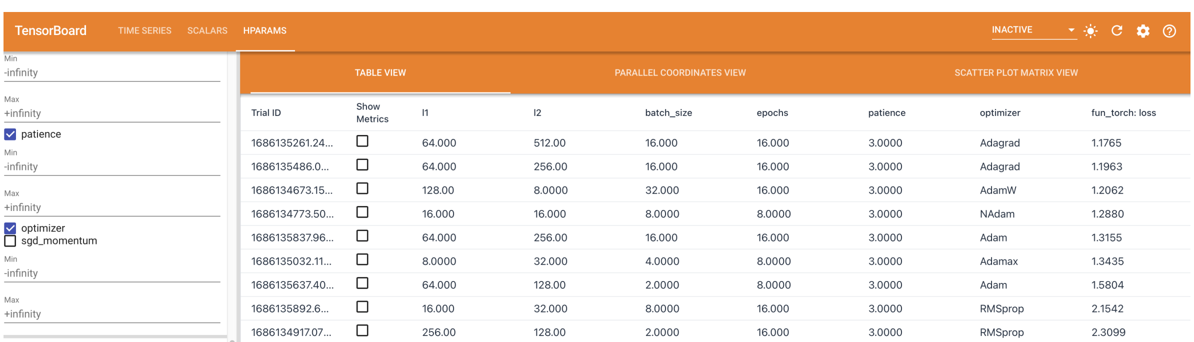


Figure 12.2: Tensorboard

```python
import pickle
SAVE = False
LOAD = False

if SAVE:
    result_file_name = "res_" + experiment_name + ".pkl"
    with open(result_file_name, 'wb') as f:
        pickle.dump(spot_tuner, f)

if LOAD:
    result_file_name = "add_the_name_of_the_result_file_here.pkl"
    with open(result_file_name, 'rb') as f:
        spot_tuner =  pickle.load(f)
```

12.10 Step 10: 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 **?@fig-progress**.

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

14_spot_ray_hpt_torch_cifar10_files/figure-pdf/cell-25-outp

Figure 12.3: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

?@fig-progress 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. **?@fig-progress** also illustrates one major difference between `ray[tune]` as used in PyTorch (2023a) 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 **?@fig-progress**. 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 **?@tbl-results**. 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.

```python
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control=fun_control, spot=spot_tuner))
```

```
| name         | type   | default   |   lower |   upper |   tuned | transform             |
|--------------|--------|-----------|---------|---------|---------|-----------------------|--
| l1           | int    | 5         |     2.0 |     9.0 |     6.0 | transform_power_2_int |
| l2           | int    | 5         |     2.0 |     9.0 |     9.0 | transform_power_2_int |
| lr_mult      | float  | 1.0       |     1.0 |     1.0 |     1.0 | None                  |
| batch_size   | int    | 4         |     1.0 |     5.0 |     4.0 | transform_power_2_int |
| epochs       | int    | 3         |     3.0 |     4.0 |     4.0 | transform_power_2_int |
| k_folds      | int    | 1         |     0.0 |     0.0 |     0.0 | None                  |
| patience     | int    | 5         |     3.0 |     3.0 |     3.0 | None                  |
| optimizer    | factor | SGD       |     0.0 |     9.0 |     1.0 | None                  |
| sgd_momentum | float  | 0.0       |     0.9 |     0.9 |     0.9 | None                  |
```

To visualize the most important hyperparameters, `spotPython` provides the function `plot_importance`. The following code generates the importance plot from **?@fig-importance**.

```python
spot_tuner.plot_importance(threshold=0.025,
    filename="./figures/" + experiment_name+"_importance.png")
```

`14_spot_ray_hpt_torch_cifar10_files/figure-pdf/cell-27-outp`

Figure 12.4: Variable importance plot, threshold 0.025.

12.10.1 Get the Tuned Architecture (SPOT Results)

The architecture of the `spotPython` model can be obtained as follows. 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:

```python
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
```

```
Net_CIFAR10(
  (conv1): Conv2d(3, 6, kernel_size=(5, 5), stride=(1, 1))
  (pool): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
  (conv2): Conv2d(6, 16, kernel_size=(5, 5), stride=(1, 1))
  (fc1): Linear(in_features=400, out_features=64, bias=True)
  (fc2): Linear(in_features=64, out_features=512, bias=True)
  (fc3): Linear(in_features=512, out_features=10, bias=True)
)
```

12.10.2 Get Default Hyperparameters

In a similar manner as in Section ??, the default hyperparameters can be obtained.

```python
# fun_control was modified, we generate a new one with the original
# default hyperparameters
from spotPython.hyperparameters.values import get_one_core_model_from_X
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
X_start = get_default_hyperparameters_as_array(fun_control)
model_default = get_one_core_model_from_X(X_start, fun_control)
model_default
```

```
Net_CIFAR10(
  (conv1): Conv2d(3, 6, kernel_size=(5, 5), stride=(1, 1))
  (pool): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
  (conv2): Conv2d(6, 16, kernel_size=(5, 5), stride=(1, 1))
  (fc1): Linear(in_features=400, out_features=32, bias=True)
  (fc2): Linear(in_features=32, out_features=32, bias=True)
  (fc3): Linear(in_features=32, out_features=10, bias=True)
)
```

12.10.3 Evaluation of the Default 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.

This evaluation is similar to the final evaluation in PyTorch (2023a).

```
from spotPython.torch.traintest import (
    train_tuned,
    test_tuned,
    )
train_tuned(net=model_default, train_dataset=train, shuffle=True,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        device = fun_control["device"], show_batch_interval=1_000_000,
        path=None,
        task=fun_control["task"],)

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

```
Epoch: 1 |

MulticlassAccuracy: 0.1013000011444092 | Loss: 2.2993141119003297 | Acc: 0.1013000000000000.
Epoch: 2 |

MulticlassAccuracy: 0.1157499998807907 | Loss: 2.2862341335296632 | Acc: 0.1157500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.1534000039100647 | Loss: 2.2558263620376588 | Acc: 0.1534000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.2099500000476837 | Loss: 2.2096788969039918 | Acc: 0.2099500000000000.
Epoch: 5 |
```

```
MulticlassAccuracy: 0.2171999961137772 | Loss: 2.1583650140762329 | Acc: 0.2172000000000000.
Epoch: 6 |

MulticlassAccuracy: 0.2302500009536743 | Loss: 2.1003214435577391 | Acc: 0.2302500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.2409500032663345 | Loss: 2.0469134126663207 | Acc: 0.2409500000000000.
Epoch: 8 |

MulticlassAccuracy: 0.2525500059127808 | Loss: 2.0065110932350159 | Acc: 0.2525500000000000.
Returned to Spot: Validation loss: 2.006511093235016

MulticlassAccuracy: 0.2576000094413757 | Loss: 2.0048375873565676 | Acc: 0.2576000000000000.
Final evaluation: Validation loss: 2.0048375873565676
Final evaluation: Validation metric: 0.25760000944137573
----------------------------------------------
```

```
(2.0048375873565676, nan, tensor(0.2576, device='mps:0'))
```

12.10.4 Evaluation of the Tuned Architecture

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.

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.

```python
train_tuned(net=model_spot, train_dataset=train,
        loss_function=fun_control["loss_function"],
        metric=fun_control["metric_torch"],
        shuffle=True,
        device = fun_control["device"],
        path=None,
        task=fun_control["task"],)
test_tuned(net=model_spot, test_dataset=test,
            shuffle=False,
            loss_function=fun_control["loss_function"],
            metric=fun_control["metric_torch"],
            device = fun_control["device"],
```

```
                task=fun_control["task"],)
```

```
Epoch: 1 |

MulticlassAccuracy: 0.4553500115871429 | Loss: 1.4807784632682801 | Acc: 0.4553500000000000.
Epoch: 2 |

MulticlassAccuracy: 0.4986500144004822 | Loss: 1.3824706964015960 | Acc: 0.4986500000000000.
Epoch: 3 |

MulticlassAccuracy: 0.5169000029563904 | Loss: 1.3429181780815125 | Acc: 0.5169000000000000.
Epoch: 4 |

MulticlassAccuracy: 0.5296999812126160 | Loss: 1.3132050466537475 | Acc: 0.5296999999999999.
Epoch: 5 |

MulticlassAccuracy: 0.5366500020027161 | Loss: 1.2941528817415238 | Acc: 0.5366500000000000.
Epoch: 6 |

MulticlassAccuracy: 0.5393499732017517 | Loss: 1.2878079622745513 | Acc: 0.5393500000000000.
Epoch: 7 |

MulticlassAccuracy: 0.5490499734878540 | Loss: 1.2646987820148468 | Acc: 0.5490500000000000.
Epoch: 8 |

MulticlassAccuracy: 0.5544499754905701 | Loss: 1.2544260616302489 | Acc: 0.5544500000000000.
Epoch: 9 |

MulticlassAccuracy: 0.5620999932289124 | Loss: 1.2338094377756119 | Acc: 0.5621000000000000.
Epoch: 10 |

MulticlassAccuracy: 0.5637500286102295 | Loss: 1.2312240300893784 | Acc: 0.5637500000000000.
Epoch: 11 |

MulticlassAccuracy: 0.5688999891281128 | Loss: 1.2254522174358369 | Acc: 0.5689000000000000.
Epoch: 12 |
```

```
MulticlassAccuracy: 0.5709999799728394 | Loss: 1.2168787500381471 | Acc: 0.5710000000000000.
Epoch: 13 |

MulticlassAccuracy: 0.5732499957084656 | Loss: 1.2131404494524003 | Acc: 0.5732500000000000.
Epoch: 14 |

MulticlassAccuracy: 0.5752500295639038 | Loss: 1.2019421347618102 | Acc: 0.5752500000000000.
Epoch: 15 |

MulticlassAccuracy: 0.5807499885559082 | Loss: 1.1982519413948058 | Acc: 0.5807500000000000.
Epoch: 16 |

MulticlassAccuracy: 0.5807999968528748 | Loss: 1.1949795161724091 | Acc: 0.5808000000000000.
Returned to Spot: Validation loss: 1.194979516172409

MulticlassAccuracy: 0.5852000117301941 | Loss: 1.2008806512832642 | Acc: 0.5852000000000001.
Final evaluation: Validation loss: 1.2008806512832642
Final evaluation: Validation metric: 0.5852000117301941
----------------------------------------------
```

```
(1.2008806512832642, nan, tensor(0.5852, device='mps:0'))
```

12.10.5 Detailed Hyperparameter Plots

The contour plots in this section visualize the interactions of the three most important 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.

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

```
l1:  0.10134443931754378
batch_size:  16.862145330943314
epochs:  100.0
optimizer:  3.487626907795692
```

14_spot_ray_hpt_torch_cifar10_files/figure-pdf/cell-32-outp

Figure 12.5: Contour plots.

14_spot_ray_hpt_torch_cifar10_files/figure-pdf/cell-32-outp

14_spot_ray_hpt_torch_cifar10_files/figure-pdf/cell-32-outp

14_spot_ray_hpt_torch_cifar10_files/figure-pdf/cell-32-outp

14_spot_ray_hpt_torch_cifar10_files/figure-pdf/cell-32-outp

14_spot_ray_hpt_torch_cifar10_files/figure-pdf/cell-32-outp

The figures (**?@fig-contour**) show the contour plots 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, **?@fig-parallel** shows the parallel plot of the hyperparameters.

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

Parallel coordinates plots

```
Unable to display output for mime type(s): text/html
```

12.11 Summary and Outlook

This tutorial presents the hyperparameter tuning open source software `spotPython` for `PyTorch`. To show its basic features, a comparison with the "official" `PyTorch` hyperparameter tuning tutorial (PyTorch 2023a) is presented. 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.
- Interaction 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`. To demonstrate its capabilities, a quick comparison with `ray[tune]` was performed. `ray[tune]` was chosen, because it is presented as "an industry standard tool for distributed hyperparameter

tuning." The results should be interpreted with care.

12.12 Appendix

12.12.1 Sample Output From Ray Tune's Run

The output from `ray[tune]` could look like this (PyTorch 2023b):

```
Number of trials: 10 (10 TERMINATED)
------+------+-------------+--------------+---------+------------+--------------------+
|   l1 |   l2 |          lr |   batch_size |    loss |   accuracy | training_iteration |
+------+------+-------------+--------------+---------+------------+--------------------|
|   64 |    4 | 0.00011629  |            2 | 1.87273 |     0.244  |                  2 |
|   32 |   64 | 0.000339763 |            8 | 1.23603 |     0.567  |                  8 |
|    8 |   16 | 0.00276249  |           16 | 1.1815  |     0.5836 |                 10 |
|    4 |   64 | 0.000648721 |            4 | 1.31131 |     0.5224 |                  8 |
|   32 |   16 | 0.000340753 |            8 | 1.26454 |     0.5444 |                  8 |
|    8 |    4 | 0.000699775 |            8 | 1.99594 |     0.1983 |                  2 |
|  256 |    8 | 0.0839654   |           16 | 2.3119  |     0.0993 |                  1 |
|   16 |  128 | 0.0758154   |           16 | 2.33575 |     0.1327 |                  1 |
|   16 |    8 | 0.0763312   |           16 | 2.31129 |     0.1042 |                  4 |
|  128 |   16 | 0.000124903 |            4 | 2.26917 |     0.1945 |                  1 |
+-----+------+------+-------------+--------------+---------+------------+----------------
Best trial config: {'l1': 8, 'l2': 16, 'lr': 0.00276249, 'batch_size': 16, 'data_dir': '..
Best trial final validation loss: 1.181501
Best trial final validation accuracy: 0.5836
Best trial test set accuracy: 0.5806
```

13 HPT: sklearn RandomForestClassifier VBDP Data

`spotPython` can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

13.1 Step 1: Setup

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

```
MAX_TIME = 1
INIT_SIZE = 5
ORIGINAL = False
PREFIX = "16"
```

```
import warnings
warnings.filterwarnings("ignore")
```

13.2 Step 2: Initialization of the Empty `fun_control` Dictionary

```
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_experiment_name, get_spot_tensorboard_path
from spotPython.utils.device import getDevice

experiment_name = get_experiment_name(prefix=PREFIX)

fun_control = fun_control_init(
    task="classification",
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name))
```

13.3 Step 3: PyTorch Data Loading

13.3.1 Load Data: Classification VBDP

```
import pandas as pd
if ORIGINAL == True:
    train_df = pd.read_csv('./data/VBDP/trainn.csv')
    test_df = pd.read_csv('./data/VBDP/testt.csv')
else:
    train_df = pd.read_csv('./data/VBDP/train.csv')
    # remove the id column
    train_df = train_df.drop(columns=['id'])
```

```
from sklearn.preprocessing import OrdinalEncoder
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# Encoder our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
train_df[target_column] = enc.fit_transform(train_df[[target_column]])
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
train_df.head()
```

```
(707, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63	x64
0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	...	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
3	0.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	0.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	...	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0

The full data set `train_df` 64 features. The target column is labeled as `prognosis`.

13.3.2 Holdout Train and Test Data

We split out a hold-out test set (25% of the data) so we can calculate an example MAP@K

```
import numpy as np
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column, axis=1),
                                                    random_state=42,
                                                    test_size=0.25,
                                                    stratify=train_df[target_column])
train = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train.shape)
print(test.shape)
train.head()
```

```
(530, 65)
(177, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63	x64
0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0
3	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
# 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})
```

13.4 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

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

A default approach for numerical data is the `StandardScaler` (mean 0, variance 1). This can be selected as follows:

```
# prep_model = StandardScaler()
# fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

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

13.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the `sklearn` implementation. For example, the `SVC` support vector machine classifier is selected as follows:

`add_core_model_to_fun_control(SVC, fun_control, SklearnHyperDict)`

Other core_models are, e.g.,:

- RidgeCV
- GradientBoostingRegressor
- ElasticNet
- RandomForestClassifier
- LogisticRegression
- KNeighborsClassifier
- RandomForestClassifier
- GradientBoostingClassifier
- HistGradientBoostingClassifier

We will use the `RandomForestClassifier` classifier in this example.

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.linear_model import ElasticNet
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
```

```
# core_model  = RidgeCV
# core_model = GradientBoostingRegressor
# core_model = ElasticNet
core_model = RandomForestClassifier
# core_model = SVC
# core_model = LogisticRegression
# core_model = KNeighborsClassifier
# core_model = GradientBoostingClassifier
add_core_model_to_fun_control(core_model=core_model,
                              fun_control=fun_control,
                              hyper_dict=SklearnHyperDict,
                              filename=None)
```

Now `fun_control` has the information from the JSON file. The available hyperparameters are:

```python
print(*fun_control["core_model_hyper_dict"].keys(), sep="\n")
```

```
n_estimators
criterion
max_depth
min_samples_split
min_samples_leaf
min_weight_fraction_leaf
max_features
max_leaf_nodes
min_impurity_decrease
bootstrap
oob_score
```

13.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

13.6.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the `modify_hyper_parameter_bounds` method. For example, to change the `tol` hyperparameter of the `SVC` model to the interval [1e-3, 1e-2], the following code can be used:

`modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3, 1e-2])`

```python
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
# modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3, 1e-2])
```

13.6.2 Modify hyperparameter of type factor

`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 were described in Section **??**.

Factors can be modified with the `modify_hyper_parameter_levels` function. For example, to exclude the `sigmoid` kernel from the tuning, the `kernel` hyperparameter of the `SVC` model can be modified as follows:

`modify_hyper_parameter_levels(fun_control, "kernel", ["linear", "rbf"])`

The new setting can be controlled via:

`fun_control["core_model_hyper_dict"]["kernel"]`

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
# XGBoost:
# modify_hyper_parameter_levels(fun_control, "loss", ["log_loss"])
```

> **Note: RandomForestClassifier and Out-of-bag Estimation**
>
> Since `oob_score` requires the `bootstrap` hyperparameter to `True`, we set the `oob_score` parameter to `False`. The `oob_score` is later discussed in Section **??**.

```
modify_hyper_parameter_bounds(fun_control, "bootstrap", bounds=[0, 1])
modify_hyper_parameter_bounds(fun_control, "oob_score", bounds=[0, 0])
```

13.6.3 Optimizers

Optimizers are described in Section **??**.

13.6.4 Selection of the Objective: Metric and Loss Functions

- Machine learning models are optimized with respect to a metric, for example, the `accuracy` function.
- Deep learning, e.g., neural networks are optimized with respect to a loss function, for example, the `cross_entropy` function and evaluated with respect to a metric, for example, the `accuracy` function.

13.7 Step 7: Selection of the Objective (Loss) Function

The loss function, that is usually used in deep learning for optimizing the weights of the net, is stored in the `fun_control` dictionary as `"loss_function"`.

13.7.1 Metric Function

There are two different types of metrics in `spotPython`:

1. `"metric_river"` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `"metric_sklearn"` is used for the sklearn based evaluation.

We will consider multi-class classification metrics, e.g., `mapk_score` and `top_k_accuracy_score`.

> **Predict Probabilities**
>
> In this multi-class classification example the machine learning algorithm should return the probabilities of the specific classes (`"predict_proba"`) instead of the predicted values.

We set `"predict_proba"` to `True` in the `fun_control` dictionary.

13.7.1.1 The MAPK Metric

To select the MAPK metric, the following two entries can be added to the `fun_control` dictionary:

`"metric_sklearn": mapk_score"`

`"metric_params": {"k": 3}`.

13.7.1.2 Other Metrics

Alternatively, other metrics for multi-class classification can be used, e.g.,: * top_k_accuracy_score or * roc_auc_score

The metric `roc_auc_score` requires the parameter `"multi_class"`, e.g.,

`"multi_class": "ovr"`.

This is set in the `fun_control` dictionary.

> **Weights**
>
> `spotPython` performs a minimization, therefore, metrics that should be maximized have to be multiplied by -1. This is done by setting `"weights"` to `-1`.

- The complete setup for the metric in our example is:

```
from spotPython.utils.metrics import mapk_score
fun_control.update({
               "weights": -1,
               "metric_sklearn": mapk_score,
               "predict_proba": True,
               "metric_params": {"k": 3},
               })
```

13.7.2 Evaluation on Hold-out Data

- The default method for computing the performance is `"eval_holdout"`.
- Alternatively, cross-validation can be used for every machine learning model.
- Specifically for RandomForests, the OOB-score can be used.

```
fun_control.update({
    "eval": "train_hold_out",
})
```

13.7.3 OOB Score

Using the OOB-Score is a very efficient way to estimate the performance of a random forest classifier. The OOB-Score is calculated on the training data and does not require a hold-out test set. If the OOB-Score is used, the key "eval" in the `fun_control` dictionary should be set to `"oob_score"` as shown below.

> **OOB-Score**
>
> In addition to setting the key `"eval"` in the `fun_control` dictionary to `"oob_score"`, the keys `"oob_score"` and `"bootstrap"` have to be set to `True`, because the OOB-Score requires the bootstrap method.

- Uncomment the following lines to use the OOB-Score:

```
fun_control.update({
    "eval": "eval_oob_score",
})
modify_hyper_parameter_bounds(fun_control, "bootstrap", bounds=[1, 1])
modify_hyper_parameter_bounds(fun_control, "oob_score", bounds=[1, 1])
```

13.7.3.1 Cross Validation

Instead of using the OOB-score, the classical cross validation can be used. The number of folds is set by the key `"k_folds"`. For example, to use 5-fold cross validation, the key `"k_folds"` is set to `5`. Uncomment the following line to use cross validation:

```
# fun_control.update({
#      "eval": "train_cv",
#      "k_folds": 10,
```

```
# })
```

13.8 Step 8: Calling the SPOT Function

13.8.1 Preparing the SPOT Call

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

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

```
| name                     | type   | default   |   lower |   upper | transform
|--------------------------|--------|-----------|---------|---------|------------------------
| n_estimators             | int    | 7         |       5 |   10    | transform_power_2_int
| criterion                | factor | gini      |       0 |    2    | None
| max_depth                | int    | 10        |       1 |   20    | transform_power_2_int
| min_samples_split        | int    | 2         |       2 |  100    | None
| min_samples_leaf         | int    | 1         |       1 |   25    | None
| min_weight_fraction_leaf | float  | 0.0       |       0 |    0.01 | None
| max_features             | factor | sqrt      |       0 |    1    | transform_none_to_None
| max_leaf_nodes           | int    | 10        |       7 |   12    | transform_power_2_int
| min_impurity_decrease    | float  | 0.0       |       0 |    0.01 | None
| bootstrap                | factor | 1         |       1 |    1    | None
| oob_score                | factor | 0         |       1 |    1    | None
```

13.8.2 The Objective Function

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

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

13.8.3 Run the Spot Optimizer

- Run SPOT for approx. x mins (max_time).
- Note: the run takes longer, because the evaluation time of initial design (here: initi_size, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
X_start = get_default_hyperparameters_as_array(fun_control)
X_start
```

```
array([[ 7.,  0., 10.,  2.,  1.,  0.,  0., 10.,  0.,  1.,  0.]])
```

```
import numpy as np
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)
```

```
spotPython tuning: -0.34276729559748426 [----------] 1.42%

spotPython tuning: -0.34276729559748426 [----------] 1.89%

spotPython tuning: -0.34276729559748426 [----------] 2.47%

spotPython tuning: -0.34276729559748426 [----------] 3.00%

spotPython tuning: -0.34276729559748426 [----------] 3.39%

spotPython tuning: -0.35062893081761004 [----------] 4.05%

spotPython tuning: -0.35062893081761004 [----------] 4.82%

spotPython tuning: -0.35062893081761004 [#---------] 5.61%

spotPython tuning: -0.35062893081761004 [#---------] 6.91%

spotPython tuning: -0.35062893081761004 [#---------] 7.57%

spotPython tuning: -0.35062893081761004 [#---------] 8.85%

spotPython tuning: -0.35062893081761004 [#---------] 9.79%

spotPython tuning: -0.35062893081761004 [#---------] 12.71%

spotPython tuning: -0.35062893081761004 [##--------] 17.57%

spotPython tuning: -0.35062893081761004 [##--------] 19.81%
```

```
spotPython tuning: -0.35062893081761004 [##--------] 23.11%

spotPython tuning: -0.35062893081761004 [###-------] 26.43%

spotPython tuning: -0.35188679245283017 [###-------] 29.78%

spotPython tuning: -0.35188679245283017 [###-------] 33.82%

spotPython tuning: -0.35188679245283017 [####------] 38.71%

spotPython tuning: -0.35188679245283017 [####------] 42.70%

spotPython tuning: -0.35188679245283017 [#####-----] 46.85%

spotPython tuning: -0.35754716981132073 [#####-----] 50.76%

spotPython tuning: -0.35754716981132073 [#####-----] 54.70%

spotPython tuning: -0.35754716981132073 [######----] 58.86%

spotPython tuning: -0.35754716981132073 [######----] 63.01%

spotPython tuning: -0.35754716981132073 [#######---] 67.70%

spotPython tuning: -0.35754716981132073 [#######---] 74.18%

spotPython tuning: -0.35754716981132073 [########--] 80.55%

spotPython tuning: -0.35754716981132073 [#########-] 87.56%

spotPython tuning: -0.3591194968553459 [#########-] 94.15%

spotPython tuning: -0.3591194968553459 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x177dc39a0>
```

13.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section **??**, see also the description in the documentation: Tensorboard.

13.10 Step 10: 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 **?@fig-progress**.

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

16_spot_hpt_sklearn_multiclass_classification_randomforest_

Figure 13.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

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

```
| name                     | type   | default   |    lower |    upper |                  tuned
|--------------------------|--------|-----------|----------|----------|-----------------------
| n_estimators             | int    | 7         |      5.0 |     10.0 |                    9.0
| criterion                | factor | gini      |      0.0 |      2.0 |                    1.0
| max_depth                | int    | 10        |      1.0 |     20.0 |                   12.0
| min_samples_split        | int    | 2         |      2.0 |    100.0 |                   11.0
| min_samples_leaf         | int    | 1         |      1.0 |     25.0 |                    1.0
| min_weight_fraction_leaf | float  | 0.0       |      0.0 |     0.01 | 0.0059164181306543325
| max_features             | factor | sqrt      |      0.0 |      1.0 |                    0.0
| max_leaf_nodes           | int    | 10        |      7.0 |     12.0 |                    9.0
| min_impurity_decrease    | float  | 0.0       |      0.0 |     0.01 |                    0.0
| bootstrap                | factor | 1         |      1.0 |      1.0 |                    1.0
| oob_score                | factor | 0         |      1.0 |      1.0 |                    1.0
```

13.10.1 Show variable importance

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

16_spot_hpt_sklearn_multiclass_classification_randomforest_

Figure 13.2: Variable importance plot, threshold 0.025.

13.10.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'n_estimators': 128,
 'criterion': 'gini',
 'max_depth': 1024,
 'min_samples_split': 2,
 'min_samples_leaf': 1,
 'min_weight_fraction_leaf': 0.0,
 'max_features': 'sqrt',
 'max_leaf_nodes': 1024,
 'min_impurity_decrease': 0.0,
 'bootstrap': 1,
 'oob_score': 0}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('nonetype', None),
                ('randomforestclassifier',
                 RandomForestClassifier(bootstrap=1, max_depth=1024,
```

```
                                            max_leaf_nodes=1024, n_estimators=128,
                                            oob_score=0))])
```

13.10.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[9.00000000e+00 1.00000000e+00 1.20000000e+01 1.10000000e+01
  1.00000000e+00 5.91641813e-03 0.00000000e+00 9.00000000e+00
  0.00000000e+00 1.00000000e+00 1.00000000e+00]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
[{'n_estimators': 512,
  'criterion': 'entropy',
  'max_depth': 4096,
  'min_samples_split': 11,
  'min_samples_leaf': 1,
  'min_weight_fraction_leaf': 0.005916418130654325,
  'max_features': 'sqrt',
  'max_leaf_nodes': 512,
  'min_impurity_decrease': 0.0,
  'bootstrap': 1,
  'oob_score': 1}]
```

```
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

```
RandomForestClassifier(bootstrap=1, criterion='entropy', max_depth=4096,
                       max_leaf_nodes=512, min_samples_split=11,
                       min_weight_fraction_leaf=0.005916418130654325,
                       n_estimators=512, oob_score=1)
```

13.10.4 Evaluate SPOT Results

- Fetch the data.

```
from spotPython.utils.convert import get_Xy_from_df
X_train, y_train = get_Xy_from_df(fun_control["train"], fun_control["target_column"])
X_test, y_test = get_Xy_from_df(fun_control["test"], fun_control["target_column"])
X_test.shape, y_test.shape
```

```
((177, 64), (177,))
```

- Fit the model with the tuned hyperparameters. This gives one result:

```
model_spot.fit(X_train, y_train)
y_pred = model_spot.predict_proba(X_test)
res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
res
```

```
0.3615819209039548
```

```
def repeated_eval(n, model):
    res_values = []
    for i in range(n):
        model.fit(X_train, y_train)
        y_pred = model.predict_proba(X_test)
        res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
        res_values.append(res)
    mean_res = np.mean(res_values)
    print(f"mean_res: {mean_res}")
    std_res = np.std(res_values)
    print(f"std_res: {std_res}")
    min_res = np.min(res_values)
    print(f"min_res: {min_res}")
    max_res = np.max(res_values)
    print(f"max_res: {max_res}")
    median_res = np.median(res_values)
    print(f"median_res: {median_res}")
    return mean_res, std_res, min_res, max_res, median_res
```

13.10.5 Handling Non-deterministic Results

- Because the model is non-determinstic, we perform $n = 30$ runs and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_spot)
```

```
mean_res: 0.3583804143126177
std_res: 0.007006898349060751
min_res: 0.34463276836158196
max_res: 0.3757062146892655
median_res: 0.3578154425612053
```

13.10.6 Evalution of the Default Hyperparameters

```
model_default.fit(X_train, y_train)["randomforestclassifier"]
```

```
RandomForestClassifier(bootstrap=1, max_depth=1024, max_leaf_nodes=1024,
                       n_estimators=128, oob_score=0)
```

- One evaluation of the default hyperparameters is performed on the hold-out test set.

```
y_pred = model_default.predict_proba(X_test)
mapk_score(y_true=y_test, y_pred=y_pred, k=3)
```

```
0.34369114877589454
```

Since one single evaluation is not meaningful, we perform, similar to the evaluation of the SPOT results, $n = 30$ runs of the default setting and and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_default)
```

```
mean_res: 0.34497802887633394
std_res: 0.01267398819635564
min_res: 0.3229755178907721
max_res: 0.36817325800376643
median_res: 0.3427495291902071
```

13.10.7 Plot: Compare Predictions

```
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```

16_spot_hpt_sklearn_multiclass_classification_randomforest_

```
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```

16_spot_hpt_sklearn_multiclass_classification_randomforest_

```
min(spot_tuner.y), max(spot_tuner.y)
```

```
(-0.3591194968553459, -0.28962264150943395)
```

13.10.8 Cross-validated Evaluations

```
from spotPython.sklearn.traintest import evaluate_cv
fun_control.update({
     "eval": "train_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.359433962264151, None)
```

```python
fun_control.update({
     "eval": "test_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.31290849673202614, None)
```

- This is the evaluation that will be used in the comparison:

```python
fun_control.update({
     "eval": "data_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3648658618376928, None)
```

13.10.9 Detailed Hyperparameter Plots

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

```
n_estimators:  38.85223485225775
criterion:  100.0
min_samples_split:  13.424756161824943
min_samples_leaf:  2.5425186088124936
max_leaf_nodes:  2.1411547457633917
```

16_spot_hpt_sklearn_multiclass_classification_randomforest_

16_spot_hpt_sklearn_multiclass_classification_randomforest_

16_spot_hpt_sklearn_multiclass_classification_randomforest_

16_spot_hpt_sklearn_multiclass_classification_randomforest_

16_spot_hpt_sklearn_multiclass_classification_randomforest_

16_spot_hpt_sklearn_multiclass_classification_randomforest_

16_spot_hpt_sklearn_multiclass_classification_randomforest_

16_spot_hpt_sklearn_multiclass_classification_randomforest_

16_spot_hpt_sklearn_multiclass_classification_randomforest_

16_spot_hpt_sklearn_multiclass_classification_randomforest_

13.10.10 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

13.10.11 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

14 HPT: sklearn XGB Classifier VBDP Data

`spotPython` can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

14.1 Step 1: Setup

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

```
MAX_TIME = 1
INIT_SIZE = 5
ORIGINAL = False
PREFIX = "17"
```

```
import warnings
warnings.filterwarnings("ignore")
```

14.2 Step 2: Initialization of the Empty `fun_control` Dictionary

```
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_experiment_name, get_spot_tensorboard_path
from spotPython.utils.device import getDevice

experiment_name = get_experiment_name(prefix=PREFIX)

fun_control = fun_control_init(
    task="classification",
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name))
```

14.3 Step 3: PyTorch Data Loading

14.3.1 1. Load Data: Classification VBDP

```
import pandas as pd
if ORIGINAL == True:
    train_df = pd.read_csv('./data/VBDP/trainn.csv')
    test_df = pd.read_csv('./data/VBDP/testt.csv')
else:
    train_df = pd.read_csv('./data/VBDP/train.csv')
    # remove the id column
    train_df = train_df.drop(columns=['id'])
```

```
from sklearn.preprocessing import OrdinalEncoder
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# Encoder our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
train_df[target_column] = enc.fit_transform(train_df[[target_column]])
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
train_df.head()
```

```
(707, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63	x64
0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	...	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
3	0.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	0.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	...	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0

The full data set `train_df` 64 features. The target column is labeled as `prognosis`.

14.3.2 Holdout Train and Test Data

We split out a hold-out test set (25% of the data) so we can calculate an example MAP@K

```
import numpy as np
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column, axis=1),
                                                     random_state=42,
                                                     test_size=0.25,
                                                     stratify=train_df[target_column])
train = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train.shape)
print(test.shape)
train.head()
```

```
(530, 65)
(177, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63	x64
0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0
3	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
# 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})
```

14.4 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

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

A default approach for numerical data is the `StandardScaler` (mean 0, variance 1). This can be selected as follows:

```
# prep_model = StandardScaler()
# fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

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

14.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the `sklearn` implementation. For example, the `SVC` support vector machine classifier is selected as follows:

```
add_core_model_to_fun_control(SVC, fun_control, SklearnHyperDict)
```

Other core_models are, e.g.,:

- RidgeCV
- GradientBoostingRegressor
- ElasticNet
- RandomForestClassifier
- LogisticRegression
- KNeighborsClassifier
- RandomForestClassifier
- GradientBoostingClassifier
- HistGradientBoostingClassifier

We will use the `RandomForestClassifier` classifier in this example.

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.linear_model import ElasticNet
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
```

```
# core_model  = RidgeCV
# core_model = GradientBoostingRegressor
# core_model = ElasticNet
core_model = RandomForestClassifier
# core_model = SVC
# core_model = LogisticRegression
# core_model = KNeighborsClassifier
# core_model = GradientBoostingClassifier
core_model = HistGradientBoostingClassifier
add_core_model_to_fun_control(core_model=core_model,
                              fun_control=fun_control,
                              hyper_dict=SklearnHyperDict,
                              filename=None)
```

Now `fun_control` has the information from the JSON file. The available hyperparameters are:

```
print(*fun_control["core_model_hyper_dict"].keys(), sep="\n")
```

```
loss
learning_rate
max_iter
max_leaf_nodes
max_depth
min_samples_leaf
l2_regularization
max_bins
early_stopping
n_iter_no_change
tol
```

14.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

14.6.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the `modify_hyper_parameter_bounds` method. For example, to change the `tol` hyperparameter of the `SVC` model to the interval [1e-3, 1e-2], the following code can be used:

`modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3, 1e-2])`

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
# modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3, 1e-2])
# modify_hyper_parameter_bounds(fun_control, "min_samples_split", bounds=[3, 20])
# modify_hyper_parameter_bounds(fun_control, "dual", bounds=[0, 0])
# modify_hyper_parameter_bounds(fun_control, "probability", bounds=[1, 1])
# fun_control["core_model_hyper_dict"]["tol"]
# modify_hyper_parameter_bounds(fun_control, "min_samples_leaf", bounds=[1, 25])
# modify_hyper_parameter_bounds(fun_control, "n_estimators", bounds=[5, 10])
```

14.6.2 Modify hyperparameter of type factor

`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 were described in Section **??**.

Factors can be modified with the `modify_hyper_parameter_levels` function. For example, to exclude the `sigmoid` kernel from the tuning, the `kernel` hyperparameter of the `SVC` model can be modified as follows:

`modify_hyper_parameter_levels(fun_control, "kernel", ["linear", "rbf"])`

The new setting can be controlled via:

`fun_control["core_model_hyper_dict"]["kernel"]`

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
# XGBoost:
modify_hyper_parameter_levels(fun_control, "loss", ["log_loss"])
```

14.6.3 Optimizers

Optimizers are described in Section **??**.

14.7 Step 7: Selection of the Objective (Loss) Function

14.7.1 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).

14.7.2 Selection of the Objective: Metric and Loss Functions

- Machine learning models are optimized with respect to a metric, for example, the `accuracy` function.
- Deep learning, e.g., neural networks are optimized with respect to a loss function, for example, the `cross_entropy` function and evaluated with respect to a metric, for example, the `accuracy` function.

14.7.3 Loss Function

The loss function, that is usually used in deep learning for optimizing the weights of the net, is stored in the `fun_control` dictionary as `"loss_function"`.

14.7.4 Metric Function

There are two different types of metrics in `spotPython`:

1. `"metric_river"` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `"metric_sklearn"` is used for the sklearn based evaluation.

We will consider multi-class classification metrics, e.g., `mapk_score` and `top_k_accuracy_score`.

> **Predict Probabilities**
>
> In this multi-class classification example the machine learning algorithm should return the probabilities of the specific classes (`"predict_proba"`) instead of the predicted values.

We set `"predict_proba"` to `True` in the `fun_control` dictionary.

14.7.4.1 The MAPK Metric

To select the MAPK metric, the following two entries can be added to the `fun_control` dictionary:

`"metric_sklearn": mapk_score"`

`"metric_params": {"k": 3}`.

14.7.4.2 Other Metrics

Alternatively, other metrics for multi-class classification can be used, e.g.,: * top_k_accuracy_score or * roc_auc_score

The metric `roc_auc_score` requires the parameter `"multi_class"`, e.g.,

`"multi_class": "ovr"`.

This is set in the `fun_control` dictionary.

> **Weights**
>
> `spotPython` performs a minimization, therefore, metrics that should be maximized have to be multiplied by -1. This is done by setting `"weights"` to `-1`.

- The complete setup for the metric in our example is:

```
from spotPython.utils.metrics import mapk_score
fun_control.update({
               "weights": -1,
               "metric_sklearn": mapk_score,
               "predict_proba": True,
               "metric_params": {"k": 3},
               })
```

14.7.5 Evaluation on Hold-out Data

- The default method for computing the performance is `"eval_holdout"`.
- Alternatively, cross-validation can be used for every machine learning model.
- Specifically for RandomForests, the OOB-score can be used.

```
fun_control.update({
    "eval": "train_hold_out",
})
```

14.7.5.1 Cross Validation

Instead of using the OOB-score, the classical cross validation can be used. The number of folds is set by the key `"k_folds"`. For example, to use 5-fold cross validation, the key `"k_folds"` is set to `5`. Uncomment the following line to use cross validation:

```
# fun_control.update({
#      "eval": "train_cv",
#      "k_folds": 10,
# })
```

14.8 Step 8: Calling the SPOT Function

14.8.1 Preparing the SPOT Call

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

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

```
| name               | type   | default   |   lower |   upper | transform              |
|--------------------|--------|-----------|---------|---------|------------------------|
| loss               | factor | log_loss  |   0     |   0     | None                   |
| learning_rate      | float  | -1.0      |  -5     |   0     | transform_power_10     |
| max_iter           | int    | 7         |   3     |  10     | transform_power_2_int  |
| max_leaf_nodes     | int    | 5         |   1     |  12     | transform_power_2_int  |
| max_depth          | int    | 2         |   1     |  20     | transform_power_2_int  |
| min_samples_leaf   | int    | 4         |   2     |  10     | transform_power_2_int  |
| l2_regularization  | float  | 0.0       |   0     |  10     | None                   |
| max_bins           | int    | 255       | 127     | 255     | None                   |
| early_stopping     | factor | 1         |   0     |   1     | None                   |
| n_iter_no_change   | int    | 10        |   5     |  20     | None                   |
| tol                | float  | 0.0001    |   1e-05 |   0.001 | None                   |
```

14.8.2 The Objective Function

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

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

14.8.3 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
X_start = get_default_hyperparameters_as_array(fun_control)
X_start
```

```
array([[ 0.00e+00, -1.00e+00,  7.00e+00,  5.00e+00,  2.00e+00,  4.00e+00,
         0.00e+00,  2.55e+02,  1.00e+00,  1.00e+01,  1.00e-04]])
```

```
import numpy as np
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,
```

```python
                                          "log_level": 50
                                          })
spot_tuner.run(X_start=X_start)
```

```
spotPython tuning: -0.40100250626566414 [#---------] 5.65%

spotPython tuning: -0.40100250626566414 [#---------] 7.74%

spotPython tuning: -0.40100250626566414 [#---------] 9.89%

spotPython tuning: -0.40100250626566414 [#---------] 13.11%

spotPython tuning: -0.40100250626566414 [#---------] 14.98%

spotPython tuning: -0.40100250626566414 [##--------] 20.09%

spotPython tuning: -0.40100250626566414 [##--------] 21.13%

spotPython tuning: -0.40100250626566414 [###-------] 26.91%

spotPython tuning: -0.40100250626566414 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2871cddb0>
```

14.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section **??**, see also the description in the documentation: Tensorboard.

14.10 Step 10: 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 **?@fig-progress**.

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

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

Figure 14.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

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

```
| name               | type   | default   |    lower |    upper |                  tuned | trans
|--------------------|--------|-----------|----------|----------|------------------------|-------
| loss               | factor | log_loss  |      0.0 |      0.0 |                    0.0 | None
| learning_rate      | float  | -1.0      |     -5.0 |      0.0 |    -0.9302847173981572 | trans
| max_iter           | int    | 7         |      3.0 |     10.0 |                    9.0 | trans
| max_leaf_nodes     | int    | 5         |      1.0 |     12.0 |                    5.0 | trans
| max_depth          | int    | 2         |      1.0 |     20.0 |                   19.0 | trans
| min_samples_leaf   | int    | 4         |      2.0 |     10.0 |                    2.0 | trans
| l2_regularization  | float  | 0.0       |      0.0 |     10.0 |     2.4029083174160553 | None
| max_bins           | int    | 255       |    127.0 |    255.0 |                  142.0 | None
| early_stopping     | factor | 1         |      0.0 |      1.0 |                    1.0 | None
| n_iter_no_change   | int    | 10        |      5.0 |     20.0 |                    6.0 | None
| tol                | float  | 0.0001    |    1e-05 |    0.001 | 0.0009512860974290124 | None
```

14.10.1 Show variable importance

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

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

Figure 14.2: Variable importance plot, threshold 0.025.

14.10.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'loss': 'log_loss',
 'learning_rate': 0.1,
 'max_iter': 128,
 'max_leaf_nodes': 32,
 'max_depth': 4,
 'min_samples_leaf': 16,
 'l2_regularization': 0.0,
 'max_bins': 255,
 'early_stopping': 1,
 'n_iter_no_change': 10,
 'tol': 0.0001}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('nonetype', None),
                ('histgradientboostingclassifier',
                 HistGradientBoostingClassifier(early_stopping=1, max_depth=4,
                                                max_iter=128, max_leaf_nodes=32,
                                                min_samples_leaf=16,
                                                tol=0.0001))])
```

14.10.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[ 0.00000000e+00 -9.30284717e-01  9.00000000e+00  5.00000000e+00
   1.90000000e+01  2.00000000e+00  2.40290832e+00  1.42000000e+02
   1.00000000e+00  6.00000000e+00  9.51286097e-04]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
[{'loss': 'log_loss',
  'learning_rate': 0.11741275609341804,
  'max_iter': 512,
  'max_leaf_nodes': 32,
  'max_depth': 524288,
  'min_samples_leaf': 4,
  'l2_regularization': 2.4029083174160553,
  'max_bins': 142,
  'early_stopping': 1,
  'n_iter_no_change': 6,
  'tol': 0.0009512860974290124}]
```

```
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

```
HistGradientBoostingClassifier(early_stopping=1,
                               l2_regularization=2.4029083174160553,
                               learning_rate=0.11741275609341804, max_bins=142,
                               max_depth=524288, max_iter=512,
                               max_leaf_nodes=32, min_samples_leaf=4,
                               n_iter_no_change=6, tol=0.0009512860974290124)
```

14.10.4 Evaluate SPOT Results

- Fetch the data.

```python
from spotPython.utils.convert import get_Xy_from_df
X_train, y_train = get_Xy_from_df(fun_control["train"], fun_control["target_column"])
X_test, y_test = get_Xy_from_df(fun_control["test"], fun_control["target_column"])
X_test.shape, y_test.shape
```

```
((177, 64), (177,))
```

- Fit the model with the tuned hyperparameters. This gives one result:

```python
model_spot.fit(X_train, y_train)
y_pred = model_spot.predict_proba(X_test)
res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
res
```

```
0.36252354048964214
```

```python
def repeated_eval(n, model):
    res_values = []
    for i in range(n):
        model.fit(X_train, y_train)
        y_pred = model.predict_proba(X_test)
        res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
        res_values.append(res)
    mean_res = np.mean(res_values)
    print(f"mean_res: {mean_res}")
    std_res = np.std(res_values)
    print(f"std_res: {std_res}")
    min_res = np.min(res_values)
    print(f"min_res: {min_res}")
    max_res = np.max(res_values)
    print(f"max_res: {max_res}")
    median_res = np.median(res_values)
    print(f"median_res: {median_res}")
    return mean_res, std_res, min_res, max_res, median_res
```

14.10.5 Handling Non-deterministic Results

- Because the model is non-determinstic, we perform $n = 30$ runs and calculate the mean and standard deviation of the performance metric.

```python
_ = repeated_eval(30, model_spot)
```

```
mean_res: 0.33983050847457624
std_res: 0.013867406540579606
min_res: 0.3088512241054614
max_res: 0.36817325800376643
median_res: 0.3385122410546139
```

14.10.6 Evalution of the Default Hyperparameters

```python
model_default.fit(X_train, y_train)["histgradientboostingclassifier"]
```

```
HistGradientBoostingClassifier(early_stopping=1, max_depth=4, max_iter=128,
                               max_leaf_nodes=32, min_samples_leaf=16,
                               tol=0.0001)
```

- One evaluation of the default hyperparameters is performed on the hold-out test set.

```python
y_pred = model_default.predict_proba(X_test)
mapk_score(y_true=y_test, y_pred=y_pred, k=3)
```

```
0.33427495291902076
```

Since one single evaluation is not meaningful, we perform, similar to the evaluation of the SPOT results, $n = 30$ runs of the default setting and and calculate the mean and standard deviation of the performance metric.

```python
_ = repeated_eval(30, model_default)
```

```
mean_res: 0.34588826114249843
std_res: 0.01672858740749801
min_res: 0.3163841807909605
max_res: 0.38229755178907715
median_res: 0.346045197740113
```

14.10.7 Plot: Compare Predictions

```
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

```
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

```
min(spot_tuner.y), max(spot_tuner.y)
```

```
(-0.40100250626566414, -0.20927318295739344)
```

14.10.8 Cross-validated Evaluations

```
from spotPython.sklearn.traintest import evaluate_cv
fun_control.update({
     "eval": "train_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3320754716981132, None)
```

```python
fun_control.update({
     "eval": "test_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.27777777777777773, None)
```

- This is the evaluation that will be used in the comparison:

```python
fun_control.update({
     "eval": "data_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3434473507712944, None)
```

14.10.9 Detailed Hyperparameter Plots

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

```
learning_rate:  85.19160867263129
max_depth:  13.509419214003497
min_samples_leaf:  100.0
early_stopping:  1.5184335190083467
```

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

17_spot_hpt_sklearn_multiclass_classification_xgb_files/fig

14.10.10 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

14.10.11 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```python
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

15 HPT: sklearn SVC VBDP Data

`spotPython` can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

15.1 Step 1: Setup

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

```
MAX_TIME = 1
INIT_SIZE = 5
ORIGINAL = False
PREFIX = "18"
```

```
import warnings
warnings.filterwarnings("ignore")
```

15.2 Step 2: Initialization of the Empty `fun_control` Dictionary

```
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_experiment_name, get_spot_tensorboard_path
from spotPython.utils.device import getDevice

experiment_name = get_experiment_name(prefix=PREFIX)

fun_control = fun_control_init(
    task="classification",
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name))
```

15.3 Step 3: PyTorch Data Loading

15.3.1 1. Load Data: Classification VBDP

```
import pandas as pd
if ORIGINAL == True:
    train_df = pd.read_csv('./data/VBDP/trainn.csv')
    test_df = pd.read_csv('./data/VBDP/testt.csv')
else:
    train_df = pd.read_csv('./data/VBDP/train.csv')
    # remove the id column
    train_df = train_df.drop(columns=['id'])
```

```
from sklearn.preprocessing import OrdinalEncoder
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# Encoder our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
train_df[target_column] = enc.fit_transform(train_df[[target_column]])
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
train_df.head()
```

```
(707, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63	x64
0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	...	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
3	0.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	0.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	...	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0

The full data set `train_df` 64 features. The target column is labeled as `prognosis`.

15.3.2 Holdout Train and Test Data

We split out a hold-out test set (25% of the data) so we can calculate an example MAP@K

```
import numpy as np
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column, axis=1),
                                                    random_state=42,
                                                    test_size=0.25,
                                                    stratify=train_df[target_column])
train = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train.shape)
print(test.shape)
train.head()
```

```
(530, 65)
(177, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63	x64
0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0
3	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
# 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})
```

15.4 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

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

A default approach for numerical data is the `StandardScaler` (mean 0, variance 1). This can be selected as follows:

```
# prep_model = StandardScaler()
# fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

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

15.5 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the `sklearn` implementation. For example, the `SVC` support vector machine classifier is selected as follows:

`add_core_model_to_fun_control(SVC, fun_control, SklearnHyperDict)`

Other core_models are, e.g.,:

- RidgeCV
- GradientBoostingRegressor
- ElasticNet
- RandomForestClassifier
- LogisticRegression
- KNeighborsClassifier
- RandomForestClassifier
- GradientBoostingClassifier
- HistGradientBoostingClassifier

We will use the `RandomForestClassifier` classifier in this example.

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.linear_model import ElasticNet
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
```

```
# core_model  = RidgeCV
# core_model = GradientBoostingRegressor
# core_model = ElasticNet
# core_model = RandomForestClassifier
core_model = SVC
# core_model = LogisticRegression
# core_model = KNeighborsClassifier
# core_model = GradientBoostingClassifier
# core_model = HistGradientBoostingClassifier
add_core_model_to_fun_control(core_model=core_model,
                              fun_control=fun_control,
                              hyper_dict=SklearnHyperDict,
                              filename=None)
```

Now `fun_control` has the information from the JSON file. The available hyperparameters are:

```
print(*fun_control["core_model_hyper_dict"].keys(), sep="\n")
```

```
C
kernel
degree
gamma
coef0
shrinking
probability
tol
cache_size
break_ties
```

15.6 Step 6: Modify `hyper_dict` Hyperparameters for the Selected Algorithm aka `core_model`

15.6.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the `modify_hyper_parameter_bounds` method. For example, to change the `tol` hyperparameter of the `SVC` model to the interval [1e-3, 1e-2], the following code can be used:

`modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3, 1e-2])`

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
modify_hyper_parameter_bounds(fun_control, "probability", bounds=[1, 1])
```

15.6.2 Modify hyperparameter of type factor

`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 were described in Section **??**.

Factors can be modified with the `modify_hyper_parameter_levels` function. For example, to exclude the `sigmoid` kernel from the tuning, the `kernel` hyperparameter of the `SVC` model can be modified as follows:

`modify_hyper_parameter_levels(fun_control, "kernel", ["linear", "rbf"])`

The new setting can be controlled via:

`fun_control["core_model_hyper_dict"]["kernel"]`

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
modify_hyper_parameter_levels(fun_control, "kernel", ["rbf"])
```

15.6.3 Optimizers

Optimizers are described in Section **??**.

15.6.4 Selection of the Objective: Metric and Loss Functions

- Machine learning models are optimized with respect to a metric, for example, the `accuracy` function.
- Deep learning, e.g., neural networks are optimized with respect to a loss function, for example, the `cross_entropy` function and evaluated with respect to a metric, for example, the `accuracy` function.

15.7 Step 7: Selection of the Objective (Loss) Function

The loss function, that is usually used in deep learning for optimizing the weights of the net, is stored in the `fun_control` dictionary as `"loss_function"`.

15.7.1 Metric Function

There are two different types of metrics in `spotPython`:

1. `"metric_river"` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `"metric_sklearn"` is used for the sklearn based evaluation.

We will consider multi-class classification metrics, e.g., `mapk_score` and `top_k_accuracy_score`.

> **Predict Probabilities**
>
> In this multi-class classification example the machine learning algorithm should return the probabilities of the specific classes (`"predict_proba"`) instead of the predicted values.

We set `"predict_proba"` to `True` in the `fun_control` dictionary.

15.7.1.1 The MAPK Metric

To select the MAPK metric, the following two entries can be added to the `fun_control` dictionary:

`"metric_sklearn": mapk_score"`

`"metric_params": {"k": 3}`.

15.7.1.2 Other Metrics

Alternatively, other metrics for multi-class classification can be used, e.g.,: * top_k_accuracy_score or * roc_auc_score

The metric `roc_auc_score` requires the parameter `"multi_class"`, e.g.,

`"multi_class": "ovr"`.

This is set in the `fun_control` dictionary.

> **Weights**
>
> `spotPython` performs a minimization, therefore, metrics that should be maximized have to be multiplied by -1. This is done by setting `"weights"` to `-1`.

- The complete setup for the metric in our example is:

```
from spotPython.utils.metrics import mapk_score
fun_control.update({
               "weights": -1,
               "metric_sklearn": mapk_score,
               "predict_proba": True,
               "metric_params": {"k": 3},
               })
```

15.7.2 Evaluation on Hold-out Data

- The default method for computing the performance is `"eval_holdout"`.
- Alternatively, cross-validation can be used for every machine learning model.
- Specifically for RandomForests, the OOB-score can be used.

```
fun_control.update({
    "eval": "train_hold_out",
```

```
})
```

15.7.2.1 Cross Validation

Instead of using the OOB-score, the classical cross validation can be used. The number of folds is set by the key "k_folds". For example, to use 5-fold cross validation, the key "k_folds" is set to 5. Uncomment the following line to use cross validation:

```
# fun_control.update({
#      "eval": "train_cv",
#      "k_folds": 10,
# })
```

15.8 Step 8: Calling the SPOT Function

15.8.1 Preparing the SPOT Call

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

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

```
| name         | type   | default   |    lower |    upper | transform    |
|--------------|--------|-----------|----------|----------|--------------|
| C            | float  | 1.0       |   0.1    |   10     | None         |
| kernel       | factor | rbf       |   0      |    0     | None         |
| degree       | int    | 3         |   3      |    3     | None         |
| gamma        | factor | scale     |   0      |    1     | None         |
| coef0        | float  | 0.0       |   0      |    0     | None         |
```

```
| shrinking   | factor | 0         |   0      |    1     | None          |
| probability | factor | 0         |   1      |    1     | None          |
| tol         | float  | 0.001     |   0.0001 |    0.01  | None          |
| cache_size  | float  | 200.0     | 100      |  400     | None          |
| break_ties  | factor | 0         |   0      |    1     | None          |
```

15.8.2 The Objective Function

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

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

15.8.3 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
X_start = get_default_hyperparameters_as_array(fun_control)
X_start
```

```
array([[1.e+00, 0.e+00, 3.e+00, 0.e+00, 0.e+00, 0.e+00, 0.e+00, 1.e-03,
        2.e+02, 0.e+00]])
```

```
import numpy as np
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,
```

```python
                         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)
```

```
spotPython tuning: -0.38345864661654133 [----------] 0.30%

spotPython tuning: -0.38345864661654133 [----------] 0.60%

spotPython tuning: -0.38345864661654133 [----------] 0.96%

spotPython tuning: -0.38345864661654133 [----------] 1.31%

spotPython tuning: -0.38345864661654133 [----------] 1.54%

spotPython tuning: -0.38345864661654133 [----------] 1.82%

spotPython tuning: -0.38345864661654133 [----------] 2.04%

spotPython tuning: -0.38345864661654133 [----------] 2.31%

spotPython tuning: -0.38345864661654133 [----------] 2.59%

spotPython tuning: -0.39473684210526316 [----------] 2.85%
```

```
spotPython tuning: -0.39473684210526316 [----------] 3.07%

spotPython tuning: -0.39473684210526316 [----------] 3.31%

spotPython tuning: -0.39473684210526316 [----------] 3.92%

spotPython tuning: -0.39473684210526316 [----------] 4.58%

spotPython tuning: -0.39473684210526316 [#---------] 5.27%

spotPython tuning: -0.39473684210526316 [#---------] 6.22%

spotPython tuning: -0.39473684210526316 [#---------] 7.59%

spotPython tuning: -0.39473684210526316 [#---------] 8.83%

spotPython tuning: -0.39473684210526316 [#---------] 9.63%

spotPython tuning: -0.39473684210526316 [#---------] 10.54%

spotPython tuning: -0.39473684210526316 [#---------] 11.42%

spotPython tuning: -0.39473684210526316 [#---------] 12.32%

spotPython tuning: -0.39473684210526316 [#---------] 13.22%

spotPython tuning: -0.39473684210526316 [#---------] 14.17%

spotPython tuning: -0.39473684210526316 [##--------] 15.38%

spotPython tuning: -0.39473684210526316 [##--------] 16.23%

spotPython tuning: -0.39473684210526316 [##--------] 16.89%

spotPython tuning: -0.39473684210526316 [##--------] 17.78%

spotPython tuning: -0.39473684210526316 [##--------] 18.99%
```

```
spotPython tuning: -0.39473684210526316 [##--------] 19.93%

spotPython tuning: -0.39473684210526316 [##--------] 20.99%

spotPython tuning: -0.39473684210526316 [##--------] 22.45%

spotPython tuning: -0.39473684210526316 [##--------] 23.93%

spotPython tuning: -0.39473684210526316 [###-------] 25.19%

spotPython tuning: -0.39473684210526316 [###-------] 26.45%

spotPython tuning: -0.39473684210526316 [###-------] 28.19%

spotPython tuning: -0.39473684210526316 [###-------] 29.46%

spotPython tuning: -0.39473684210526316 [###-------] 30.80%

spotPython tuning: -0.39473684210526316 [###-------] 32.24%

spotPython tuning: -0.39473684210526316 [###-------] 33.64%

spotPython tuning: -0.39473684210526316 [###-------] 34.97%

spotPython tuning: -0.39473684210526316 [####------] 36.29%

spotPython tuning: -0.39473684210526316 [####------] 37.52%

spotPython tuning: -0.39473684210526316 [####------] 39.57%

spotPython tuning: -0.39473684210526316 [####------] 41.22%

spotPython tuning: -0.39473684210526316 [####------] 42.67%

spotPython tuning: -0.39473684210526316 [####------] 44.10%

spotPython tuning: -0.39473684210526316 [#####-----] 45.91%
```

```
spotPython tuning: -0.39473684210526316 [#####-----] 47.26%

spotPython tuning: -0.39473684210526316 [#####-----] 48.85%

spotPython tuning: -0.39473684210526316 [#####-----] 50.40%

spotPython tuning: -0.39473684210526316 [#####-----] 52.23%

spotPython tuning: -0.39473684210526316 [#####-----] 53.83%

spotPython tuning: -0.39473684210526316 [######----] 55.30%

spotPython tuning: -0.39473684210526316 [######----] 56.72%

spotPython tuning: -0.39473684210526316 [######----] 58.15%

spotPython tuning: -0.39473684210526316 [######----] 59.52%

spotPython tuning: -0.39473684210526316 [######----] 60.98%

spotPython tuning: -0.39473684210526316 [#######---] 65.14%

spotPython tuning: -0.39473684210526316 [#######---] 69.00%

spotPython tuning: -0.39473684210526316 [#######---] 72.56%

spotPython tuning: -0.39473684210526316 [########--] 76.09%

spotPython tuning: -0.39473684210526316 [#########-] 86.54%

spotPython tuning: -0.39473684210526316 [#########-] 90.03%

spotPython tuning: -0.39473684210526316 [#########-] 93.12%

spotPython tuning: -0.39473684210526316 [##########] 96.94%

spotPython tuning: -0.39473684210526316 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x2b040e7d0>
```

15.9 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section **??**, see also the description in the documentation: Tensorboard.

15.10 Step 10: 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 **?@fig-progress**.

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

18_spot_hpt_sklearn_multiclass_classification_svc_files/fig

Figure 15.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

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

name	type	default	lower	upper	tuned	transform
C	float	1.0	0.1	10.0	4.211117448021866	None
kernel	factor	rbf	0.0	0.0	0.0	None
degree	int	3	3.0	3.0	3.0	None
gamma	factor	scale	0.0	1.0	1.0	None
coef0	float	0.0	0.0	0.0	0.0	None
shrinking	factor	0	0.0	1.0	1.0	None
probability	factor	0	1.0	1.0	1.0	None
tol	float	0.001	0.0001	0.01	0.004278044656534419	None
cache_size	float	200.0	100.0	400.0	319.49898598118955	None
break_ties	factor	0	0.0	1.0	1.0	None

15.10.1 Show variable importance

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

18_spot_hpt_sklearn_multiclass_classification_svc_files/fig

Figure 15.2: Variable importance plot, threshold 0.025.

15.10.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'C': 1.0,
 'kernel': 'rbf',
 'degree': 3,
 'gamma': 'scale',
 'coef0': 0.0,
 'shrinking': 0,
 'probability': 0,
 'tol': 0.001,
 'cache_size': 200.0,
 'break_ties': 0}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('nonetype', None),
                ('svc',
                 SVC(break_ties=0, cache_size=200.0, probability=0,
                     shrinking=0))])
```

> **Note**
>
> - Default value for "probability" is False, but we need it to be True for the metric "mapk_score".
>
> ```
> values_default.update({"probability": 1})
> ```

15.10.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[4.21111745e+00 0.00000000e+00 3.00000000e+00 1.00000000e+00
  0.00000000e+00 1.00000000e+00 1.00000000e+00 4.27804466e-03
  3.19498986e+02 1.00000000e+00]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
[{'C': 4.211117448021866,
  'kernel': 'rbf',
  'degree': 3,
  'gamma': 'auto',
  'coef0': 0.0,
  'shrinking': 1,
  'probability': 1,
  'tol': 0.004278044656534419,
  'cache_size': 319.49898598118955,
  'break_ties': 1}]
```

```
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

```
SVC(C=4.211117448021866, break_ties=1, cache_size=319.49898598118955,
    gamma='auto', probability=1, shrinking=1, tol=0.004278044656534419)
```

15.10.4 Evaluate SPOT Results

- Fetch the data.

```
from spotPython.utils.convert import get_Xy_from_df
X_train, y_train = get_Xy_from_df(fun_control["train"], fun_control["target_column"])
X_test, y_test = get_Xy_from_df(fun_control["test"], fun_control["target_column"])
X_test.shape, y_test.shape
```

```
((177, 64), (177,))
```

- Fit the model with the tuned hyperparameters. This gives one result:

```
model_spot.fit(X_train, y_train)
y_pred = model_spot.predict_proba(X_test)
res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
res
```

```
0.37664783427495285
```

```
def repeated_eval(n, model):
    res_values = []
    for i in range(n):
        model.fit(X_train, y_train)
        y_pred = model.predict_proba(X_test)
        res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
        res_values.append(res)
    mean_res = np.mean(res_values)
    print(f"mean_res: {mean_res}")
    std_res = np.std(res_values)
    print(f"std_res: {std_res}")
    min_res = np.min(res_values)
    print(f"min_res: {min_res}")
    max_res = np.max(res_values)
    print(f"max_res: {max_res}")
    median_res = np.median(res_values)
    print(f"median_res: {median_res}")
    return mean_res, std_res, min_res, max_res, median_res
```

15.10.5 Handling Non-deterministic Results

- Because the model is non-determinstic, we perform $n = 30$ runs and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_spot)
```

```
mean_res: 0.37696170747018193
std_res: 0.003689846079017097
min_res: 0.3700564971751412
max_res: 0.3860640301318267
median_res: 0.37664783427495285
```

15.10.6 Evalution of the Default Hyperparameters

```
model_default["svc"].probability = True
model_default.fit(X_train, y_train)["svc"]
```

```
SVC(break_ties=0, cache_size=200.0, probability=True, shrinking=0)
```

- One evaluation of the default hyperparameters is performed on the hold-out test set.

```
y_pred = model_default.predict_proba(X_test)
mapk_score(y_true=y_test, y_pred=y_pred, k=3)
```

```
0.3870056497175141
```

Since one single evaluation is not meaningful, we perform, similar to the evaluation of the SPOT results, $n = 30$ runs of the default setting and and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_default)
```

```
mean_res: 0.384557438794727
std_res: 0.004693007832157095
min_res: 0.37476459510357824
max_res: 0.396421845574388
median_res: 0.38465160075329563
```

15.10.7 Plot: Compare Predictions

```
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```

18_spot_hpt_sklearn_multiclass_classification_svc_files/fig

```
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```

18_spot_hpt_sklearn_multiclass_classification_svc_files/fig

```
min(spot_tuner.y), max(spot_tuner.y)
```

```
(-0.39473684210526316, -0.3370927318295739)
```

15.10.8 Cross-validated Evaluations

```
from spotPython.sklearn.traintest import evaluate_cv
fun_control.update({
     "eval": "train_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3474842767295597, None)
```

```python
fun_control.update({
     "eval": "test_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3616013071895425, None)
```

- This is the evaluation that will be used in the comparison:

```python
fun_control.update({
     "eval": "data_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3612508383635144, None)
```

15.10.9 Detailed Hyperparameter Plots

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

```
C:  100.0
gamma:  100.0
cache_size:  0.9414624306295091
```

18_spot_hpt_sklearn_multiclass_classification_svc_files/fig

18_spot_hpt_sklearn_multiclass_classification_svc_files/fig

18_spot_hpt_sklearn_multiclass_classification_svc_files/fig

15.10.10 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

15.10.11 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

16 HPT: sklearn KNN Classifier VBDP Data

spotPython can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

```
!pip install spotPython
```

- Uncomment the following lines if you want to for (re-)installation the latest version of spotPython from gitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

16.1 Step 1: Setup

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

```
MAX_TIME = 1
INIT_SIZE = 5
ORIGINAL = False
PREFIX = "19"
```

```
import warnings
warnings.filterwarnings("ignore")
```

16.2 Step 2: Initialization of the Empty `fun_control` Dictionary

```
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_experiment_name, get_spot_tensorboard_path
from spotPython.utils.device import getDevice

experiment_name = get_experiment_name(prefix=PREFIX)

fun_control = fun_control_init(
    task="classification",
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name))
```

16.2.1 Load Data: Classification VBDP

```
import pandas as pd
if ORIGINAL == True:
    train_df = pd.read_csv('./data/VBDP/trainn.csv')
    test_df = pd.read_csv('./data/VBDP/testt.csv')
else:
    train_df = pd.read_csv('./data/VBDP/train.csv')
    # remove the id column
    train_df = train_df.drop(columns=['id'])
```

```
from sklearn.preprocessing import OrdinalEncoder
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# Encoder our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
train_df[target_column] = enc.fit_transform(train_df[[target_column]])
train_df.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train_df.shape)
train_df.head()
```

```
(707, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63	x64
0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	...	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0
3	0.0	0.0	1.0	1.0	1.0	1.0	0.0	1.0	0.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	...	0.0	1.0	0.0	0.0	1.0	1.0	1.0	0.0

The full data set `train_df` 64 features. The target column is labeled as `prognosis`.

16.2.2 Holdout Train and Test Data

We split out a hold-out test set (25% of the data) so we can calculate an example MAP@K

```
import numpy as np
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(train_df.drop(target_column, axis=1),
                                                    random_state=42,
                                                    test_size=0.25,
                                                    stratify=train_df[target_column])
train = pd.DataFrame(np.hstack((X_train, np.array(y_train).reshape(-1, 1))))
test = pd.DataFrame(np.hstack((X_test, np.array(y_test).reshape(-1, 1))))
train.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
test.columns = [f"x{i}" for i in range(1, n_features+1)] + [target_column]
print(train.shape)
print(test.shape)
train.head()
```

```
(530, 65)
(177, 65)
```

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x56	x57	x58	x59	x60	x61	x62	x63	x64
0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	1.0	1.0	1.0	0.0
3	1.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```python
# 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})
```

16.3 Step 4: Specification of the Preprocessing Model

Data preprocesssing can be very simple, e.g., you can ignore it. Then you would choose the `prep_model` "None":

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

A default approach for numerical data is the `StandardScaler` (mean 0, variance 1). This can be selected as follows:

```python
# prep_model = StandardScaler()
# fun_control.update({"prep_model": prep_model})
```

Even more complicated pre-processing steps are possible, e.g., the follwing pipeline:

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

16.4 Step 5: Select Model (`algorithm`) and `core_model_hyper_dict`

The selection of the algorithm (ML model) that should be tuned is done by specifying the its name from the `sklearn` implementation. For example, the `SVC` support vector machine classifier is selected as follows:

```
add_core_model_to_fun_control(SVC, fun_control, SklearnHyperDict)
```

Other core_models are, e.g.,:

- RidgeCV
- GradientBoostingRegressor
- ElasticNet
- RandomForestClassifier
- LogisticRegression
- KNeighborsClassifier
- RandomForestClassifier
- GradientBoostingClassifier
- HistGradientBoostingClassifier

We will use the `RandomForestClassifier` classifier in this example.

```
from sklearn.linear_model import RidgeCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.linear_model import ElasticNet
from spotPython.hyperparameters.values import add_core_model_to_fun_control
from spotPython.data.sklearn_hyper_dict import SklearnHyperDict
from spotPython.fun.hypersklearn import HyperSklearn
```

```
# core_model  = RidgeCV
# core_model = GradientBoostingRegressor
# core_model = ElasticNet
# core_model = RandomForestClassifier
core_model = KNeighborsClassifier
# core_model = LogisticRegression
# core_model = KNeighborsClassifier
# core_model = GradientBoostingClassifier
# core_model = HistGradientBoostingClassifier
add_core_model_to_fun_control(core_model=core_model,
                              fun_control=fun_control,
                              hyper_dict=SklearnHyperDict,
                              filename=None)
```

Now fun_control has the information from the JSON file. The available hyperparameters are:

```
print(*fun_control["core_model_hyper_dict"].keys(), sep="\n")
```

```
n_neighbors
weights
algorithm
leaf_size
p
```

16.5 Step 6: Modify hyper_dict Hyperparameters for the Selected Algorithm aka core_model

16.5.1 Modify hyperparameter of type numeric and integer (boolean)

Numeric and boolean values can be modified using the modify_hyper_parameter_bounds method. For example, to change the tol hyperparameter of the SVC model to the interval [1e-3, 1e-2], the following code can be used:

`modify_hyper_parameter_bounds(fun_control, "tol", bounds=[1e-3, 1e-2])`

```
# from spotPython.hyperparameters.values import modify_hyper_parameter_bounds
# modify_hyper_parameter_bounds(fun_control, "probability", bounds=[1, 1])
```

16.5.2 Modify hyperparameter of type factor

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 were described in Section **??**.

Factors can be modified with the modify_hyper_parameter_levels function. For example, to exclude the sigmoid kernel from the tuning, the kernel hyperparameter of the SVC model can be modified as follows:

`modify_hyper_parameter_levels(fun_control, "kernel", ["linear", "rbf"])`

The new setting can be controlled via:

`fun_control["core_model_hyper_dict"]["kernel"]`

```
# from spotPython.hyperparameters.values import modify_hyper_parameter_levels
# modify_hyper_parameter_levels(fun_control, "kernel", ["rbf"])
```

16.5.3 Optimizers

Optimizers are described in Section ??.

16.5.4 Selection of the Objective: Metric and Loss Functions

- Machine learning models are optimized with respect to a metric, for example, the `accuracy` function.
- Deep learning, e.g., neural networks are optimized with respect to a loss function, for example, the `cross_entropy` function and evaluated with respect to a metric, for example, the `accuracy` function.

16.6 Step 7: Selection of the Objective (Loss) Function

The loss function, that is usually used in deep learning for optimizing the weights of the net, is stored in the `fun_control` dictionary as `"loss_function"`.

16.6.1 Metric Function

There are two different types of metrics in `spotPython`:

1. `"metric_river"` is used for the river based evaluation via `eval_oml_iter_progressive`.
2. `"metric_sklearn"` is used for the sklearn based evaluation.

We will consider multi-class classification metrics, e.g., `mapk_score` and `top_k_accuracy_score`.

> **Predict Probabilities**
>
> In this multi-class classification example the machine learning algorithm should return the probabilities of the specific classes (`"predict_proba"`) instead of the predicted values.

We set `"predict_proba"` to `True` in the `fun_control` dictionary.

16.6.1.1 The MAPK Metric

To select the MAPK metric, the following two entries can be added to the `fun_control` dictionary:

`"metric_sklearn": mapk_score"`

`"metric_params": {"k": 3}`.

16.6.1.2 Other Metrics

Alternatively, other metrics for multi-class classification can be used, e.g.,: * top_k_accuracy_score or * roc_auc_score

The metric `roc_auc_score` requires the parameter `"multi_class"`, e.g.,

`"multi_class": "ovr"`.

This is set in the `fun_control` dictionary.

> **Weights**
>
> `spotPython` performs a minimization, therefore, metrics that should be maximized have to be multiplied by -1. This is done by setting `"weights"` to `-1`.

- The complete setup for the metric in our example is:

```
from spotPython.utils.metrics import mapk_score
fun_control.update({
               "weights": -1,
               "metric_sklearn": mapk_score,
               "predict_proba": True,
               "metric_params": {"k": 3},
               })
```

16.6.2 Evaluation on Hold-out Data

- The default method for computing the performance is `"eval_holdout"`.
- Alternatively, cross-validation can be used for every machine learning model.
- Specifically for RandomForests, the OOB-score can be used.

```
fun_control.update({
    "eval": "train_hold_out",
```

```
})
```

16.6.2.1 Cross Validation

Instead of using the OOB-score, the classical cross validation can be used. The number of folds is set by the key "k_folds". For example, to use 5-fold cross validation, the key "k_folds" is set to 5. Uncomment the following line to use cross validation:

```
# fun_control.update({
#       "eval": "train_cv",
#       "k_folds": 10,
# })
```

16.7 Step 8: Calling the SPOT Function

16.7.1 Preparing the SPOT Call

- Get types and variable names as well as lower and upper bounds for the hyperparameters.

```
# extract the variable types, names, and bounds
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

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

```
| name        | type   | default   |   lower |   upper | transform             |
|-------------|--------|-----------|---------|---------|-----------------------|
| n_neighbors | int    | 2         |       1 |       7 | transform_power_2_int |
| weights     | factor | uniform   |       0 |       1 | None                  |
| algorithm   | factor | auto      |       0 |       3 | None                  |
| leaf_size   | int    | 5         |       2 |       7 | transform_power_2_int |
| p           | int    | 2         |       1 |       2 | None                  |
```

16.7.2 The Objective Function

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

```
from spotPython.fun.hypersklearn import HyperSklearn
fun = HyperSklearn().fun_sklearn
```

16.7.3 Run the `Spot` Optimizer

- Run SPOT for approx. x mins (`max_time`).
- Note: the run takes longer, because the evaluation time of initial design (here: `initi_size`, 20 points) is not considered.

```
from spotPython.hyperparameters.values import get_default_hyperparameters_as_array
X_start = get_default_hyperparameters_as_array(fun_control)
X_start
```

```
array([[2, 0, 0, 5, 2]])
```

```
import numpy as np
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,
```

```python
                     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)
```

```
spotPython tuning: -0.3107769423558897 [----------] 0.24%

spotPython tuning: -0.3107769423558897 [----------] 0.51%

spotPython tuning: -0.3107769423558897 [----------] 0.79%

spotPython tuning: -0.3107769423558897 [----------] 1.03%

spotPython tuning: -0.3107769423558897 [----------] 1.29%

spotPython tuning: -0.3107769423558897 [----------] 1.60%

spotPython tuning: -0.3107769423558897 [----------] 1.97%

spotPython tuning: -0.3107769423558897 [----------] 2.30%

spotPython tuning: -0.3107769423558897 [----------] 2.62%

spotPython tuning: -0.3107769423558897 [----------] 2.90%

spotPython tuning: -0.3107769423558897 [----------] 3.18%

spotPython tuning: -0.3107769423558897 [----------] 4.16%

spotPython tuning: -0.3107769423558897 [#---------] 5.16%
```

```
spotPython tuning: -0.3107769423558897 [#---------] 6.33%

spotPython tuning: -0.3107769423558897 [#---------] 7.51%

spotPython tuning: -0.3107769423558897 [#---------] 8.74%

spotPython tuning: -0.3107769423558897 [#---------] 10.17%

spotPython tuning: -0.3107769423558897 [#---------] 11.28%

spotPython tuning: -0.3107769423558897 [#---------] 13.26%

spotPython tuning: -0.3107769423558897 [#---------] 14.56%

spotPython tuning: -0.3107769423558897 [##--------] 15.60%

spotPython tuning: -0.3107769423558897 [##--------] 16.51%

spotPython tuning: -0.3107769423558897 [##--------] 17.55%

spotPython tuning: -0.3107769423558897 [##--------] 18.80%

spotPython tuning: -0.3107769423558897 [##--------] 19.78%

spotPython tuning: -0.3107769423558897 [##--------] 21.03%

spotPython tuning: -0.3107769423558897 [##--------] 22.46%

spotPython tuning: -0.3107769423558897 [##--------] 23.96%

spotPython tuning: -0.3107769423558897 [###-------] 25.67%

spotPython tuning: -0.3107769423558897 [###-------] 27.43%

spotPython tuning: -0.3107769423558897 [###-------] 29.07%

spotPython tuning: -0.3107769423558897 [###-------] 31.43%
```

```
spotPython tuning: -0.3107769423558897 [###-------] 33.49%

spotPython tuning: -0.3107769423558897 [####------] 36.03%

spotPython tuning: -0.3107769423558897 [####------] 39.84%

spotPython tuning: -0.3107769423558897 [####------] 42.72%

spotPython tuning: -0.3107769423558897 [#####-----] 45.55%

spotPython tuning: -0.3107769423558897 [#####-----] 48.73%

spotPython tuning: -0.3107769423558897 [#####-----] 51.61%

spotPython tuning: -0.3107769423558897 [#####-----] 54.38%

spotPython tuning: -0.3107769423558897 [######----] 57.39%

spotPython tuning: -0.3107769423558897 [######----] 60.35%

spotPython tuning: -0.3107769423558897 [######----] 63.52%

spotPython tuning: -0.3107769423558897 [#######---] 66.66%

spotPython tuning: -0.3107769423558897 [#######---] 69.44%

spotPython tuning: -0.3107769423558897 [#######---] 72.55%

spotPython tuning: -0.3107769423558897 [########--] 81.33%

spotPython tuning: -0.3107769423558897 [#########-] 85.04%

spotPython tuning: -0.3107769423558897 [#########-] 88.62%

spotPython tuning: -0.3107769423558897 [#########-] 92.31%

spotPython tuning: -0.3107769423558897 [##########] 96.25%

spotPython tuning: -0.3107769423558897 [##########] 100.00% Done...

<spotPython.spot.spot.Spot at 0x289d1bb20>
```

16.8 Step 9: Tensorboard

The textual output shown in the console (or code cell) can be visualized with Tensorboard as described in Section **??**, see also the description in the documentation: Tensorboard.

16.9 Step 10: 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 **?@fig-progress**.

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

19_spot_hpt_sklearn_multiclass_classification_knn_files/fig

Figure 16.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

- Print the results

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

```
| name        | type   | default   |   lower |   upper |   tuned | transform             |
|-------------|--------|-----------|---------|---------|---------|-----------------------|---
| n_neighbors | int    | 2         |       1 |       7 |     4.0 | transform_power_2_int |
| weights     | factor | uniform   |       0 |       1 |     1.0 | None                  |
| algorithm   | factor | auto      |       0 |       3 |     2.0 | None                  |
| leaf_size   | int    | 5         |       2 |       7 |     6.0 | transform_power_2_int |
| p           | int    | 2         |       1 |       2 |     1.0 | None                  |
```

16.9.1 Show variable importance

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

19_spot_hpt_sklearn_multiclass_classification_knn_files/fig

Figure 16.2: Variable importance plot, threshold 0.025.

16.9.2 Get Default Hyperparameters

```
from spotPython.hyperparameters.values import get_default_values, transform_hyper_paramete
values_default = get_default_values(fun_control)
values_default = transform_hyper_parameter_values(fun_control=fun_control, hyper_parameter
values_default
```

```
{'n_neighbors': 4,
 'weights': 'uniform',
 'algorithm': 'auto',
 'leaf_size': 32,
 'p': 2}
```

```
from sklearn.pipeline import make_pipeline
model_default = make_pipeline(fun_control["prep_model"], fun_control["core_model"](**value
model_default
```

```
Pipeline(steps=[('nonetype', None),
                ('kneighborsclassifier',
                 KNeighborsClassifier(leaf_size=32, n_neighbors=4))])
```

16.9.3 Get SPOT Results

```
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
print(X)
```

```
[[4. 1. 2. 6. 1.]]
```

```
from spotPython.hyperparameters.values import assign_values, return_conf_list_from_var_dic
v_dict = assign_values(X, fun_control["var_name"])
return_conf_list_from_var_dict(var_dict=v_dict, fun_control=fun_control)
```

```
[{'n_neighbors': 16,
  'weights': 'distance',
  'algorithm': 'kd_tree',
  'leaf_size': 64,
  'p': 1}]
```

```
from spotPython.hyperparameters.values import get_one_sklearn_model_from_X
model_spot = get_one_sklearn_model_from_X(X, fun_control)
model_spot
```

```
KNeighborsClassifier(algorithm='kd_tree', leaf_size=64, n_neighbors=16, p=1,
                     weights='distance')
```

16.9.4 Evaluate SPOT Results

- Fetch the data.

```
from spotPython.utils.convert import get_Xy_from_df
X_train, y_train = get_Xy_from_df(fun_control["train"], fun_control["target_column"])
X_test, y_test = get_Xy_from_df(fun_control["test"], fun_control["target_column"])
X_test.shape, y_test.shape
```

```
((177, 64), (177,))
```

- Fit the model with the tuned hyperparameters. This gives one result:

```python
model_spot.fit(X_train, y_train)
y_pred = model_spot.predict_proba(X_test)
res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
res
```

```
0.3267419962335216
```

```python
def repeated_eval(n, model):
    res_values = []
    for i in range(n):
        model.fit(X_train, y_train)
        y_pred = model.predict_proba(X_test)
        res = mapk_score(y_true=y_test, y_pred=y_pred, k=3)
        res_values.append(res)
    mean_res = np.mean(res_values)
    print(f"mean_res: {mean_res}")
    std_res = np.std(res_values)
    print(f"std_res: {std_res}")
    min_res = np.min(res_values)
    print(f"min_res: {min_res}")
    max_res = np.max(res_values)
    print(f"max_res: {max_res}")
    median_res = np.median(res_values)
    print(f"median_res: {median_res}")
    return mean_res, std_res, min_res, max_res, median_res
```

16.9.5 Handling Non-deterministic Results

- Because the model is non-determinstic, we perform $n = 30$ runs and calculate the mean and standard deviation of the performance metric.

```python
_ = repeated_eval(30, model_spot)
```

```
mean_res: 0.3267419962335218
std_res: 1.6653345369377348e-16
min_res: 0.3267419962335216
max_res: 0.3267419962335216
median_res: 0.3267419962335216
```

16.9.6 Evalution of the Default Hyperparameters

```
model_default.fit(X_train, y_train)["kneighborsclassifier"]
```

```
KNeighborsClassifier(leaf_size=32, n_neighbors=4)
```

- One evaluation of the default hyperparameters is performed on the hold-out test set.

```
y_pred = model_default.predict_proba(X_test)
mapk_score(y_true=y_test, y_pred=y_pred, k=3)
```

```
0.2768361581920904
```

Since one single evaluation is not meaningful, we perform, similar to the evaluation of the SPOT results, $n = 30$ runs of the default setting and and calculate the mean and standard deviation of the performance metric.

```
_ = repeated_eval(30, model_default)
```

```
mean_res: 0.2768361581920903
std_res: 1.1102230246251565e-16
min_res: 0.2768361581920904
max_res: 0.2768361581920904
median_res: 0.2768361581920904
```

16.9.7 Plot: Compare Predictions

```
from spotPython.plot.validation import plot_confusion_matrix
plot_confusion_matrix(model_default, fun_control, title = "Default")
```

19_spot_hpt_sklearn_multiclass_classification_knn_files/fig

```
plot_confusion_matrix(model_spot, fun_control, title="SPOT")
```

19_spot_hpt_sklearn_multiclass_classification_knn_files/fig

```
min(spot_tuner.y), max(spot_tuner.y)
```

```
(-0.3107769423558897, -0.23558897243107768)
```

16.9.8 Cross-validated Evaluations

```
from spotPython.sklearn.traintest import evaluate_cv
fun_control.update({
     "eval": "train_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3157232704402516, None)
```

```
fun_control.update({
     "eval": "test_cv",
     "k_folds": 10,
})
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.2832788671023965, None)
```

- This is the evaluation that will be used in the comparison:

```
fun_control.update({
     "eval": "data_cv",
     "k_folds": 10,
})
```

```
evaluate_cv(model=model_spot, fun_control=fun_control, verbose=0)
```

```
(0.3061904761904762, None)
```

16.9.9 Detailed Hyperparameter Plots

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

```
n_neighbors:  100.0
p:  0.025665817779093207
```

19_spot_hpt_sklearn_multiclass_classification_knn_files/fig

16.9.10 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

```
Unable to display output for mime type(s): text/html
```

16.9.11 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
    for i in range(n-1):
        for j in range(i+1, n):
```

```
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

17 HPT PyTorch Lightning: VBDP

In this tutorial, we will show how `spotPython` can be integrated into the `PyTorch` Lightning training workflow for a classification task.

> Caution: Data must be downloaded manually
>
> - Ensure that the corresponding data is available as `./data/VBDP/train.csv`.

This document refers to the latest `spotPython` version, which can be installed via pip. Alternatively, the source code can be downloaded from gitHub: https://github.com/sequential-parameter-optimization/spotPython.

- Uncomment the following lines if you want to for (re-)installation the latest version of `spotPython` from GitHub.

```
# import sys
# !{sys.executable} -m pip install --upgrade build
# !{sys.executable} -m pip install --upgrade --force-reinstall spotPython
```

17.1 Step 1: Setup

- Before we consider the detailed experimental setup, we select the parameters that affect run time, initial design size, etc.
- The parameter `MAX_TIME` specifies the maximum run time in seconds.
- The parameter `INIT_SIZE` specifies the initial design size.
- The parameter `WORKERS` specifies the number of workers.
- The prefix `PREFIX` is used for the experiment name and the name of the log file.

```
MAX_TIME = 1
INIT_SIZE = 5
WORKERS = 0
PREFIX="31"
```

Caution: Run time and initial design size should be increased for real experiments

- `MAX_TIME` is set to one minute for demonstration purposes. For real experiments, this should be increased to at least 1 hour.
- `INIT_SIZE` is set to 5 for demonstration purposes. For real experiments, this should be increased to at least 10.
- `WORKERS` is set to 0 for demonstration purposes. For real experiments, this should be increased. See the warnings that are printed when the number of workers is set to 0.

Note: Device selection

- Although there are no .cuda() or .to(device) calls required, because Lightning does these for you, see LIGHTNINGMODULE, we would like to know which device is used. Threrefore, we imitate the LightningModule behaviour which selects the highest device.
- The method `spotPython.utils.device.getDevice()` returns the device that is used by Lightning.

17.2 Step 2: Initialization of the `fun_control` Dictionary

`spotPython` uses a Python dictionary for storing the information required for the hyperparameter tuning process, which was described in Section ??, see Initialization of the fun_control Dictionary in the documentation.

```
from spotPython.utils.init import fun_control_init
from spotPython.utils.file import get_experiment_name, get_spot_tensorboard_path
from spotPython.utils.device import getDevice

experiment_name = get_experiment_name(prefix=PREFIX)
fun_control = fun_control_init(
    spot_tensorboard_path=get_spot_tensorboard_path(experiment_name),
    num_workers=WORKERS,
    device=getDevice(),
    _L_in=64,
    _L_out=11,
    TENSORBOARD_CLEAN=True)
```

```
fun_control["device"]
```

```
'mps'
```

17.3 Step 3: PyTorch Data Loading

17.3.1 Lightning Dataset and DataModule

The data loading and preprocessing is handled by `Lightning` and `PyTorch`. It comprehends the following classes:

- `CSVDataset`: A class that loads the data from a CSV file. [SOURCE]
- `CSVDataModule`: A class that prepares the data for training and testing. [SOURCE]

Section Section **??** illustrates how to access the data.

17.4 Step 4: Preprocessing

Preprocessing is handled by `Lightning` and `PyTorch`. It can be implemented in the `CSVDataModule` class [SOURCE] and is described in the LIGHTNINGDATAMODULE documentation. Here you can find information about the `transforms` methods.

17.5 Step 5: Select the NN Model (`algorithm`) and `core_model_hyper_dict`

`spotPython` includes the `NetLightBase` class [SOURCE] for configurable neural networks. The class is imported here. It inherits from the class `Lightning.LightningModule`, which is the base class for all models in `Lightning`. `Lightning.LightningModule` is a subclass of `torch.nn.Module` and provides additional functionality for the training and testing of neural networks. The class `Lightning.LightningModule` is described in the Lightning documentation.

- Here we simply add the NN Model to the fun_control dictionary by calling the function `add_core_model_to_fun_control`:

```
from spotPython.light.netlightbase import NetLightBase
from spotPython.data.light_hyper_dict import LightHyperDict
from spotPython.hyperparameters.values import add_core_model_to_fun_control
add_core_model_to_fun_control(core_model=NetLightBase,
                              fun_control=fun_control,
                              hyper_dict= LightHyperDict)
```

The NetLightBase is a configurable neural network. The hyperparameters of the model are specified in the core_model_hyper_dict dictionary [SOURCE].

17.6 Step 6: Modify hyper_dict Hyperparameters for the Selected Algorithm aka core_model

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 were described in Section ??.

> Caution: Small number of epochs for demonstration purposes
>
> - epochs and patience are set to small values for demonstration purposes. These values are too small for a real application.
> - More resonable values are, e.g.:
>   - modify_hyper_parameter_bounds(fun_control, "epochs", bounds=[7, 9]) and
>   - modify_hyper_parameter_bounds(fun_control, "patience", bounds=[2, 7])

```
from spotPython.hyperparameters.values import modify_hyper_parameter_bounds

modify_hyper_parameter_bounds(fun_control, "l1", bounds=[5,8])
modify_hyper_parameter_bounds(fun_control, "epochs", bounds=[6,13])
modify_hyper_parameter_bounds(fun_control, "batch_size", bounds=[2, 8])
```

```
from spotPython.hyperparameters.values import modify_hyper_parameter_levels
modify_hyper_parameter_levels(fun_control, "optimizer",["Adam", "AdamW", "Adamax", "NAdam"
# modify_hyper_parameter_levels(fun_control, "optimizer", ["Adam"])
```

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 [SOURCE] generates a design table as follows:

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

```
| name           | type   | default    |    lower |    upper | transform              |
```

```
|----------------|--------|-----------|---------|---------|-----------------------|
| l1             | int    | 3         |     5   |     8   | transform_power_2_int |
| epochs         | int    | 4         |     6   |    13   | transform_power_2_int |
| batch_size     | int    | 4         |     2   |     8   | transform_power_2_int |
| act_fn         | factor | ReLU      |     0   |     5   | None                  |
| optimizer      | factor | SGD       |     0   |     3   | None                  |
| dropout_prob   | float  | 0.01      |     0   |     0.25 | None                 |
| lr_mult        | float  | 1.0       |     0.1 |    10   | None                  |
| patience       | int    | 2         |     2   |     6   | transform_power_2_int |
| initialization | factor | Default   |     0   |     2   | None                  |
```

This allows to check if all information is available and if the information is correct.

Note: Hyperparameters of the Tuned Model and the `fun_control` Dictionary

The updated `fun_control` dictionary can be shown with the command `fun_control["core_model_hyper_dict"]`.

17.7 Step 7: Data Splitting, the Objective (Loss) Function and the Metric

17.7.1 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 (see Section **??**)
2. the loss function (and a metric).

Caution: Data Splitting in Lightning

- The data splitting is handled by `Lightning`.

17.7.2 Loss Functions and Metrics

The loss function is specified in the configurable network class [SOURCE] We will use CrossEntropy loss for the multiclass-classification task.

17.7.3 Metric

- We will use the MAP@k metric [SOURCE] for the evaluation of the model.
- An example, how this metric works, is shown in the Appendix, see Section {Section **??**}.

Similar to the loss function, the metric is specified in the configurable network class [SOURCE].

> Caution: Loss Function and Metric in Lightning
>
> - The loss function and the metric are not hyperparameters that can be tuned with `spotPython`.
> - They are handled by `Lightning`.

17.8 Step 8: Calling the SPOT Function

17.8.1 Preparing the SPOT Call

The following code passes the information about the parameter ranges and bounds to `spot`. It extracts the variable types, names, and bounds

```
from spotPython.hyperparameters.values import (get_bound_values,
    get_var_name,
    get_var_type,)
var_type = get_var_type(fun_control)
var_name = get_var_name(fun_control)
lower = get_bound_values(fun_control, "lower")
upper = get_bound_values(fun_control, "upper")
```

17.8.2 The Objective Function `fun`

The objective function `fun` from the class `HyperLight` [SOURCE] is selected next. It implements an interface from `PyTorch`'s training, validation, and testing methods to `spotPython`.

```
from spotPython.fun.hyperlight import HyperLight
fun = HyperLight().fun
```

17.8.3 Starting the Hyperparameter Tuning

The spotPython hyperparameter tuning is started by calling the Spot function [SOURCE] as described in Section ??.

```
import numpy as np
from spotPython.spot import spot
from math import inf
spot_tuner = spot.Spot(fun=fun,
                   lower = lower,
                   upper = upper,
                   fun_evals = inf,
                   max_time = MAX_TIME,
                   tolerance_x = np.sqrt(np.spacing(1)),
                   var_type = var_type,
                   var_name = var_name,
                   show_progress= True,
                   fun_control = fun_control,
                   design_control={"init_size": INIT_SIZE},
                   surrogate_control={"noise": True,
                                      "min_theta": -4,
                                      "max_theta": 3,
                                      "n_theta": len(var_name),
                                      "model_fun_evals": 10_000,
                                      })
spot_tuner.run()
```

```
config: {'l1': 256, 'epochs': 4096, 'batch_size': 32, 'act_fn': ReLU(), 'optimizer': 'AdamW'
```

```
      Validate metric            DataLoader 0

         hp_metric           2.2778313159942627
          val_acc             0.268551230430603
         val_loss            2.2778313159942627
        valid_mapk           0.36781978607177734
```

```
config: {'l1': 32, 'epochs': 128, 'batch_size': 256, 'act_fn': LeakyReLU(), 'optimizer': 'Ada
```

```
  Validate metric           DataLoader 0

     hp_metric           2.3127529621124268
      val_acc            0.2226148396730423
     val_loss            2.3127529621124268
    valid_mapk           0.3133559823036194
```

```
config: {'l1': 128, 'epochs': 256, 'batch_size': 8, 'act_fn': Swish(), 'optimizer': 'NAdam',
```

```
  Validate metric           DataLoader 0

     hp_metric           2.4299659729003906
      val_acc            0.11307420581579208
     val_loss            2.4299659729003906
    valid_mapk            0.196180522441864
```

```
config: {'l1': 64, 'epochs': 512, 'batch_size': 16, 'act_fn': Sigmoid(), 'optimizer': 'Adam'
```

```
  Validate metric           DataLoader 0

     hp_metric           2.3009538650512695
      val_acc            0.23674911260604858
     val_loss            2.3009538650512695
    valid_mapk           0.31565654277801514
```

```
config: {'l1': 64, 'epochs': 4096, 'batch_size': 64, 'act_fn': ReLU(), 'optimizer': 'Adamax'
```

```
  Validate metric           DataLoader 0

     hp_metric           2.2806520462036133
      val_acc            0.23674911260604858
```

```
val_loss              2.2806520462036133
valid_mapk             0.330941379070282
```

```
config: {'l1': 32, 'epochs': 4096, 'batch_size': 128, 'act_fn': ReLU(), 'optimizer': 'Adamax
```

```
Validate metric            DataLoader 0

   hp_metric              2.321744680404663
    val_acc              0.18727914988994598
   val_loss               2.321744680404663
  valid_mapk             0.3122909963130951
```

```
spotPython tuning: 2.2778313159942627 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x2b8e6f370>
```

17.9 Step 9: Tensorboard

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

```
tensorboard --logdir="runs/"
```

Further information can be found in the PyTorch Lightning documentation for Tensorboard.

17.10 Step 10: Results

After the hyperparameter tuning run is finished, the results can be analyzed as described in Section **??**.

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

31_spot_lightning_csv_files/figure-pdf/cell-13-output-1.pdf

Figure 17.1: Progress plot. *Black* dots denote results from the initial design. *Red* dots illustrate the improvement found by the surrogate model based optimization.

```
from spotPython.utils.eda import gen_design_table
print(gen_design_table(fun_control=fun_control, spot=spot_tuner))
```

```
| name           | type   | default   |   lower |   upper |                tuned | transform
|----------------|--------|-----------|---------|---------|----------------------|-----------
| l1             | int    | 3         |     5.0 |     8.0 |                  8.0 | transform_
| epochs         | int    | 4         |     6.0 |    13.0 |                 12.0 | transform_
| batch_size     | int    | 4         |     2.0 |     8.0 |                  5.0 | transform_
| act_fn         | factor | ReLU      |     0.0 |     5.0 |                  2.0 | None
| optimizer      | factor | SGD       |     0.0 |     3.0 |                  1.0 | None
| dropout_prob   | float  | 0.01      |     0.0 |    0.25 |  0.10939527466721133 | None
| lr_mult        | float  | 1.0       |     0.1 |    10.0 |    4.211776903906428 | None
| patience       | int    | 2         |     2.0 |     6.0 |                  4.0 | transform_
| initialization | factor | Default   |     0.0 |     2.0 |                  0.0 | None
```

```
spot_tuner.plot_importance(threshold=0.025,
    filename="./figures/" + experiment_name+"_importance.png")
```

31_spot_lightning_csv_files/figure-pdf/cell-15-output-1.pdf

Figure 17.2: Variable importance plot, threshold 0.025.

17.10.1 Get the Tuned Architecture

```
from spotPython.light.utils import get_tuned_architecture
config = get_tuned_architecture(spot_tuner, fun_control)
```

- Test on the full data set

```
from spotPython.light.traintest import test_model
test_model(config, fun_control)
```

```
       Test metric             DataLoader 0

        hp_metric            2.1490375995635986
     test_mapk_epoch         0.4713163673877716
         val_acc             0.3932107388973236
        val_loss             2.1490375995635986
```

```
(2.1490375995635986, 0.3932107388973236)
```

```
from spotPython.light.traintest import load_light_from_checkpoint

model_loaded = load_light_from_checkpoint(config, fun_control)
```

```
Loading model from runs/lightning_logs/256_4096_32_ReLU()_AdamW_0.10939527466721133_4.211776
```

17.10.2 Cross Validation With Lightning

- The KFold class from sklearn.model_selection is used to generate the folds for cross-validation.
- These mechanism is used to generate the folds for the final evaluation of the model.
- The CrossValidationDataModule class [SOURCE] is used to generate the folds for the hyperparameter tuning process.
- It is called from the cv_model function [SOURCE].

```
from spotPython.light.traintest import cv_model
# set the number of folds to 10
fun_control["k_folds"] = 10
```

```
cv_model(config, fun_control)
```

```
k: 0
Train Dataset Size: 636
Val Dataset Size: 71


      Validate metric             DataLoader 0

         hp_metric             2.2597849369049072
          val_acc              0.26760563254356384
         val_loss              2.2597849369049072
        valid_mapk              0.37028768658638


train_model result: {'valid_mapk': 0.37028768658638, 'val_loss': 2.2597849369049072, 'val_acc
k: 1
Train Dataset Size: 636
Val Dataset Size: 71


      Validate metric             DataLoader 0

         hp_metric              2.200228691101074
          val_acc              0.3239436745643616
         val_loss               2.200228691101074
        valid_mapk             0.5409225821495056


train_model result: {'valid_mapk': 0.5409225821495056, 'val_loss': 2.200228691101074, 'val_ac
k: 2
Train Dataset Size: 636
Val Dataset Size: 71


      Validate metric             DataLoader 0

         hp_metric             2.3468029499053955
          val_acc              0.18309858441352844
         val_loss              2.3468029499053955
```

```
        valid_mapk            0.2470238208770752


train_model result: {'valid_mapk': 0.2470238208770752, 'val_loss': 2.3468029499053955, 'val_a
k: 3
Train Dataset Size: 636
Val Dataset Size: 71



      Validate metric            DataLoader 0

         hp_metric           2.2228169441223145
          val_acc            0.30985915660858154
         val_loss            2.2228169441223145
        valid_mapk            0.367807537317276


train_model result: {'valid_mapk': 0.367807537317276, 'val_loss': 2.2228169441223145, 'val_ac
k: 4
Train Dataset Size: 636
Val Dataset Size: 71



      Validate metric            DataLoader 0

         hp_metric           2.3275797367095947
          val_acc            0.2112676054239273
         val_loss            2.3275797367095947
        valid_mapk            0.294394850730896


train_model result: {'valid_mapk': 0.294394850730896, 'val_loss': 2.3275797367095947, 'val_ac
k: 5
Train Dataset Size: 636
Val Dataset Size: 71



      Validate metric            DataLoader 0

         hp_metric           2.2334837913513184
          val_acc            0.3239436745643616
```

```
         val_loss             2.2334837913513184
        valid_mapk            0.4871031939983368


train_model result: {'valid_mapk': 0.4871031939983368, 'val_loss': 2.2334837913513184, 'val_a
k: 6
Train Dataset Size: 636
Val Dataset Size: 71


      Validate metric             DataLoader 0

         hp_metric            2.3447251319885254
          val_acc             0.18309858441352844
         val_loss             2.3447251319885254
        valid_mapk            0.2688492238521576


train_model result: {'valid_mapk': 0.2688492238521576, 'val_loss': 2.3447251319885254, 'val_a
k: 7
Train Dataset Size: 637
Val Dataset Size: 70


      Validate metric             DataLoader 0

         hp_metric            2.2224338054656982
          val_acc             0.30000001192092896
         val_loss             2.2224338054656982
        valid_mapk            0.48900464177131653


train_model result: {'valid_mapk': 0.48900464177131653, 'val_loss': 2.2224338054656982, 'val_
k: 8
Train Dataset Size: 637
Val Dataset Size: 70


      Validate metric             DataLoader 0

         hp_metric            2.3125994205474854
```

```
val_acc             0.2142857164144516
val_loss            2.3125994205474854
valid_mapk          0.3628472089767456
```

```
train_model result: {'valid_mapk': 0.3628472089767456, 'val_loss': 2.3125994205474854, 'val_a
k: 9
Train Dataset Size: 637
Val Dataset Size: 70
```

```
Validate metric            DataLoader 0

hp_metric           2.2290546894073486
val_acc             0.3142857253551483
val_loss            2.2290546894073486
valid_mapk          0.3229166567325592
```

```
train_model result: {'valid_mapk': 0.3229166567325592, 'val_loss': 2.2290546894073486, 'val_a
```

```
0.37511574029922484
```

> **Note: Evaluation for the Final Comaprison**
>
> - This is the evaluation that will be used in the comparison.

17.10.3 Detailed Hyperparameter Plots

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

```
epochs:  82.46345406242555
act_fn:  100.0
dropout_prob:  0.12389681147506997
```

31_spot_lightning_csv_files/figure-pdf/cell-20-output-2.pdf

Figure 17.3: Contour plots.

31_spot_lightning_csv_files/figure-pdf/cell-20-output-3.pdf

31_spot_lightning_csv_files/figure-pdf/cell-20-output-4.pdf

17.10.4 Parallel Coordinates Plot

```
spot_tuner.parallel_plot()
```

```
Unable to display output for mime type(s): text/html
```

Parallel coordinates plots

```
Unable to display output for mime type(s): text/html
```

17.10.5 Plot all Combinations of Hyperparameters

- Warning: this may take a while.

```
PLOT_ALL = False
if PLOT_ALL:
    n = spot_tuner.k
```

```python
    for i in range(n-1):
        for j in range(i+1, n):
            spot_tuner.plot_contour(i=i, j=j, min_z=min_z, max_z = max_z)
```

17.10.6 Visualizing the Activation Distribution

Reference:

- The following code is based on [PyTorch Lightning TUTORIAL 2: ACTIVATION FUNCTIONS], Author: Phillip Lippe, License: [CC BY-SA], Generated: 2023-03-15T09:52:39.179933.

After we have trained the models, we can look at the actual activation values that find inside the model. For instance, how many neurons are set to zero in ReLU? Where do we find most values in Tanh? To answer these questions, we can write a simple function which takes a trained model, applies it to a batch of images, and plots the histogram of the activations inside the network:

```python
from spotPython.torch.activation import Sigmoid, Tanh, ReLU, LeakyReLU, ELU, Swish
act_fn_by_name = {"sigmoid": Sigmoid, "tanh": Tanh, "relu": ReLU, "leakyrelu": LeakyReLU,
```

```python
from spotPython.hyperparameters.values import get_one_config_from_X
X = spot_tuner.to_all_dim(spot_tuner.min_X.reshape(1,-1))
config = get_one_config_from_X(X, fun_control)
model = fun_control["core_model"](**config, _L_in=64, _L_out=11)
model
```

```
NetLightBase(
  (train_mapk): MAPK()
  (valid_mapk): MAPK()
  (test_mapk): MAPK()
  (layers): Sequential(
    (0): Linear(in_features=64, out_features=256, bias=True)
    (1): ReLU()
    (2): Dropout(p=0.10939527466721133, inplace=False)
    (3): Linear(in_features=256, out_features=128, bias=True)
    (4): ReLU()
    (5): Dropout(p=0.10939527466721133, inplace=False)
    (6): Linear(in_features=128, out_features=128, bias=True)
    (7): ReLU()
```

```
    (8): Dropout(p=0.10939527466721133, inplace=False)
    (9): Linear(in_features=128, out_features=64, bias=True)
    (10): ReLU()
    (11): Dropout(p=0.10939527466721133, inplace=False)
    (12): Linear(in_features=64, out_features=11, bias=True)
  )
)
```

```python
from spotPython.utils.eda import visualize_activations
visualize_activations(model, color=f"C{0}")
```

31_spot_lightning_csv_files/figure-pdf/cell-25-output-1.pdf

17.11 Submission

```python
import numpy as np
import pandas as pd
from sklearn.preprocessing import OrdinalEncoder
```

```python
import pandas as pd
from sklearn.preprocessing import OrdinalEncoder
train_df = pd.read_csv('./data/VBDP/train.csv', index_col=0)
# remove the id column
# train_df = train_df.drop(columns=['id'])
n_samples = train_df.shape[0]
n_features = train_df.shape[1] - 1
target_column = "prognosis"
# Encode our prognosis labels as integers for easier decoding later
enc = OrdinalEncoder()
y = enc.fit_transform(train_df[[target_column]])
test_df = pd.read_csv('./data/VBDP/test.csv', index_col=0)
test_df
```

id	sudden_fever	headache	mouth_bleed	nose_bleed	muscle_pain	joint_pain	vomiting	rash	dia
707	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
708	1.0	1.0	0.0	1.0	0.0	1.0	1.0	1.0	
709	1.0	1.0	0.0	1.0	1.0	1.0	1.0	0.0	
710	0.0	1.0	0.0	0.0	0.0	1.0	1.0	1.0	
711	0.0	0.0	1.0	0.0	1.0	1.0	0.0	0.0	
...	...	...	...	...	...	...	...	...	
1005	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	
1006	1.0	0.0	1.0	0.0	1.0	1.0	0.0	1.0	
1007	1.0	0.0	0.0	1.0	1.0	0.0	1.0	1.0	
1008	1.0	0.0	1.0	1.0	1.0	0.0	1.0	0.0	
1009	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	

```python
import torch
X_tensor = torch.Tensor(test_df.values)
X_tensor = X_tensor.to(fun_control["device"])
```

```python
y = model_loaded(X_tensor)
y.shape
```

```
torch.Size([303, 11])
```

```python
# convert the predictions to a numpy array
y = y.cpu().detach().numpy()
y
```

```
array([[4.8564044e-07, 1.6487252e-04, 5.4398137e-01, ..., 3.4355637e-02,
        4.0643147e-01, 4.8128068e-03],
       [9.9994564e-01, 5.0947194e-05, 4.9569702e-15, ..., 3.3718368e-06,
        1.4148394e-08, 3.3289385e-10],
       [6.4826966e-04, 1.7104080e-04, 9.8287100e-03, ..., 2.1993841e-01,
        8.8195398e-02, 1.6476467e-01],
       ...,
       [2.9529277e-09, 2.8129137e-09, 1.1018859e-07, ..., 1.0940506e-03,
        2.4432049e-07, 8.2061818e-04],
       [3.0594871e-12, 1.4670589e-09, 2.0237121e-06, ..., 6.4277177e-05,
        2.5600203e-08, 1.9252108e-04],
       [1.3348927e-08, 9.2245477e-07, 1.6618009e-03, ..., 3.2895284e-03,
```

```
       2.6913152e-05, 6.2432229e-03]], dtype=float32)
```

```
test_sorted_prediction_ids = np.argsort(-y, axis=1)
test_top_3_prediction_ids = test_sorted_prediction_ids[:,:3]
original_shape = test_top_3_prediction_ids.shape
test_top_3_prediction = enc.inverse_transform(test_top_3_prediction_ids.reshape(-1, 1))
test_top_3_prediction = test_top_3_prediction.reshape(original_shape)
test_df['prognosis'] = np.apply_along_axis(lambda x: np.array(' '.join(x), dtype="object")
test_df['prognosis'].reset_index().to_csv('./data/VBDP/submission.csv', index=False)
```

17.12 Appendix

17.12.1 Differences to the spotPython Approaches for `torch`, `sklearn` and `river`

> **Caution: Data Loading in Lightning**
>
> - Data loading is handled independently from the `fun_control` dictionary by `Lightning` and `PyTorch`.
> - In contrast to `spotPython` with `torch`, `river` and `sklearn`, the data sets are not added to the `fun_control` dictionary.

17.12.1.1 Specification of the Preprocessing Model

The `fun_control` dictionary, the `torch`, `sklearn`and `river` versions of `spotPython` allow the specification of a data preprocessing pipeline, e.g., for the scaling of the data or for the one-hot encoding of categorical variables, see Section **??**. This feature is not used in the `Lightning` version.

> **Caution: Data preprocessing in Lightning**
>
> Lightning allows the data preprocessing to be specified in the `LightningDataModule` class. It is not considered here, because it should be computed at one location only.

17.12.2 Taking a Look at the Data

```
import torch
from spotPython.light.csvdataset import CSVDataset
from torch.utils.data import DataLoader
from torchvision.transforms import ToTensor

# Create an instance of CSVDataset
dataset = CSVDataset(csv_file="./data/VBDP/train.csv", train=True)
# show the dimensions of the input data
print(dataset[0][0].shape)
# show the first element of the input data
print(dataset[0][0])
# show the size of the dataset
print(f"Dataset Size: {len(dataset)}")
```

```
torch.Size([64])
tensor([1., 1., 0., 1., 1., 1., 1., 0., 1., 1., 1., 1., 0., 0., 1., 1., 0., 0.,
        1., 0., 1., 0., 1., 1., 1., 1., 1., 1., 1., 0., 0., 1., 0., 0., 0., 0.,
        1., 0., 0., 0., 0., 0., 1., 0., 1., 0., 1., 0., 0., 0., 0., 1., 0., 1.,
        0., 0., 0., 0., 0., 0., 0., 0., 0., 0.])
Dataset Size: 707
```

```
# Set batch size for DataLoader
batch_size = 3
# Create DataLoader
dataloader = DataLoader(dataset, batch_size=batch_size, shuffle=True)

# Iterate over the data in the DataLoader
for batch in dataloader:
    inputs, targets = batch
    print(f"Batch Size: {inputs.size(0)}")
    print("---------------")
    print(f"Inputs: {inputs}")
    print(f"Targets: {targets}")
    break
```

```
Batch Size: 3
---------------
Inputs: tensor([[1., 0., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0., 1., 0., 0., 1., 0., 0.,
```

```
         1., 1., 0., 0., 1., 1., 1., 1., 0., 1., 1., 0., 0., 0., 0., 0., 0., 0.,
         0., 0., 0., 0., 1., 0., 0., 0., 0., 1., 0., 0., 1., 0., 0., 0., 0., 0.,
         0., 0., 0., 0., 0., 0., 0., 0., 0., 0.],
        [1., 1., 1., 0., 1., 0., 0., 0., 0., 0., 1., 1., 0., 0., 0., 1., 0., 0.,
         0., 0., 0., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0., 1., 1., 0., 1., 0.,
         1., 1., 1., 0., 1., 0., 0., 0., 0., 1., 0., 0., 0., 1., 1., 1., 1., 1.,
         0., 0., 0., 0., 0., 0., 0., 0., 0., 0.],
        [0., 0., 1., 0., 0., 0., 1., 0., 1., 1., 1., 0., 0., 0., 1., 0., 0., 0.,
         0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 1., 0., 0., 0., 1., 1., 1., 1.,
         1., 1., 1., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
         0., 0., 0., 0., 0., 0., 0., 0., 0., 0.]])
Targets: tensor([7, 8, 9])
```

17.12.3 The MAPK Metric

Here is an example how the MAPK metric is calculated.

```python
from spotPython.torch.mapk import MAPK
import torch
mapk = MAPK(k=2)
target = torch.tensor([0, 1, 2, 2])
preds = torch.tensor(
    [
        [0.5, 0.2, 0.2],  # 0 is in top 2
        [0.3, 0.4, 0.2],  # 1 is in top 2
        [0.2, 0.4, 0.3],  # 2 is in top 2
        [0.7, 0.2, 0.1],  # 2 isn't in top 2
    ]
)
mapk.update(preds, target)
print(mapk.compute()) # tensor(0.6250)
```

```
tensor(0.6250)
```

A Documentation of the Sequential Parameter Optimization

This document describes the `Spot` features.

A.1 Example: spot

```
import numpy as np
from math import inf
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
from scipy.optimize import shgo
from scipy.optimize import direct
from scipy.optimize import differential_evolution
import matplotlib.pyplot as plt
```

A.1.1 The Objective Function

The `spotPython` package provides several classes of objective functions. We will use an analytical objective function, i.e., a function that can be described by a (closed) formula:

$$f(x) = x^2$$

```
fun = analytical().fun_sphere
```

```
x = np.linspace(-1,1,100).reshape(-1,1)
y = fun(x)
plt.figure()
plt.plot(x,y, "k")
plt.show()
```

99_spot_doc_files/figure-pdf/cell-4-output-1.pdf

```
spot_1 = spot.Spot(fun=fun,
                   lower = np.array([-10]),
                   upper = np.array([100]),
                   fun_evals = 7,
                   fun_repeats = 1,
                   max_time = inf,
                   noise = False,
                   tolerance_x = np.sqrt(np.spacing(1)),
                   var_type=["num"],
                   infill_criterion = "y",
                   n_points = 1,
                   seed=123,
                   log_level = 50,
                   show_models=True,
                   fun_control = {},
                   design_control={"init_size": 5,
                                   "repeats": 1},
                   surrogate_control={"noise": False,
                                      "cod_type": "norm",
                                      "min_theta": -4,
                                      "max_theta": 3,
                                      "n_theta": 1,
                                      "model_optimizer": differential_evolution,
                                      "model_fun_evals": 1000,
                                      })
```

`spot`'s `__init__` method sets the control parameters. There are two parameter groups:

1. external parameters can be specified by the user
2. internal parameters, which are handled by `spot`.

A.1.2 External Parameters

external parameter	type	description	default	mandatory
`fun`	object	objective function		yes
`lower`	array	lower bound		yes
`upper`	array	upper bound		yes
`fun_evals`	int	number of function evaluations	15	no
`fun_evals`	int	number of function evaluations	15	no
`fun_control`	dict	noise etc.	{}	n
`max_time`	int	max run time budget	`inf`	no
`noise`	bool	if repeated evaluations of `fun` results in different values, then `noise` should be set to `True`.	`False`	no
`tolerance_x`	float	tolerance for new x solutions. Minimum distance of new solutions, generated by `suggest_new_X`, to already existing solutions. If zero (which is the default), every new solution is accepted.	`0`	no
`var_type`	list	list of type information, can be either `"num"` or `"factor"`	`["num"]`	no

external parameter	type	description	default	mandatory
`infill_criterion`	string	Can be `"y"`, `"s"`, `"ei"` (negative expected improvement), or `"all"`	`"y"`	no
`n_points`	int	number of infill points	1	no
`seed`	int	initial seed. If `Spot.run()` is called twice, different results will be generated. To reproduce results, the `seed` can be used.	`123`	no

external parameter	type	description	default	mandatory
`log_level`	int	log level with the following settings: `NOTSET` (`0`), `DEBUG` (`10`: Detailed information, typically of interest only when diagnosing problems.), `INFO` (`20`: Confirmation that things are working as expected.), `WARNING` (`30`: An indication that something unexpected happened, or indicative of some problem in the near future (e.g. 'disk space low'). The software is still working as expected.), `ERROR` (`40`: Due to a more serious problem, the software has not been able to perform some function.), and `CRITICAL` (`50`: A serious error, indicating that the program itself may be unable to continue running.)	`50`	no

external parameter	type	description	default	mandatory
`show_models`	bool	Plot model. Currently only 1-dim functions are supported	`False`	no
`design`	object	experimental design	`None`	no
`design_control`	dict	control parameters	see below	no
`surrogate`		surrogate model	`kriging`	no
`surrogate_control`	dict	control parameters	see below	no
`optimizer`	object	optimizer	see below	no
`optimizer_control`	dict	control parameters	see below	no

- Besides these single parameters, the following parameter dictionaries can be specified by the user:
  - `fun_control`
  - `design_control`
  - `surrogate_control`
  - `optimizer_control`

A.2 The `fun_control` Dictionary

	external parameter	type	description	default	mandatory
`sigma`		float	noise: standard deviation	`0`	yes
`seed`		int	seed for rng	`124`	yes

A.3 The `design_control` Dictionary

external parameter	type	description	default	mandatory
`init_size`	int	initial sample size	`10`	yes

external parameter	type	description	default	mandatory
`repeats`	int	number of repeats of the initial sammples	1	yes

A.4 The `surrogate_control` Dictionary

external parameter	type	description	default	mandatory
`noise`				
`model_optimizer`	object	optimizer	`differential_evolution`	
`model_fun_evals`				
`min_theta`			`-3.`	
`max_theta`			`3.`	
`n_theta`			`1`	
`n_p`			`1`	
`optim_p`			`False`	
`cod_type`			`"norm"`	
`var_type`				
`use_cod_y`	bool		`False`	

A.5 The `optimizer_control` Dictionary

external parameter	type	description	default	mandatory
`max_iter`	int	max number of iterations. Note: these are the cheap evaluations on the surrogate.	1000	no

A.6 Run

```
spot_1.run()
```

99_spot_doc_files/figure-pdf/cell-6-output-1.pdf

99_spot_doc_files/figure-pdf/cell-6-output-2.pdf

```
spotPython tuning: 1.6282181269484761 [#########-] 85.71%
```

99_spot_doc_files/figure-pdf/cell-6-output-4.pdf

```
spotPython tuning: 0.30656551286610595 [##########] 100.00% Done...
```

```
<spotPython.spot.spot.Spot at 0x17cb96a40>
```

A.7 Print the Results

```
spot_1.print_results()
```

```
min y: 0.30656551286610595
x0: -0.5536835855126157
```

```
[['x0', -0.5536835855126157]]
```

A.8 Show the Progress

```python
spot_1.plot_progress()
```

99_spot_doc_files/figure-pdf/cell-8-output-1.pdf

A.9 Visualize the Surrogate

- The plot method of the `kriging` surrogate is used.
- Note: the plot uses the interval defined by the ranges of the natural variables.

```python
spot_1.surrogate.plot()
```

```
<Figure size 2700x1800 with 0 Axes>
```

99_spot_doc_files/figure-pdf/cell-9-output-2.pdf

A.10 Init: Build Initial Design

```python
from spotPython.design.spacefilling import spacefilling
from spotPython.build.kriging import Kriging
from spotPython.fun.objectivefunctions import analytical
gen = spacefilling(2)
rng = np.random.RandomState(1)
lower = np.array([-5,-0])
upper = np.array([10,15])
fun = analytical().fun_branin
```

```
fun_control = {"sigma": 0,
               "seed": 123}

X = gen.scipy_lhd(10, lower=lower, upper = upper)
print(X)
y = fun(X, fun_control=fun_control)
print(y)
```

```
[[ 8.97647221 13.41926847]
 [ 0.66946019  1.22344228]
 [ 5.23614115 13.78185824]
 [ 5.6149825  11.5851384 ]
 [-1.72963184  1.66516096]
 [-4.26945568  7.1325531 ]
 [ 1.26363761 10.17935555]
 [ 2.88779942  8.05508969]
 [-3.39111089  4.15213772]
 [ 7.30131231  5.22275244]]
[128.95676449  31.73474356 172.89678121 126.71295908  64.34349975
  70.16178611  48.71407916  31.77322887  76.91788181  30.69410529]
```

A.11 Replicability

Seed

```
gen = spacefilling(2, seed=123)
X0 = gen.scipy_lhd(3)
gen = spacefilling(2, seed=345)
X1 = gen.scipy_lhd(3)
X2 = gen.scipy_lhd(3)
gen = spacefilling(2, seed=123)
X3 = gen.scipy_lhd(3)
X0, X1, X2, X3
```

```
(array([[0.77254938, 0.31539299],
        [0.59321338, 0.93854273],
        [0.27469803, 0.3959685 ]]),
 array([[0.78373509, 0.86811887],
        [0.06692621, 0.6058029 ],
```

```
       [0.41374778, 0.00525456]]),
array([[0.121357  , 0.69043832],
       [0.41906219, 0.32838498],
       [0.86742658, 0.52910374]]),
array([[0.77254938, 0.31539299],
       [0.59321338, 0.93854273],
       [0.27469803, 0.3959685 ]]))
```

A.12 Surrogates

A.12.1 A Simple Predictor

The code below shows how to use a simple model for prediction. Assume that only two (very costly) measurements are available:

1. f(0) = 0.5
2. f(2) = 2.5

We are interested in the value at $x_0 = 1$, i.e., $f(x_0 = 1)$, but cannot run an additional, third experiment.

```
from sklearn import linear_model
X = np.array([[0], [2]])
y = np.array([0.5, 2.5])
S_lm = linear_model.LinearRegression()
S_lm = S_lm.fit(X, y)
X0 = np.array([[1]])
y0 = S_lm.predict(X0)
print(y0)
```

```
[1.5]
```

Central Idea: Evaluation of the surrogate model `S_lm` is much cheaper (or / and much faster) than running the real-world experiment f.

A.13 Demo/Test: Objective Function Fails

SPOT expects `np.nan` values from failed objective function values. These are handled. Note: SPOT's counter considers only successful executions of the objective function.

```python
import numpy as np
from spotPython.fun.objectivefunctions import analytical
from spotPython.spot import spot
import numpy as np
from math import inf
# number of initial points:
ni = 20
# number of points
n = 30

fun = analytical().fun_random_error
lower = np.array([-1])
upper = np.array([1])
design_control={"init_size": ni}

spot_1 = spot.Spot(fun=fun,
            lower = lower,
            upper= upper,
            fun_evals = n,
            show_progress=False,
            design_control=design_control,)
spot_1.run()
# To check whether the run was successfully completed,
# we compare the number of evaluated points to the specified
# number of points.
assert spot_1.y.shape[0] == n
```

```
[ 0.53176481 -0.9053821  -0.02203599         nan  0.78240941 -0.58120945
 -0.3923345   0.67234256  0.31802454 -0.68898927 -0.75129705  0.97550354
  0.41757584         nan  0.82585329  0.23700598 -0.49274073 -0.82319082
 -0.17991251         nan]
[-1.]
[-0.47259301]

[0.95541987]




[0.17335968]

[-0.58552368]
```

```
[-0.20126111]

[-0.60100809]
[-0.97897336]

[nan]
[-0.2748985]

[0.8359486]
[0.99035591]

[0.01641232]
[0.5629346]
```

A.14 PyTorch: Detailed Description of the Data Splitting

A.14.1 Description of the "train_hold_out" Setting

The "train_hold_out" setting is used by default. It uses the loss function specfied in fun_control and the metric specified in fun_control.

1. First, the method HyperTorch().fun_torch is called.
2. fun_torc(), which is implemented in the file hypertorch.py, calls evaluate_hold_out() as follows:

```
df_eval, _ = evaluate_hold_out(
    model,
    train_dataset=fun_control["train"],
    shuffle=self.fun_control["shuffle"],
    loss_function=self.fun_control["loss_function"],
    metric=self.fun_control["metric_torch"],
    device=self.fun_control["device"],
    show_batch_interval=self.fun_control["show_batch_interval"],
    path=self.fun_control["path"],
    task=self.fun_control["task"],
    writer=self.fun_control["writer"],
    writerId=config_id,
)
```

Note: Only the data set fun_control["train"] is used for training and validation. It is used in evaluate_hold_out as follows:

```
trainloader, valloader = create_train_val_data_loaders(
                dataset=train_dataset, batch_size=batch_size_instance, shuffle=shuffle
            )
```

create_train_val_data_loaders() splits the train_dataset into trainloader and valloader using torch.utils.data.random_split() as follows:

```
def create_train_val_data_loaders(dataset, batch_size, shuffle, num_workers=0):
    test_abs = int(len(dataset) * 0.6)
    train_subset, val_subset = random_split(dataset, [test_abs, len(dataset) - test_abs])
    trainloader = torch.utils.data.DataLoader(
        train_subset, batch_size=int(batch_size), shuffle=shuffle, num_workers=num_workers
    )
    valloader = torch.utils.data.DataLoader(
```

```
        val_subset, batch_size=int(batch_size), shuffle=shuffle, num_workers=num_workers
    )
    return trainloader, valloader
```

The optimizer is set up as follows:

```
optimizer_instance = net.optimizer
lr_mult_instance = net.lr_mult
sgd_momentum_instance = net.sgd_momentum
optimizer = optimizer_handler(
    optimizer_name=optimizer_instance,
    params=net.parameters(),
    lr_mult=lr_mult_instance,
    sgd_momentum=sgd_momentum_instance,
)
```

3. `evaluate_hold_out()` sets the `net` attributes such as `epochs`, `batch_size`, `optimizer`, and `patience`. For each epoch, the methods `train_one_epoch()` and `validate_one_epoch()` are called, the former for training and the latter for validation and early stopping. The validation loss from the last epoch (not the best validation loss) is returned from `evaluate_hold_out`.
4. The method `train_one_epoch()` is implemented as follows:

```
def train_one_epoch(
    net,
    trainloader,
    batch_size,
    loss_function,
    optimizer,
    device,
    show_batch_interval=10_000,
    task=None,
):
    running_loss = 0.0
    epoch_steps = 0
    for batch_nr, data in enumerate(trainloader, 0):
        input, target = data
        input, target = input.to(device), target.to(device)
        optimizer.zero_grad()
        output = net(input)
        if task == "regression":
```

```
            target = target.unsqueeze(1)
            if target.shape == output.shape:
                loss = loss_function(output, target)
            else:
                raise ValueError(f"Shapes of target and output do not match:
                 {target.shape} vs {output.shape}")
        elif task == "classification":
            loss = loss_function(output, target)
        else:
            raise ValueError(f"Unknown task: {task}")
        loss.backward()
        torch.nn.utils.clip_grad_norm_(net.parameters(), max_norm=1.0)
        optimizer.step()
        running_loss += loss.item()
        epoch_steps += 1
        if batch_nr % show_batch_interval == (show_batch_interval - 1):
            print(
                "Batch: %5d. Batch Size: %d. Training Loss (running): %.3f"
                % (batch_nr + 1, int(batch_size), running_loss / epoch_steps)
            )
            running_loss = 0.0
    return loss.item()
```

5. The method `validate_one_epoch()` is implemented as follows:

```
def validate_one_epoch(net, valloader, loss_function, metric, device, task):
    val_loss = 0.0
    val_steps = 0
    total = 0
    correct = 0
    metric.reset()
    for i, data in enumerate(valloader, 0):
        # get batches
        with torch.no_grad():
            input, target = data
            input, target = input.to(device), target.to(device)
            output = net(input)
            # print(f"target: {target}")
            # print(f"output: {output}")
            if task == "regression":
                target = target.unsqueeze(1)
```

```
                if target.shape == output.shape:
                    loss = loss_function(output, target)
                else:
                    raise ValueError(f"Shapes of target and output
                        do not match: {target.shape} vs {output.shape}")
                metric_value = metric.update(output, target)
            elif task == "classification":
                loss = loss_function(output, target)
                metric_value = metric.update(output, target)
                _, predicted = torch.max(output.data, 1)
                total += target.size(0)
                correct += (predicted == target).sum().item()
            else:
                raise ValueError(f"Unknown task: {task}")
            val_loss += loss.cpu().numpy()
            val_steps += 1
    loss = val_loss / val_steps
    print(f"Loss on hold-out set: {loss}")
    if task == "classification":
        accuracy = correct / total
        print(f"Accuracy on hold-out set: {accuracy}")
    # metric on all batches using custom accumulation
    metric_value = metric.compute()
    metric_name = type(metric).__name__
    print(f"{metric_name} value on hold-out data: {metric_value}")
    return metric_value, loss
```

A.14.1.1 Description of the `"test_hold_out"` Setting

It uses the loss function specfied in `fun_control` and the metric specified in `fun_control`.

1. First, the method `HyperTorch().fun_torch` is called.
2. `fun_torc()` calls `spotPython.torch.traintest.evaluate_hold_out()` similar to the `"train_hold_out"` setting with one exception: It passes an additional `test` data set to `evaluate_hold_out()` as follows:

```
test_dataset=fun_control["test"]
```

`evaluate_hold_out()` calls `create_train_test_data_loaders` instead of `create_train_val_data_loaders`: The two data sets are used in `create_train_test_data_loaders` as follows:

```
def create_train_test_data_loaders(dataset, batch_size, shuffle, test_dataset,
        num_workers=0):
    trainloader = torch.utils.data.DataLoader(
        dataset, batch_size=int(batch_size), shuffle=shuffle,
        num_workers=num_workers
    )
    testloader = torch.utils.data.DataLoader(
        test_dataset, batch_size=int(batch_size), shuffle=shuffle,
        num_workers=num_workers
    )
    return trainloader, testloader
```

3. The following steps are identical to the `"train_hold_out"` setting. Only a different data loader is used for testing.

A.14.1.2 Detailed Description of the `"train_cv"` Setting

It uses the loss function specfied in `fun_control` and the metric specified in `fun_control`.

1. First, the method `HyperTorch().fun_torch` is called.
2. `fun_torc()` calls `spotPython.torch.traintest.evaluate_cv()` as follows (Note: Only the data set `fun_control["train"]` is used for CV.):

```
df_eval, _ = evaluate_cv(
    model,
    dataset=fun_control["train"],
    shuffle=self.fun_control["shuffle"],
    device=self.fun_control["device"],
    show_batch_interval=self.fun_control["show_batch_interval"],
    task=self.fun_control["task"],
    writer=self.fun_control["writer"],
    writerId=config_id,
)
```

3. In ‘evaluate_cv(), the following steps are performed: The optimizer is set up as follows:

```
optimizer_instance = net.optimizer
lr_instance = net.lr
sgd_momentum_instance = net.sgd_momentum
optimizer = optimizer_handler(optimizer_name=optimizer_instance,
     params=net.parameters(), lr_mult=lr_mult_instance)
```

`evaluate_cv()` sets the `net` attributes such as `epochs`, `batch_size`, `optimizer`, and `patience`. CV is implemented as follows:

```
def evaluate_cv(
    net,
    dataset,
    shuffle=False,
    loss_function=None,
    num_workers=0,
    device=None,
    show_batch_interval=10_000,
    metric=None,
    path=None,
    task=None,
    writer=None,
    writerId=None,
):
    lr_mult_instance = net.lr_mult
    epochs_instance = net.epochs
    batch_size_instance = net.batch_size
    k_folds_instance = net.k_folds
    optimizer_instance = net.optimizer
    patience_instance = net.patience
    sgd_momentum_instance = net.sgd_momentum
    removed_attributes, net = get_removed_attributes_and_base_net(net)
    metric_values = {}
    loss_values = {}
    try:
        device = getDevice(device=device)
        if torch.cuda.is_available():
            device = "cuda:0"
            if torch.cuda.device_count() > 1:
                print("We will use", torch.cuda.device_count(), "GPUs!")
                net = nn.DataParallel(net)
        net.to(device)
        optimizer = optimizer_handler(
            optimizer_name=optimizer_instance,
            params=net.parameters(),
            lr_mult=lr_mult_instance,
            sgd_momentum=sgd_momentum_instance,
        )
        kfold = KFold(n_splits=k_folds_instance, shuffle=shuffle)
```

```
for fold, (train_ids, val_ids) in enumerate(kfold.split(dataset)):
    print(f"Fold: {fold + 1}")
    train_subsampler = torch.utils.data.SubsetRandomSampler(train_ids)
    val_subsampler = torch.utils.data.SubsetRandomSampler(val_ids)
    trainloader = torch.utils.data.DataLoader(
        dataset, batch_size=batch_size_instance,
        sampler=train_subsampler, num_workers=num_workers
    )
    valloader = torch.utils.data.DataLoader(
        dataset, batch_size=batch_size_instance,
        sampler=val_subsampler, num_workers=num_workers
    )
    # each fold starts with new weights:
    reset_weights(net)
    # Early stopping parameters
    best_val_loss = float("inf")
    counter = 0
    for epoch in range(epochs_instance):
        print(f"Epoch: {epoch + 1}")
        # training loss from one epoch:
        training_loss = train_one_epoch(
            net=net,
            trainloader=trainloader,
            batch_size=batch_size_instance,
            loss_function=loss_function,
            optimizer=optimizer,
            device=device,
            show_batch_interval=show_batch_interval,
            task=task,
        )
        # Early stopping check. Calculate validation loss from one epoch:
        metric_values[fold], loss_values[fold] = validate_one_epoch(
            net, valloader=valloader, loss_function=loss_function,
            metric=metric, device=device, task=task
        )
        # Log the running loss averaged per batch
        metric_name = "Metric"
        if metric is None:
            metric_name = type(metric).__name__
            print(f"{metric_name} value on hold-out data:
                {metric_values[fold]}")
```

```
                if writer is not None:
                    writer.add_scalars(
                        "evaluate_cv fold:" + str(fold + 1) +
                        ". Train & Val Loss and Val Metric" + writerId,
                        {"Train loss": training_loss, "Val loss":
                        loss_values[fold], metric_name: metric_values[fold]},
                        epoch + 1,
                    )
                    writer.flush()
                if loss_values[fold] < best_val_loss:
                    best_val_loss = loss_values[fold]
                    counter = 0
                    # save model:
                    if path is not None:
                        torch.save(net.state_dict(), path)
                else:
                    counter += 1
                    if counter >= patience_instance:
                        print(f"Early stopping at epoch {epoch}")
                        break
        df_eval = sum(loss_values.values()) / len(loss_values.values())
        df_metrics = sum(metric_values.values()) / len(metric_values.values())
        df_preds = np.nan
    except Exception as err:
        print(f"Error in Net_Core. Call to evaluate_cv() failed. {err=},
            {type(err)=}")
        df_eval = np.nan
        df_preds = np.nan
    add_attributes(net, removed_attributes)
    if writer is not None:
        metric_name = "Metric"
        if metric is None:
            metric_name = type(metric).__name__
        writer.add_scalars(
            "CV: Val Loss and Val Metric" + writerId,
            {"CV-loss": df_eval, metric_name: df_metrics},
            epoch + 1,
        )
        writer.flush()
    return df_eval, df_preds, df_metrics
```

4. The method `train_fold()` is implemented as shown above.

5. The method `validate_one_epoch()` is implemented as shown above. In contrast to the hold-out setting, it is called for each of the k folds. The results are stored in a dictionaries `metric_values` and `loss_values`. The results are averaged over the k folds and returned as `df_eval`.

A.14.1.3 Detailed Description of the "test_cv" Setting

It uses the loss function specfied in `fun_control` and the metric specified in `fun_control`.

1. First, the method `HyperTorch().fun_torch` is called.
2. `fun_torc()` calls `spotPython.torch.traintest.evaluate_cv()` as follows:

```
df_eval, _ = evaluate_cv(
    model,
    dataset=fun_control["test"],
    shuffle=self.fun_control["shuffle"],
    device=self.fun_control["device"],
    show_batch_interval=self.fun_control["show_batch_interval"],
    task=self.fun_control["task"],
    writer=self.fun_control["writer"],
    writerId=config_id,
)
```

Note: The data set `fun_control["test"]` is used for CV. The rest is the same as for the `"train_cv"` setting.

A.14.1.4 Detailed Description of the Final Model Training and Evaluation

There are two methods that can be used for the final evaluation of a Pytorch model:

1. `"train_tuned` and
2. `"test_tuned"`.

`train_tuned()` is just a wrapper to `evaluate_hold_out` using the `train` data set. It is implemented as follows:

```
def train_tuned(
    net,
    train_dataset,
    shuffle,
    loss_function,
    metric,
```

```
        device=None,
        show_batch_interval=10_000,
        path=None,
        task=None,
        writer=None,
):
    evaluate_hold_out(
        net=net,
        train_dataset=train_dataset,
        shuffle=shuffle,
        test_dataset=None,
        loss_function=loss_function,
        metric=metric,
        device=device,
        show_batch_interval=show_batch_interval,
        path=path,
        task=task,
        writer=writer,
    )
```

The `test_tuned()` procedure is implemented as follows:

```
def test_tuned(net, shuffle, test_dataset=None, loss_function=None,
    metric=None, device=None, path=None, task=None):
    batch_size_instance = net.batch_size
    removed_attributes, net = get_removed_attributes_and_base_net(net)
    if path is not None:
        net.load_state_dict(torch.load(path))
        net.eval()
    try:
        device = getDevice(device=device)
        if torch.cuda.is_available():
            device = "cuda:0"
            if torch.cuda.device_count() > 1:
                print("We will use", torch.cuda.device_count(), "GPUs!")
                net = nn.DataParallel(net)
        net.to(device)
        valloader = torch.utils.data.DataLoader(
            test_dataset, batch_size=int(batch_size_instance),
            shuffle=shuffle,
            num_workers=0
        )
```

```
        metric_value, loss = validate_one_epoch(
            net, valloader=valloader, loss_function=loss_function,
            metric=metric, device=device, task=task
        )
        df_eval = loss
        df_metric = metric_value
        df_preds = np.nan
    except Exception as err:
        print(f"Error in Net_Core. Call to test_tuned() failed. {err=},
            {type(err)=}")
        df_eval = np.nan
        df_metric = np.nan
        df_preds = np.nan
    add_attributes(net, removed_attributes)
    print(f"Final evaluation: Validation loss: {df_eval}")
    print(f"Final evaluation: Validation metric: {df_metric}")
    print("----------------------------------------------")
    return df_eval, df_preds, df_metric
```

References

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, Jürgen Branke, Jörn Mehnen, and Olaf Mersmann. 2014. "Evolutionary Algorithms." *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery* 4 (3): 178–95.

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.

Bartz-Beielstein, Thomas, Christian Lasarczyk, and Mike Preuss. 2005. "Sequential Parameter Optimization." In *Proceedings 2005 Congress on Evolutionary Computation (CEC'05), Edinburgh, Scotland*, edited by B McKay et al., 773–80. Piscataway NJ: IEEE Press.

Lewis, R M, V Torczon, and M W Trosset. 2000. "Direct search methods: Then and now." *Journal of Computational and Applied Mathematics* 124 (1–2): 191–207.

Li, Lisha, Kevin Jamieson, Giulia DeSalvo, Afshin Rostamizadeh, and Ameet Talwalkar. 2016. "Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization." *arXiv e-Prints*, March, arXiv:1603.06560.

Meignan, David, Sigrid Knust, Jean-Marc Frayet, Gilles Pesant, and Nicolas Gaud. 2015. "A Review and Taxonomy of Interactive Optimization Methods in Operations Research." *ACM Transactions on Interactive Intelligent Systems*, September.

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. 2023a. "Hyperparameter Tuning with Ray Tune." https://pytorch.org/tutorials/beginner/hyperparameter_tuning_tutorial.html.

———. 2023b. "Training a Classifier." https://pytorch.org/tutorials/beginner/blitz/cifar10_tutorial.html.