Sequential Parameter Optimization

Using `scipy` Optimizers

- This notebook describes how different optimizers form 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
import matplotlib.pyplot as plt
```

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].

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

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

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

```
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": 2,
                                       "model_optimizer": differential_evolution,
                                       "model_fun_evals": 1000,
                                       })
spot_de.run()
```

```
<spotPython.spot.spot.Spot at 0x166b83eb0>
```

Print the Results

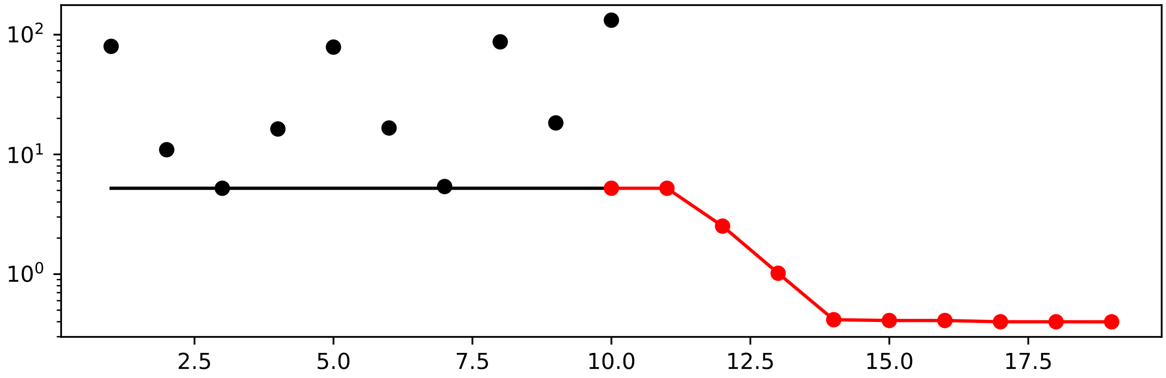
```
spot_de.print_results()
```

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

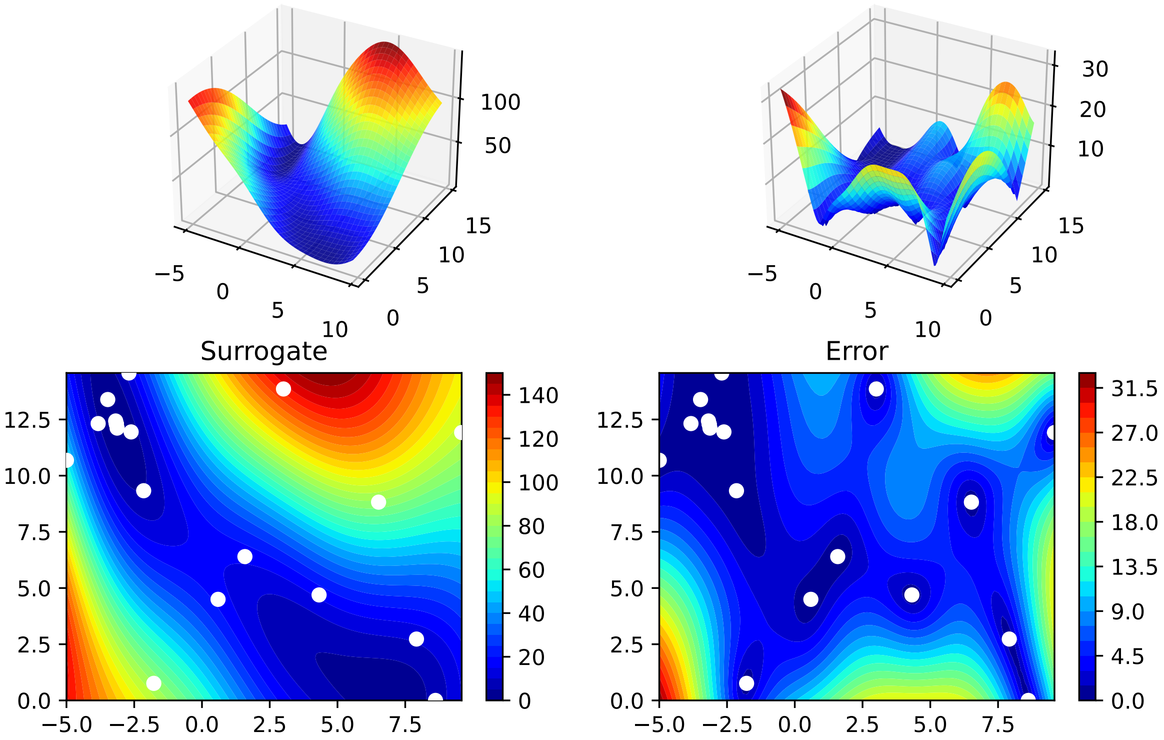
```
[['x0', -3.1570201165683587], ['x1', 12.289980569430284]]
```

Show the Progress

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



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


100
50
−5
0
5
10
0
5
10
15
30
20
10
−5
0
5
10
0
5
10
15
Surrogate
Error
12.5
10.0
7.5
5.0
2.5
0.0
−5.0
−2.5
0.0
2.5
5.0
7.5
140
120
100
80
60
40
20
0
31.5
27.0
22.5
18.0
13.5
9.0
4.5
0.0

Exercises

- Important:
  - 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 (see http://www.gm.fh-koeln.de/~bartz/site/download/

Exercise 1

- Each team member should choose one of the following optimization algorithms.
- Please add your name to the section title!

1. `dual_annealing`

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

2. `direct`

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

3. `shgo`

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

4. `basinhopping`

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

Exercise 2

(All group members): * 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?