BayesO Documentation

Release 0.5.0 alpha

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Contents

BayesO

BayesO (pronounced "bayes-o") is a simple, but essential Bayesian optimization package, written in Python. It is developed by machine learning group at POSTECH. This project is licensed under the MIT license.

This documentation describes the details of implementation, getting started guides, some examples with BayesO, and Python API specifications. The code can be found in our GitHub repository.

CHAPTER 1

About BayesO

Simple, but essential Bayesian optimization package. It is designed to run advanced Bayesian optimization with implementation-specific and application-specific modifications as well as to run Bayesian optimization in various applications simply. This package contains the codes for Gaussian process regression and Gaussian process-based Bayesian optimization. Some famous benchmark and custom benchmark functions for Bayesian optimization are included in bayeso-benchmarks, which can be used to test the Bayesian optimization strategy. If you are interested in this package, please refer to that repository.

1.1 Supported Python Version

We test our package in the following versions.

- Python 3.6
- Python 3.7
- Python 3.8
- Python 3.9

1.2 Related Package for Benchmark Functions

The related package **bayeso-benchmarks**, which contains some famous benchmark functions and custom benchmark functions is hosted in this repository. It can be used to test a Bayesian optimization strategy.

The details of benchmark functions implemented in **bayeso-benchmarks** are described in these notes.

1.3 Contributor

- Jungtaek Kim (POSTECH)

1.4 Citation

```
@misc{KimJ2017bayeso,
    author={Kim, Jungtaek and Choi, Seungjin},
    title={{BayesO}: A {Bayesian} optimization framework in {Python}},
    howpublished={\url{http://bayeso.org}},
    year={2017}
}
```

1.5 Contact

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1.6 License

CHAPTER 2

About Bayesian Optimization

Bayesian optimization is a **global optimization** strategy for **black-box** and **expensive-to-evaluate** functions. Generic Bayesian optimization follows these steps:

1. Build a **surrogate function** with historical inputs and their observations.
2. Compute and maximize an **acquisition function**, defined by the outputs of surrogate function.
3. Observe the **maximizer** of acquisition function from a true objective function.
4. Accumulate the maximizer and its observation.

This project helps us to execute this Bayesian optimization procedure. In particular, **Gaussian process regression** is used as a surrogate function, and various acquisition functions such as **probability improvement**, **expected improvement**, and **Gaussian process upper confidence bound** are included in this project.

CHAPTER 3

Installing BayesO

We recommend installing it with **virtualenv**. You can choose one of three installation options.

3.1 Installing from PyPI

It is for user installation. To install the released version from PyPI repository, command it.

```
$ pip install bayeso
```

3.2 Compiling from Source

It is for developer installation. To install **bayeso** from source code, command

```
$ pip install .
```

in the **bayeso** root.

3.3 Compiling from Source (Editable)

It is for editable development mode. To use editable development mode, command

```
$ pip install -r requirements.txt
$ python setup.py develop
```

in the **bayeso** root.

3.4 Uninstalling

If you would like to uninstall **bayeso**, command it.

```
$ pip uninstall bayeso
```

3.5 Required Packages

Mandatory pacakges are inlcuded in **requirements.txt**. The following **requirements** files include the package list, the purpose of which is described as follows.

- **requirements-optional.txt**: It is an optional package list, but it needs to be installed to execute some features of **bayeso**.
- **requirements-dev.txt**: It is for developing the **bayeso** package.
- **requirements-examples.txt**: It needs to be installed to execute the examples included in the **bayeso** repository.

CHAPTER 4

Building Gaussian Process Regression

This example is for building Gaussian process regression models. First of all, import the packages we need and **bayeso**.

```
import numpy as np

from bayeso import covariance
from bayeso.gp import gp
from bayeso.utils import utils_covariance
from bayeso.utils import utils_plotting
```

Declare some parameters to control this example.

```
use_tex = False
num_test = 200
str_cov = 'matern52'
```

Make a simple synthetic dataset, which produces with cosine functions.

```
X_train = np.array([
    [-3.0],
    [-2.0],
    [-1.0],
    [2.0],
    [1.2],
    [1.1],
])
Y_train = np.cos(X_train) + 10.0
X_test = np.linspace(-3, 3, num_test)
X_test = X_test.reshape((num_test, 1))
Y_test = np.cos(X_test) + 10.0
```

Sample functions from a prior distribution, which is zero mean.

```
mu = np.zeros(num_test)
hyps = utils_covariance.get_hyps(str_cov, 1)
```

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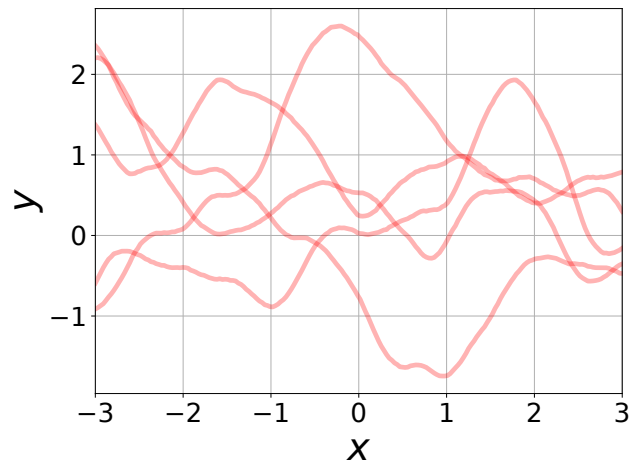
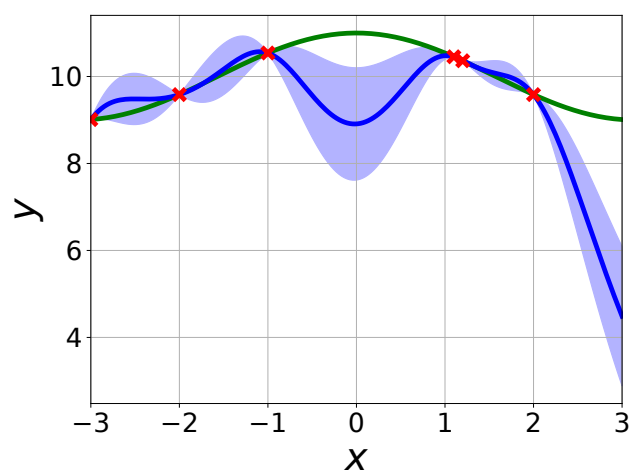
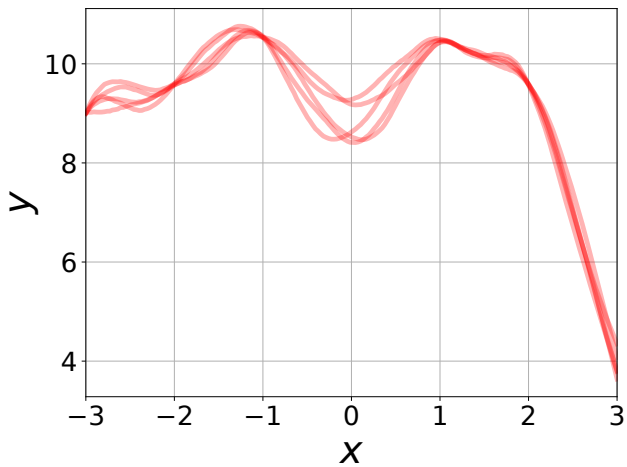
```
Sigma = covariance.cov_main(str_cov, X_test, X_test, hyps, True)

Ys = gp.sample_functions(mu, Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')
```



Build a Gaussian process regression model with fixed hyperparameters. Then, plot the result.

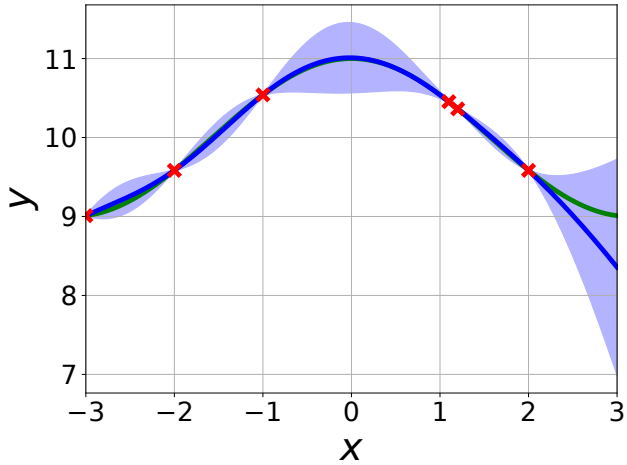
```
hyps = utils_covariance.get_hyps(str_cov, 1)
mu, sigma, Sigma = gp.predict_with_hyps(X_train, Y_train, X_test, hyps, str_cov=str_
↪cov)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')
```

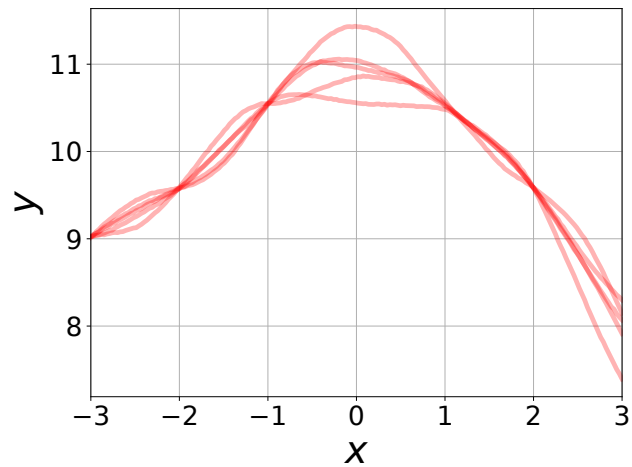




Build a Gaussian process regression model with the hyperparameters optimized by marginal likelihood maximization, and plot the result.

```
mu, sigma, Sigma = gp.predict_with_optimized_hyps(X_train, Y_train, X_test, str_
↪cov=str_cov)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')
```





Declare some functions that would be employed as prior functions.

```
def cosine(X):
    return np.cos(X)

def linear_down(X):
    list_up = []
    for elem_X in X:
        list_up.append([-0.5 * np.sum(elem_X)])
    return np.array(list_up)

def linear_up(X):
    list_up = []
    for elem_X in X:
        list_up.append([0.5 * np.sum(elem_X)])
    return np.array(list_up)
```

Make an another synthetic dataset using a cosine function.

```
X_train = np.array([
    [-3.0],
    [-2.0],
    [-1.0],
])
Y_train = np.cos(X_train) + 2.0
X_test = np.linspace(-3, 6, num_test)
X_test = X_test.reshape((num_test, 1))
Y_test = np.cos(X_test) + 2.0
```

Build Gaussian process regression models with the prior functions we declare above and the hyperparameters optimized by marginal likelihood maximization, and plot the result.

```
def cosine(X):
    return np.cos(X)

def linear_down(X):
    list_up = []
    for elem_X in X:
        list_up.append([-0.5 * np.sum(elem_X)])
    return np.array(list_up)
```

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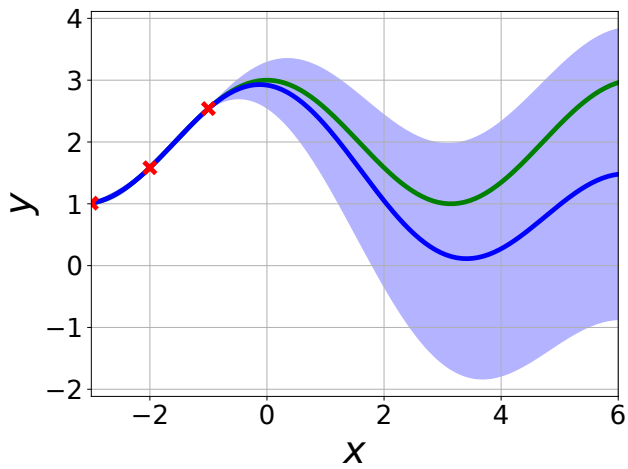
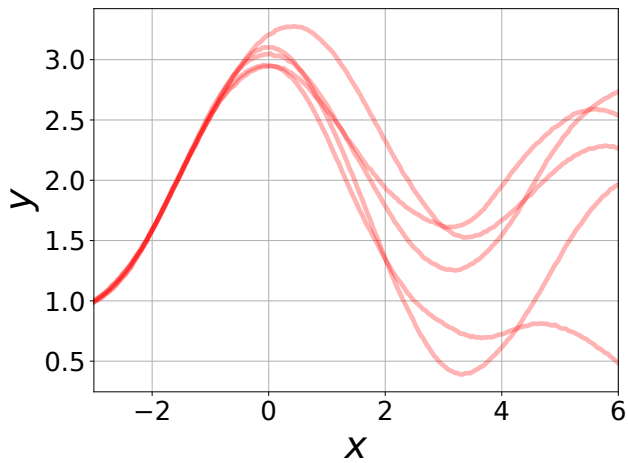
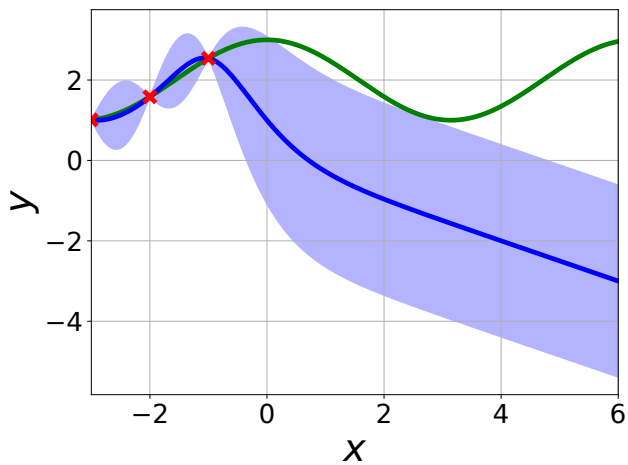
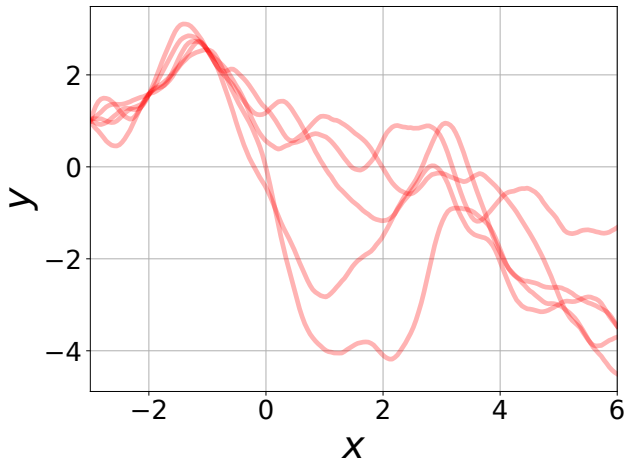
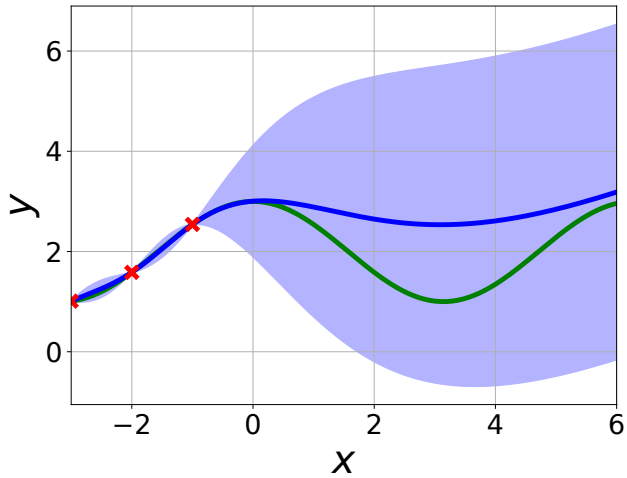
```
def linear_up(X):
    list_up = []
    for elem_X in X:
        list_up.append([0.5 * np.sum(elem_X)])
    return np.array(list_up)

X_train = np.array([
    [-3.0],
    [-2.0],
    [-1.0],
])
Y_train = np.cos(X_train) + 2.0
X_test = np.linspace(-3, 6, num_test)
X_test = X_test.reshape((num_test, 1))
Y_test = np.cos(X_test) + 2.0

prior_mu = cosine
mu, sigma, Sigma = gp.predict_with_optimized_hyps(X_train, Y_train, X_test,
                                                  str_cov=str_cov, prior_mu=prior_mu)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')

prior_mu = linear_down
mu, sigma, Sigma = gp.predict_with_optimized_hyps(X_train, Y_train, X_test,
                                                  str_cov=str_cov, prior_mu=prior_mu)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')

prior_mu = linear_up
mu, sigma, Sigma = gp.predict_with_optimized_hyps(X_train, Y_train, X_test,
                                                  str_cov=str_cov, prior_mu=prior_mu)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')
```

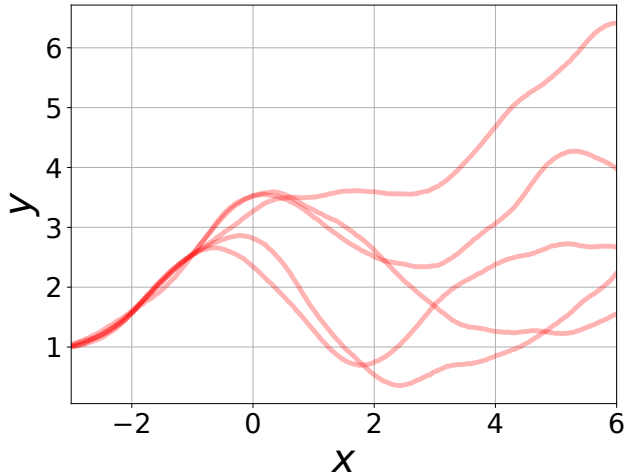

4
3
2
1
0
−1
−2
y
−2
0
2
4
6
x


3.0
2.5
2.0
1.5
1.0
0.5
y
−2
0
2
4
6
x


2
0
−2
−4
y
−2
0
2
4
6
x







Full code:

```
import numpy as np

from bayeso import covariance
from bayeso.gp import gp
```

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```
from bayeso.utils import utils_covariance
from bayeso.utils import utils_plotting

use_tex = False
num_test = 200
str_cov = 'matern52'

X_train = np.array([
    [-3.0],
    [-2.0],
    [-1.0],
    [2.0],
    [1.2],
    [1.1],
])
Y_train = np.cos(X_train) + 10.0
X_test = np.linspace(-3, 3, num_test)
X_test = X_test.reshape((num_test, 1))
Y_test = np.cos(X_test) + 10.0

mu = np.zeros(num_test)
hyps = utils_covariance.get_hyps(str_cov, 1)
Sigma = covariance.cov_main(str_cov, X_test, X_test, hyps, True)

Ys = gp.sample_functions(mu, Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')

hyps = utils_covariance.get_hyps(str_cov, 1)
mu, sigma, Sigma = gp.predict_with_hyps(X_train, Y_train, X_test, hyps, str_cov=str_
↪cov)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')

mu, sigma, Sigma = gp.predict_with_optimized_hyps(X_train, Y_train, X_test, str_
↪cov=str_cov)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')

def cosine(X):
    return np.cos(X)

def linear_down(X):
```

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```
    list_up = []
    for elem_X in X:
        list_up.append([-0.5 * np.sum(elem_X)])
    return np.array(list_up)

def linear_up(X):
    list_up = []
    for elem_X in X:
        list_up.append([0.5 * np.sum(elem_X)])
    return np.array(list_up)

X_train = np.array([
    [-3.0],
    [-2.0],
    [-1.0],
])
Y_train = np.cos(X_train) + 2.0
X_test = np.linspace(-3, 6, num_test)
X_test = X_test.reshape((num_test, 1))
Y_test = np.cos(X_test) + 2.0

prior_mu = cosine
mu, sigma, Sigma = gp.predict_with_optimized_hyps(X_train, Y_train, X_test,
                                                  str_cov=str_cov, prior_mu=prior_mu)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')

prior_mu = linear_down
mu, sigma, Sigma = gp.predict_with_optimized_hyps(X_train, Y_train, X_test,
                                                  str_cov=str_cov, prior_mu=prior_mu)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')

prior_mu = linear_up
mu, sigma, Sigma = gp.predict_with_optimized_hyps(X_train, Y_train, X_test,
                                                  str_cov=str_cov, prior_mu=prior_mu)
utils_plotting.plot_gp_via_distribution(
    X_train, Y_train, X_test, mu, sigma,
    Y_test=Y_test, use_tex=use_tex,
    str_x_axis='$x$', str_y_axis='$y$'
)

Ys = gp.sample_functions(mu.flatten(), Sigma, num_samples=5)
```

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```
utils_plotting.plot_gp_via_sample(X_test, Ys, use_tex=use_tex,
                                  str_x_axis='$x$', str_y_axis='$y$')
```

CHAPTER 5

Optimizing Sampled Function via Thompson Sampling

This example is to optimize a function sampled from a Gaussian process prior via Thompson sampling. First of all, import the packages we need and **bayeso**.

```
import numpy as np

from bayeso import covariance
from bayeso.gp import gp
from bayeso.utils import utils_covariance
from bayeso.utils import utils_plotting
```

Declare some parameters to control this example, including zero-mean prior, and compute a covariance matrix.

```
num_points = 1000
str_cov = 'se'
num_iter = 50
num_ts = 10

list_Y_min = []

X = np.expand_dims(np.linspace(-5, 5, num_points), axis=1)
mu = np.zeros(num_points)
hyps = utils_covariance.get_hyps(str_cov, 1)
Sigma = covariance.cov_main(str_cov, X, X, hyps, True)
```

Optimize a function sampled from a Gaussian process prior. At each iteration, we sample a query point that outputs the mininum value of the function sampled from a Gaussian process posterior.

```
for ind_ts in range(0, num_ts):
    print('TS:', ind_ts + 1, 'round')
    Y = gp.sample_functions(mu, Sigma, num_samples=1)[0]

    ind_init = np.argmin(Y)
    bx_min = X[ind_init]
    y_min = Y[ind_init]
```

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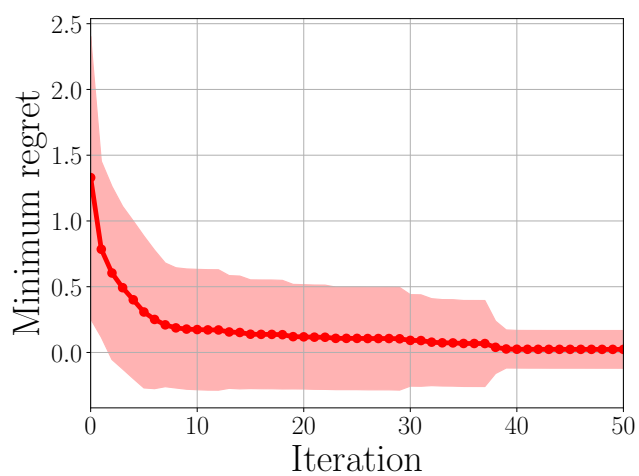
```
    ind_random = np.random.choice(num_points)

    X_ = np.expand_dims(X[ind_random], axis=0)
    Y_ = np.expand_dims(np.expand_dims(Y[ind_random], axis=0), axis=1)

    for ind_iter in range(0, num_iter):
        print(ind_iter + 1, 'iteration')

        mu_, sigma_, Sigma_ = gp.predict_with_optimized_hyps(X_, Y_, X, str_cov=str_
↪cov)
        ind_ = np.argmin(gp.sample_functions(np.squeeze(mu_, axis=1), Sigma_, num_
↪samples=1)[0])

        X_ = np.concatenate([X_, [X[ind_]]], axis=0)
        Y_ = np.concatenate([Y_, [[Y[ind_]]]], axis=0)

    list_Y_min.append(Y_ - y_min)

Ys = np.array(list_Y_min)
Ys = np.squeeze(Ys, axis=2)
print(Ys.shape)
```

Plot the result obtained from the code block above.

```
utils_plotting.plot_minimum_vs_iter(
    np.array([Ys]), ['TS'], 1, True,
    use_tex=True, range_shade=1.0,
    str_x_axis=r'\textrm{Iteration}',
    str_y_axis=r'\textrm{Minimum regret}'
)
```



Full code:

```
import numpy as np

from bayeso import covariance
from bayeso.gp import gp
from bayeso.utils import utils_covariance
```

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```
from bayeso.utils import utils_plotting

num_points = 1000
str_cov = 'se'
num_iter = 50
num_ts = 10

list_Y_min = []

X = np.expand_dims(np.linspace(-5, 5, num_points), axis=1)
mu = np.zeros(num_points)
hyps = utils_covariance.get_hyps(str_cov, 1)
Sigma = covariance.cov_main(str_cov, X, X, hyps, True)

for ind_ts in range(0, num_ts):
    print('TS:', ind_ts + 1, 'round')
    Y = gp.sample_functions(mu, Sigma, num_samples=1)[0]

    ind_init = np.argmin(Y)
    bx_min = X[ind_init]
    y_min = Y[ind_init]

    ind_random = np.random.choice(num_points)

    X_ = np.expand_dims(X[ind_random], axis=0)
    Y_ = np.expand_dims(np.expand_dims(Y[ind_random], axis=0), axis=1)

    for ind_iter in range(0, num_iter):
        print(ind_iter + 1, 'iteration')

        mu_, sigma_, Sigma_ = gp.predict_with_optimized_hyps(X_, Y_, X, str_cov=str_
↪cov)
        ind_ = np.argmin(gp.sample_functions(np.squeeze(mu_, axis=1), Sigma_, num_
↪samples=1)[0])

        X_ = np.concatenate([X_, [X[ind_]]], axis=0)
        Y_ = np.concatenate([Y_, [[Y[ind_]]]], axis=0)

    list_Y_min.append(Y_ - y_min)

Ys = np.array(list_Y_min)
Ys = np.squeeze(Ys, axis=2)
print(Ys.shape)

utils_plotting.plot_minimum_vs_iter(
    np.array([Ys]), ['TS'], 1, True,
    use_tex=True, range_shade=1.0,
    str_x_axis=r'\textrm{Iteration}',
    str_y_axis=r'\textrm{Minimum regret}'
)
```

CHAPTER 6

Optimizing Branin Function

This example is for optimizing Branin function. It needs to install **bayeso-benchmarks**, which is included in **requirements-optional.txt**. First, import some packages we need.

```
import numpy as np

from bayeso import bo
from bayeso_benchmarks.two_dim_branin import Branin
from bayeso.wrappers import wrappers_bo
from bayeso.utils import utils_plotting
```

Then, declare Branin function we will optimize and a search space for the function.

```
obj_fun = Branin()
bounds = obj_fun.get_bounds()

def fun_target(X):
    return obj_fun.output(X)
```

We optimize the objective function with 10 Bayesian optimization rounds and 50 iterations per round with 3 initial random evaluations.

```
str_fun = 'branin'

num_bo = 10
num_iter = 50
num_init = 3
```

With BO class in *bayeso.bo*, optimize the objective function.

```
model_bo = bo.BO(bounds, debug=False)
list_Y = []
list_time = []

for ind_bo in range(0, num_bo):
```

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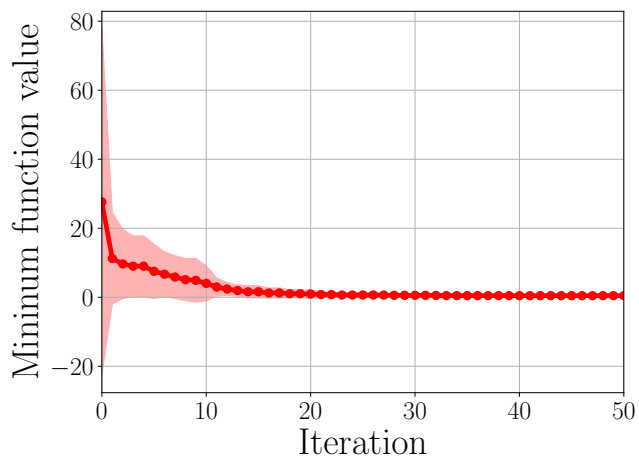
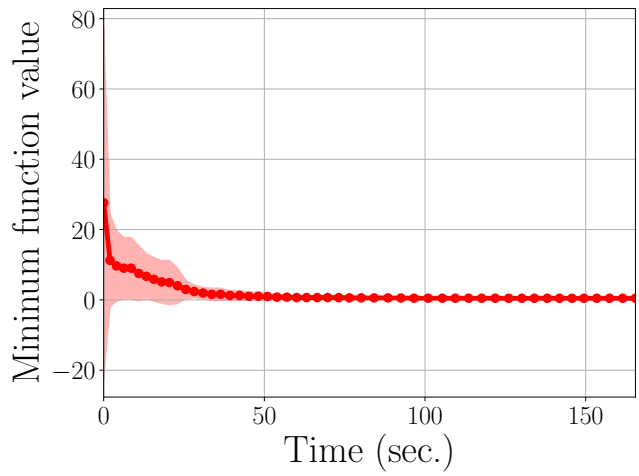
```
    print('BO Round', ind_bo + 1)
    X_final, Y_final, time_final, _, _ = wrappers_bo.run_single_round(
        model_bo, fun_target, num_init, num_iter,
        str_initial_method_bo='uniform', str_sampling_method_ao='uniform', num_
↪samples_ao=100,
        seed=42 * ind_bo
    )
    list_Y.append(Y_final)
    list_time.append(time_final)

arr_Y = np.array(list_Y)
arr_time = np.array(list_time)

arr_Y = np.expand_dims(np.squeeze(arr_Y), axis=0)
arr_time = np.expand_dims(arr_time, axis=0)
```

Plot the results in terms of the number of iterations and time.

```
utils_plotting.plot_minimum_vs_iter(arr_Y, [str_fun], num_init, True,
    use_tex=True,
    str_x_axis=r'\textrm{Iteration}',
    str_y_axis=r'\textrm{Mininum function value}')
utils_plotting.plot_minimum_vs_time(arr_time, arr_Y, [str_fun], num_init, True,
    use_tex=True,
    str_x_axis=r'\textrm{Time (sec.)}',
    str_y_axis=r'\textrm{Mininum function value}')
```





Full code:

```
import numpy as np

from bayeso import bo
from bayeso_benchmarks.two_dim_branin import Branin
from bayeso.wrappers import wrappers_bo
from bayeso.utils import utils_plotting

obj_fun = Branin()
bounds = obj_fun.get_bounds()

def fun_target(X):
    return obj_fun.output(X)

str_fun = 'branin'

num_bo = 10
num_iter = 50
num_init = 3

model_bo = bo.BO(bounds, debug=False)
list_Y = []
list_time = []

for ind_bo in range(0, num_bo):
    print('BO Round', ind_bo + 1)
    X_final, Y_final, time_final, _, _ = wrappers_bo.run_single_round(
        model_bo, fun_target, num_init, num_iter,
        str_initial_method_bo='uniform', str_sampling_method_ao='uniform', num_
↪samples_ao=100,
        seed=42 * ind_bo
    )
    list_Y.append(Y_final)
    list_time.append(time_final)

arr_Y = np.array(list_Y)
arr_time = np.array(list_time)

arr_Y = np.expand_dims(np.squeeze(arr_Y), axis=0)
arr_time = np.expand_dims(arr_time, axis=0)
```

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```
utils_plotting.plot_minimum_vs_iter(arr_Y, [str_fun], num_init, True,
    use_tex=True,
    str_x_axis=r'\textrm{Iteration}',
    str_y_axis=r'\textrm{Mininum function value}')
utils_plotting.plot_minimum_vs_time(arr_time, arr_Y, [str_fun], num_init, True,
    use_tex=True,
    str_x_axis=r'\textrm{Time (sec.)}',
    str_y_axis=r'\textrm{Mininum function value}')
```

CHAPTER 7

Constructing xgboost Classifier with Hyperparameter Optimization

This example is for optimizing hyperparameters for **xgboost** classifier. In this example, we optimize *max_depth* and *n_estimators* for *xgboost.XGBClassifier*. It needs to install **xgboost**, which is included in **requirements-examples.txt**. First, import some packages we need.

```
import numpy as np
import xgboost as xgb
import sklearn.datasets
import sklearn.metrics
import sklearn.model_selection

from bayeso import bo
from bayeso.wrappers import wrappers_bo
from bayeso.utils import utils_plotting
```

Get handwritten digits dataset, which contains digit images of 0 to 9, and split the dataset to training and test datasets.

```
digits = sklearn.datasets.load_digits()
data_digits = digits.images
data_digits = np.reshape(data_digits,
    (data_digits.shape[0], data_digits.shape[1] * data_digits.shape[2]))
labels_digits = digits.target

data_train, data_test, labels_train, labels_test = sklearn.model_selection.train_test_
↪split(
    data_digits, labels_digits, test_size=0.3, stratify=labels_digits)
```

Declare an objective function we would like to optimize. This function trains *xgboost.XGBClassifier* with the training dataset and given hyerparameter vector *bx* and returns (1 - accuracy), which computed by the test dataset.

```
def fun_target(bx):
    model_xgb = xgb.XGBClassifier(
        max_depth=int(bx[0]),
        n_estimators=int(bx[1])
    )
```

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```
    model_xgb.fit(data_train, labels_train)
    preds_test = model_xgb.predict(data_test)
    return 1.0 - sklearn.metrics.accuracy_score(labels_test, preds_test)
```

We optimize the objective function with our *bayeso.bo.BO* for 50 iterations. 5 initial points would be given and 10 rounds would be run.

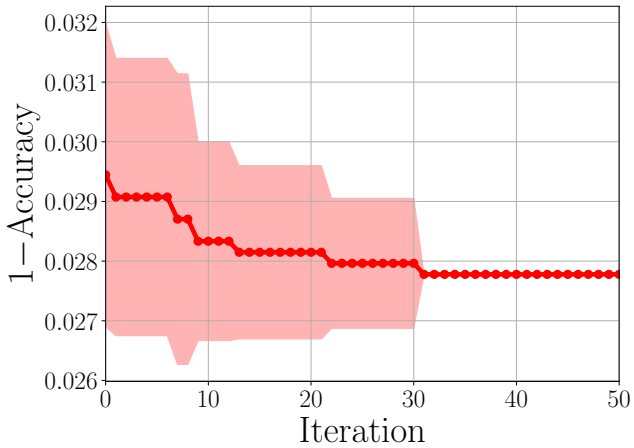
```
str_fun = 'xgboost'

# (max_depth, n_estimators)
bounds = np.array([[1, 10], [100, 500]])
num_bo = 10
num_iter = 50
num_init = 5
```

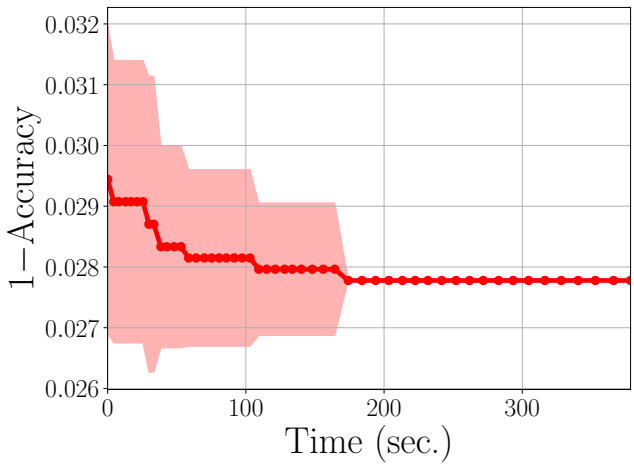
Optimze the objective function, after declaring the *bayeso.bo.BO* object.

```
model_bo = bo.BO(bounds, debug=False)

list_Y = []
list_time = []

for ind_bo in range(0, num_bo):
    print('BO Round:', ind_bo + 1)
    X_final, Y_final, time_final, _, _ = wrappers_bo.run_single_round(
        model_bo, fun_target, num_init, num_iter,
        str_initial_method_bo='uniform', str_sampling_method_ao='uniform',
        num_samples_ao=100, seed=42 * ind_bo)
    list_Y.append(Y_final)
    list_time.append(time_final)

arr_Y = np.array(list_Y)
arr_time = np.array(list_time)

arr_Y = np.expand_dims(np.squeeze(arr_Y), axis=0)
arr_time = np.expand_dims(arr_time, axis=0)
```

Plot the results in terms of the number of iterations and time.

```
utils_plotting.plot_minimum_vs_iter(arr_Y, [str_fun], num_init, True,
    use_tex=True,
    str_x_axis=r'\textrm{Iteration}',
    str_y_axis=r'$1 - $\textrm{Accuracy}')
utils_plotting.plot_minimum_vs_time(arr_time, arr_Y, [str_fun], num_init, True,
    use_tex=True,
    str_x_axis=r'\textrm{Time (sec.)}',
    str_y_axis=r'$1 - $\textrm{Accuracy}')
```





Full code:

```
import numpy as np
import xgboost as xgb
import sklearn.datasets
import sklearn.metrics
import sklearn.model_selection

from bayeso import bo
from bayeso.wrappers import wrappers_bo
from bayeso.utils import utils_plotting

digits = sklearn.datasets.load_digits()
data_digits = digits.images
data_digits = np.reshape(data_digits,
    (data_digits.shape[0], data_digits.shape[1] * data_digits.shape[2]))
labels_digits = digits.target

data_train, data_test, labels_train, labels_test = sklearn.model_selection.train_test_
↪split(
    data_digits, labels_digits, test_size=0.3, stratify=labels_digits)

def fun_target(bx):
    model_xgb = xgb.XGBClassifier(
        max_depth=int(bx[0]),
```

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```
        n_estimators=int(bx[1])
    )
    model_xgb.fit(data_train, labels_train)
    preds_test = model_xgb.predict(data_test)
    return 1.0 - sklearn.metrics.accuracy_score(labels_test, preds_test)

str_fun = 'xgboost'

# (max_depth, n_estimators)
bounds = np.array([[1, 10], [100, 500]])
num_bo = 10
num_iter = 50
num_init = 5

model_bo = bo.BO(bounds, debug=False)

list_Y = []
list_time = []

for ind_bo in range(0, num_bo):
    print('BO Round:', ind_bo + 1)
    X_final, Y_final, time_final, _, _ = wrappers_bo.run_single_round(
        model_bo, fun_target, num_init, num_iter,
        str_initial_method_bo='uniform', str_sampling_method_ao='uniform',
        num_samples_ao=100, seed=42 * ind_bo)
    list_Y.append(Y_final)
    list_time.append(time_final)

arr_Y = np.array(list_Y)
arr_time = np.array(list_time)

arr_Y = np.expand_dims(np.squeeze(arr_Y), axis=0)
arr_time = np.expand_dims(arr_time, axis=0)

utils_plotting.plot_minimum_vs_iter(arr_Y, [str_fun], num_init, True,
    use_tex=True,
    str_x_axis=r'\textrm{Iteration}',
    str_y_axis=r'$1 - $\textrm{Accuracy}')
utils_plotting.plot_minimum_vs_time(arr_time, arr_Y, [str_fun], num_init, True,
    use_tex=True,
    str_x_axis=r'\textrm{Time (sec.)}',
    str_y_axis=r'$1 - $\textrm{Accuracy}')
```

CHAPTER 8

bayeso

BayesO is a simple, but essential Bayesian optimization package, implemented in Python.

8.1 bayeso.acquisition

It defines acquisition functions, each of which is employed to determine where next to evaluate.

`bayeso.acquisition.ei`(*pred_mean: numpy.ndarray*, *pred_std: numpy.ndarray*, *Y_train: numpy.ndarray*, *noise: float*, *jitter: float = 1e-05*) → numpy.ndarray

It is an augmented expected improvement criterion.

Parameters

- **pred_mean** (*numpy.ndarray*) – posterior predictive mean function over *X_test*. Shape: (l,).
- **pred_std** (*numpy.ndarray*) – posterior predictive standard deviation function over *X_test*. Shape: (l,).
- **Y_train** (*numpy.ndarray*) – outputs of *X_train*. Shape: (n, 1).
- **noise** (*float*) – noise for augmenting exploration.
- **jitter** (*float, optional*) – jitter for *pred_std*.

Returns acquisition function values. Shape: (l,).

Return type numpy.ndarray

Raises AssertionError

`bayeso.acquisition.ei`(*pred_mean: numpy.ndarray*, *pred_std: numpy.ndarray*, *Y_train: numpy.ndarray*, *jitter: float = 1e-05*) → numpy.ndarray

It is an expected improvement criterion.

Parameters

- **pred_mean** (*numpy.ndarray*) – posterior predictive mean function over *X_test*. Shape: (l,).
- **pred_std** (*numpy.ndarray*) – posterior predictive standard deviation function over *X_test*. Shape: (l,).
- **Y_train** (*numpy.ndarray*) – outputs of *X_train*. Shape: (n, 1).
- **jitter** (*float, optional*) – jitter for *pred_std*.

Returns acquisition function values. Shape: (l,).

Return type numpy.ndarray

Raises AssertionError

bayeso.acquisition.**pi**(*pred_mean: numpy.ndarray, pred_std: numpy.ndarray, Y_train: numpy.ndarray, jitter: float = 1e-05*) → numpy.ndarray

It is a probability of improvement criterion.

Parameters

- **pred_mean** (*numpy.ndarray*) – posterior predictive mean function over *X_test*. Shape: (l,).
- **pred_std** (*numpy.ndarray*) – posterior predictive standard deviation function over *X_test*. Shape: (l,).
- **Y_train** (*numpy.ndarray*) – outputs of *X_train*. Shape: (n, 1).
- **jitter** (*float, optional*) – jitter for *pred_std*.

Returns acquisition function values. Shape: (l,).

Return type numpy.ndarray

Raises AssertionError

bayeso.acquisition.**pure_exploit**(*pred_mean: numpy.ndarray*) → numpy.ndarray

It is a pure exploitation criterion.

Parameters **pred_mean** (*numpy.ndarray*) – posterior predictive mean function over *X_test*. Shape: (l,).

Returns acquisition function values. Shape: (l,).

Return type numpy.ndarray

Raises AssertionError

bayeso.acquisition.**pure_explore**(*pred_std: numpy.ndarray*) → numpy.ndarray

It is a pure exploration criterion.

Parameters **pred_std** (*numpy.ndarray*) – posterior predictive standard deviation function over *X_test*. Shape: (l,).

Returns acquisition function values. Shape: (l,).

Return type numpy.ndarray

Raises AssertionError

bayeso.acquisition.**ucb**(*pred_mean: numpy.ndarray, pred_std: numpy.ndarray, Y_train: Optional[numpy.ndarray] = None, kappa: float = 2.0, increase_kappa: bool = True*) → numpy.ndarray

It is a Gaussian process upper confidence bound criterion.

Parameters

- **pred_mean** (*numpy.ndarray*) – posterior predictive mean function over *X_test*. Shape: (l,).
- **pred_std** (*numpy.ndarray*) – posterior predictive standard deviation function over *X_test*. Shape: (l,).
- **Y_train** (*numpy.ndarray, optional*) – outputs of *X_train*. Shape: (n, 1).
- **kappa** (*float, optional*) – trade-off hyperparameter between exploration and exploitation.
- **increase_kappa** (*bool., optional*) – flag for increasing a kappa value as *Y_train* grows. If *Y_train* is None, it is ignored, which means *kappa* is fixed.

Returns acquisition function values. Shape: (l,).

Return type numpy.ndarray

Raises AssertionError

8.2 bayeso.constants

This file declares various default constants. If you would like to see the details, check out the Python script in the repository directly.

8.3 bayeso.covariance

It defines covariance functions and their associated functions. Derivatives of covariance functions with respect to hyperparameters are described in these notes.

`bayeso.covariance.`**`choose_fun_cov`**(*str_cov: str*) → Callable

It chooses a covariance function.

Parameters **str_cov** (*str.*) – the name of covariance function.

Returns covariance function.

Return type callable

Raises AssertionError

`bayeso.covariance.`**`choose_fun_grad_cov`**(*str_cov: str*) → Callable

It chooses a function for computing gradients of covariance function.

Parameters **str_cov** (*str.*) – the name of covariance function.

Returns function for computing gradients of covariance function.

Return type callable

Raises AssertionError

`bayeso.covariance.`**`cov_main`**(*str_cov: str, X: numpy.ndarray, Xp: numpy.ndarray, hyps: dict, same_X_Xp: bool, jitter: float = 1e-05*) → numpy.ndarray

It computes kernel matrix over *X* and *Xp*, where *hyps* is given.

Parameters

- **str_cov** (*str.*) – the name of covariance function.
- **X** (*numpy.ndarray*) – one inputs. Shape: (n, d).

- **Xp** (*numpy.ndarray*) – another inputs. Shape: (m, d).
- **hyps** (*dict.*) – dictionary of hyperparameters for covariance function.
- **same_X_Xp** (*bool.*) – flag for checking *X* and *Xp* are same.
- **jitter** (*float, optional*) – jitter for diagonal entries.

Returns kernel matrix over *X* and *Xp*. Shape: (n, m).

Return type numpy.ndarray

Raises AssertionError, ValueError

bayeso.covariance.**cov_matern32**(*X: numpy.ndarray, Xp: numpy.ndarray, lengthscales: Union[numpy.ndarray, float], signal: float*) → numpy.ndarray

It computes Matern 3/2 kernel over *X* and *Xp*, where *lengthscales* and *signal* are given.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **Xp** (*numpy.ndarray*) – another inputs. Shape: (m, d).
- **lengthscales** (*numpy.ndarray, or float*) – length scales. Shape: (d,) or ().
- **signal** (*float*) – coefficient for signal.

Returns kernel values over *X* and *Xp*. Shape: (n, m).

Return type numpy.ndarray

Raises AssertionError

bayeso.covariance.**cov_matern52**(*X: numpy.ndarray, Xp: numpy.ndarray, lengthscales: Union[numpy.ndarray, float], signal: float*) → numpy.ndarray

It computes Matern 5/2 kernel over *X* and *Xp*, where *lengthscales* and *signal* are given.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **Xp** (*numpy.ndarray*) – another inputs. Shape: (m, d).
- **lengthscales** (*numpy.ndarray, or float*) – length scales. Shape: (d,) or ().
- **signal** (*float*) – coefficient for signal.

Returns kernel values over *X* and *Xp*. Shape: (n, m).

Return type numpy.ndarray

Raises AssertionError

bayeso.covariance.**cov_se**(*X: numpy.ndarray, Xp: numpy.ndarray, lengthscales: Union[numpy.ndarray, float], signal: float*) → numpy.ndarray

It computes squared exponential kernel over *X* and *Xp*, where *lengthscales* and *signal* are given.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **Xp** (*numpy.ndarray*) – another inputs. Shape: (m, d).
- **lengthscales** (*numpy.ndarray, or float*) – length scales. Shape: (d,) or ().
- **signal** (*float*) – coefficient for signal.

Returns kernel values over *X* and *Xp*. Shape: (n, m).

Return type numpy.ndarray

Raises AssertionError

`bayeso.covariance.`**`cov_set`**(*str_cov: str, X: numpy.ndarray, Xp: numpy.ndarray, lengthscales: Union[numpy.ndarray, float], signal: float*) → numpy.ndarray

It computes set kernel matrix over *X* and *Xp*, where *lengthscales* and *signal* are given.

Parameters

- **str_cov** (*str.*) – the name of covariance function.
- **X** (*numpy.ndarray*) – one inputs. Shape: (n, m, d).
- **Xp** (*numpy.ndarray*) – another inputs. Shape: (l, m, d).
- **lengthscales** (*numpy.ndarray, or float*) – length scales. Shape: (d,) or ().
- **signal** (*float*) – coefficient for signal.

Returns set kernel matrix over *X* and *Xp*. Shape: (n, l).

Return type numpy.ndarray

Raises AssertionError

`bayeso.covariance.`**`get_kernel_cholesky`**(*X_train: numpy.ndarray, hyps: dict, str_cov: str, fix_noise: bool = True, use_gradient: bool = False, debug: bool = False*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]

This function computes a kernel inverse with Cholesky decomposition.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **hyps** (*dict.*) – dictionary of hyperparameters for Gaussian process.
- **str_cov** (*str.*) – the name of covariance function.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.
- **use_gradient** (*bool., optional*) – flag for computing and returning gradients of negative log marginal likelihood.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of kernel matrix over *X_train*, lower matrix computed by Cholesky decomposition, and gradients of kernel matrix. If *use_gradient* is False, gradients of kernel matrix would be None.

Return type tuple of (numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

`bayeso.covariance.`**`get_kernel_inverse`**(*X_train: numpy.ndarray, hyps: dict, str_cov: str, fix_noise: bool = True, use_gradient: bool = False, debug: bool = False*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]

This function computes a kernel inverse without any matrix decomposition techniques.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **hyps** (*dict.*) – dictionary of hyperparameters for Gaussian process.
- **str_cov** (*str.*) – the name of covariance function.

- **fix_noise** (*bool., optional*) – flag for fixing a noise.
- **use_gradient** (*bool., optional*) – flag for computing and returning gradients of negative log marginal likelihood.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of kernel matrix over *X_train*, kernel matrix inverse, and gradients of kernel matrix. If *use_gradient* is False, gradients of kernel matrix would be None.

Return type tuple of (numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

bayeso.covariance.**grad_cov_main**(*str_cov: str*, *X: numpy.ndarray*, *Xp: numpy.ndarray*, *hyps: dict*, *fix_noise: bool*, *same_X_Xp: bool = True*, *jitter: float = 1e-05*) → numpy.ndarray

It computes gradients of kernel matrix over hyperparameters, where *hyps* is given.

Parameters

- **str_cov** (*str.*) – the name of covariance function.
- **X** (*numpy.ndarray*) – one inputs. Shape: (n, d).
- **Xp** (*numpy.ndarray*) – another inputs. Shape: (m, d).
- **hyps** (*dict.*) – dictionary of hyperparameters for covariance function.
- **fix_noise** (*bool.*) – flag for fixing a noise.
- **same_X_Xp** (*bool., optional*) – flag for checking *X* and *Xp* are same.
- **jitter** (*float, optional*) – jitter for diagonal entries.

Returns gradient matrix over hyperparameters. Shape: (n, m, l) where l is the number of hyperparameters.

Return type numpy.ndarray

Raises AssertionError

bayeso.covariance.**grad_cov_matern32**(*cov_X_Xp: numpy.ndarray*, *X: numpy.ndarray*, *Xp: numpy.ndarray*, *hyps: dict*, *num_hyps: int*, *fix_noise: bool*) → numpy.ndarray

It computes gradients of Matern 3/2 kernel over *X* and *Xp*, where *hyps* is given.

Parameters

- **cov_X_Xp** (*numpy.ndarray*) – covariance matrix. Shape: (n, m).
- **X** (*numpy.ndarray*) – one inputs. Shape: (n, d).
- **Xp** (*numpy.ndarray*) – another inputs. Shape: (m, d).
- **hyps** (*dict.*) – dictionary of hyperparameters for covariance function.
- **num_hyps** (*int.*) – the number of hyperparameters == l.
- **fix_noise** (*bool.*) – flag for fixing a noise.

Returns gradient matrix over hyperparameters. Shape: (n, m, l).

Return type numpy.ndarray

Raises AssertionError

bayeso.covariance.**grad_cov_matern52**(*cov_X_Xp: numpy.ndarray, X: numpy.ndarray, Xp: numpy.ndarray, hyps: dict, num_hyps: int, fix_noise: bool*) → numpy.ndarray

It computes gradients of Matern 5/2 kernel over *X* and *Xp*, where *hyps* is given.

Parameters

- **cov_X_Xp** (*numpy.ndarray*) – covariance matrix. Shape: (n, m).
- **X** (*numpy.ndarray*) – one inputs. Shape: (n, d).
- **Xp** (*numpy.ndarray*) – another inputs. Shape: (m, d).
- **hyps** (*dict.*) – dictionary of hyperparameters for covariance function.
- **num_hyps** (*int.*) – the number of hyperparameters == l.
- **fix_noise** (*bool.*) – flag for fixing a noise.

Returns gradient matrix over hyperparameters. Shape: (n, m, l).

Return type numpy.ndarray

Raises AssertionError

bayeso.covariance.**grad_cov_se**(*cov_X_Xp: numpy.ndarray, X: numpy.ndarray, Xp: numpy.ndarray, hyps: dict, num_hyps: int, fix_noise: bool*) → numpy.ndarray

It computes gradients of squared exponential kernel over *X* and *Xp*, where *hyps* is given.

Parameters

- **cov_X_Xp** (*numpy.ndarray*) – covariance matrix. Shape: (n, m).
- **X** (*numpy.ndarray*) – one inputs. Shape: (n, d).
- **Xp** (*numpy.ndarray*) – another inputs. Shape: (m, d).
- **hyps** (*dict.*) – dictionary of hyperparameters for covariance function.
- **num_hyps** (*int.*) – the number of hyperparameters == l.
- **fix_noise** (*bool.*) – flag for fixing a noise.

Returns gradient matrix over hyperparameters. Shape: (n, m, l).

Return type numpy.ndarray

Raises AssertionError

CHAPTER 9

bayeso.bo

These files are for implementing Bayesian optimization classes.

9.1 bayeso.bo.base_bo

It defines an abstract class of Bayesian optimization.

class bayeso.bo.base_bo.**BaseBO**(*range_X: numpy.ndarray*, *str_surrogate: str*, *str_acq: str*, *str_optimizer_method_bo: str*, *normalize_Y: bool*, *debug: bool*)

Bases: abc.ABC

It is a Bayesian optimization class.

Parameters

- **range_X** (*numpy.ndarray*) – a search space. Shape: (d, 2).
- **str_surrogate** (*str.*) – the name of surrogate model.
- **str_acq** (*str.*) – the name of acquisition function.
- **str_optimizer_method_bo** (*str.*) – the name of optimization method for Bayesian optimization.
- **normalize_Y** (*bool.*) – flag for normalizing outputs.
- **debug** (*bool.*) – flag for printing log messages.

_abc_impl = <_abc_data object>

_get_bounds() → List[T]

It returns list of range tuples, obtained from *self.range_X*.

Returns list of range tuples.

Return type list

_get_random_state(*seed: Optional[int]*)

It returns a random state, defined by *seed*.

Parameters **seed** (*NoneType or int.*) – None, or a random seed.

Returns a random state.

Return type numpy.random.RandomState

Raises AssertionError

_get_samples_gaussian(*num_samples: int*, *seed: Optional[int] = None*) → numpy.ndarray

It returns *num_samples* examples sampled from Gaussian distribution.

Parameters

- **num_samples** (*int.*) – the number of samples.
- **seed** (*NoneType or int., optional*) – None, or random seed.

Returns random examples. Shape: (*num_samples*, d).

Return type numpy.ndarray

Raises AssertionError

_get_samples_grid(*num_grids: int = 50*) → numpy.ndarray

It returns grids of *self.range_X*.

Parameters **num_grids** (*int., optional*) – the number of grids.

Returns grids of *self.range_X*. Shape: (num_grids^d, d).

Return type numpy.ndarray

Raises AssertionError

_get_samples_halton(*num_samples: int*, *seed: Optional[int] = None*) → numpy.ndarray

It returns *num_samples* examples sampled by Halton algorithm.

Parameters

- **num_samples** (*int.*) – the number of samples.
- **seed** (*NoneType or int., optional*) – None, or random seed.

Returns examples sampled by Halton algorithm. Shape: (*num_samples*, d).

Return type numpy.ndarray

Raises AssertionError

_get_samples_sobol(*num_samples: int*, *seed: Optional[int] = None*) → numpy.ndarray

It returns *num_samples* examples sampled from Sobol' sequence.

Parameters

- **num_samples** (*int.*) – the number of samples.
- **seed** (*NoneType or int., optional*) – None, or random seed.

Returns examples sampled from Sobol' sequence. Shape: (*num_samples*, d).

Return type numpy.ndarray

Raises AssertionError

_get_samples_uniform(*num_samples: int*, *seed: Optional[int] = None*) → numpy.ndarray

It returns *num_samples* examples uniformly sampled.

Parameters

- **num_samples** (*int.*) – the number of samples.

- **seed** (*NoneType or int., optional*) – None, or random seed.

Returns random examples. Shape: (*num_samples*, d).

Return type numpy.ndarray

Raises AssertionError

compute_acquisitions()

It is an abstract method.

compute_posteriors()

It is an abstract method.

get_initials(*str_initial_method: str*, *num_initials: int*, *seed: Optional[int] = None*) → numpy.ndarray

It returns *num_initials* examples, sampled by a sampling method *str_initial_method*.

Parameters

- **str_initial_method** (*str.*) – the name of sampling method.
- **num_initials** (*int.*) – the number of samples.
- **seed** (*NoneType or int., optional*) – None, or random seed.

Returns sampled examples. Shape: (*num_samples*, d).

Return type numpy.ndarray

Raises AssertionError

get_samples(*str_sampling_method: str*, *fun_objective: Optional[Callable] = None*, *num_samples: int = 100*, *seed: Optional[int] = None*) → numpy.ndarray

It returns *num_samples* examples, sampled by a sampling method *str_sampling_method*.

Parameters

- **str_sampling_method** (*str.*) – the name of sampling method.
- **fun_objective** (*NoneType or callable, optional*) – None, or objective function.
- **num_samples** (*int., optional*) – the number of samples.
- **seed** (*NoneType or int., optional*) – None, or random seed.

Returns sampled examples. Shape: (*num_samples*, d).

Return type numpy.ndarray

Raises AssertionError

optimize()

It is an abstract method.

9.2 bayeso.bo.bo_w_gp

It defines a class of Bayesian optimization with Gaussian process regression.

class bayeso.bo.bo_w_gp.**BOwGP**(*range_X: numpy.ndarray*, *str_cov: str = 'matern52'*, *str_acq: str = 'ei'*, *normalize_Y: bool = True*, *use_ard: bool = True*, *prior_mu: Optional[Callable] = None*, *str_optimizer_method_gp: str = 'BFGS'*, *str_optimizer_method_bo: str = 'L-BFGS-B'*, *str_modelselection_method: str = 'ml'*, *debug: bool = False*)

Bases: *bayeso.bo.base_bo.BaseBO*

It is a Bayesian optimization class with Gaussian process regression.

Parameters

- **range_X** (*numpy.ndarray*) – a search space. Shape: (d, 2).
- **str_cov** (*str., optional*) – the name of covariance function.
- **str_acq** (*str., optional*) – the name of acquisition function.
- **normalize_Y** (*bool., optional*) – flag for normalizing outputs.
- **use_ard** (*bool., optional*) – flag for automatic relevance determination.
- **prior_mu** (*NoneType, or callable, optional*) – None, or prior mean function.
- **str_optimizer_method_gp** (*str., optional*) – the name of optimization method for Gaussian process regression.
- **str_optimizer_method_bo** (*str., optional*) – the name of optimization method for Bayesian optimization.
- **str_modelselection_method** (*str., optional*) – the name of model selection method for Gaussian process regression.
- **debug** (*bool., optional*) – flag for printing log messages.

_abc_impl = <_abc_data object>

_optimize(*fun_negative_acquisition: Callable*, *str_sampling_method: str*, *num_samples: int*) → Tuple[numpy.ndarray, numpy.ndarray]

It optimizes *fun_negative_function* with *self.str_optimizer_method_bo*. *num_samples* examples are determined by *str_sampling_method*, to start acquisition function optimization.

Parameters

- **fun_objective** (*callable*) – negative acquisition function.
- **str_sampling_method** (*str.*) – the name of sampling method.
- **num_samples** (*int.*) – the number of samples.

Returns tuple of next point to evaluate and all candidates determined by acquisition function optimization. Shape: ((d,), (*num_samples*, d)).

Return type (numpy.ndarray, numpy.ndarray)

compute_acquisitions(*X: numpy.ndarray*, *X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *cov_X_X: numpy.ndarray*, *inv_cov_X_X: numpy.ndarray*, *hyps: dict*) → numpy.ndarray

It computes acquisition function values over 'X', where *X_train*, *Y_train*, *cov_X_X*, *inv_cov_X_X*, and *hyps* are given.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).
- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).

- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **cov_X_X** (*numpy.ndarray*) – kernel matrix over *X_train*. Shape: (n, n).
- **inv_cov_X_X** (*numpy.ndarray*) – kernel matrix inverse over *X_train*. Shape: (n, n).
- **hyps** (*dict.*) – dictionary of hyperparameters.

Returns acquisition function values over *X*. Shape: (l,).

Return type numpy.ndarray

Raises AssertionError

compute_posteriors(*X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *X_test: numpy.ndarray*, *cov_X_X: numpy.ndarray*, *inv_cov_X_X: numpy.ndarray*, *hyps: dict*) → numpy.ndarray

It returns posterior mean and standard deviation functions over *X_test*.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).
- **cov_X_X** (*numpy.ndarray*) – kernel matrix over *X_train*. Shape: (n, n).
- **inv_cov_X_X** (*numpy.ndarray*) – kernel matrix inverse over *X_train*. Shape: (n, n).
- **hyps** (*dict.*) – dictionary of hyperparameters for Gaussian process.

Returns posterior mean and standard deviation functions over *X_test*. Shape: ((l,), (l,)).

Return type (numpy.ndarray, numpy.ndarray)

Raises AssertionError

optimize(*X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *str_sampling_method: str = 'sobol'*, *num_samples: int = 100*, *str_mlm_method: str = 'regular'*) → Tuple[numpy.ndarray, dict]

It computes acquired example, candidates of acquired examples, acquisition function values for the candidates, covariance matrix, inverse matrix of the covariance matrix, hyperparameters optimized, and execution times.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **str_sampling_method** (*str., optional*) – the name of sampling method for acquisition function optimization.
- **num_samples** (*int., optional*) – the number of samples.
- **str_mlm_method** (*str., optional*) – the name of marginal likelihood maximization method for Gaussian process regression.

Returns acquired example and dictionary of information. Shape: ((d,), dict.).

Return type (numpy.ndarray, dict.)

Raises AssertionError

9.3 bayeso.bo.bo_w_tp

It defines a class of Bayesian optimization with Student-t process regression.

class bayeso.bo.bo_w_tp.**BOwTP**(*range_X: numpy.ndarray*, *str_cov: str = 'matern52'*, *str_acq: str = 'ei'*, *normalize_Y: bool = True*, *use_ard: bool = True*, *prior_mu: Optional[Callable] = None*, *str_optimizer_method_tp: str = 'SLSQP'*, *str_optimizer_method_bo: str = 'L-BFGS-B'*, *debug: bool = False*)

Bases: *bayeso.bo.base_bo.BaseBO*

It is a Bayesian optimization class with Student-t process regression.

Parameters

- **range_X** (*numpy.ndarray*) – a search space. Shape: (d, 2).
- **str_cov** (*str., optional*) – the name of covariance function.
- **str_acq** (*str., optional*) – the name of acquisition function.
- **normalize_Y** (*bool., optional*) – flag for normalizing outputs.
- **use_ard** (*bool., optional*) – flag for automatic relevance determination.
- **prior_mu** (*NoneType, or callable, optional*) – None, or prior mean function.
- **str_optimizer_method_tp** (*str., optional*) – the name of optimization method for Student-t process regression.
- **str_optimizer_method_bo** (*str., optional*) – the name of optimization method for Bayesian optimization.
- **debug** (*bool., optional*) – flag for printing log messages.

_abc_impl = <_abc_data object>

_optimize(*fun_negative_acquisition: Callable*, *str_sampling_method: str*, *num_samples: int*) → Tuple[numpy.ndarray, numpy.ndarray]

It optimizes *fun_negative_function* with *self.str_optimizer_method_bo*. *num_samples* examples are determined by *str_sampling_method*, to start acquisition function optimization.

Parameters

- **fun_objective** (*callable*) – negative acquisition function.
- **str_sampling_method** (*str.*) – the name of sampling method.
- **num_samples** (*int.*) – the number of samples.

Returns tuple of next point to evaluate and all candidates determined by acquisition function optimization. Shape: ((d,), (*num_samples*, d)).

Return type (numpy.ndarray, numpy.ndarray)

compute_acquisitions(*X: numpy.ndarray*, *X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *cov_X_X: numpy.ndarray*, *inv_cov_X_X: numpy.ndarray*, *hyps: dict*) → numpy.ndarray

It computes acquisition function values over 'X', where *X_train*, *Y_train*, *cov_X_X*, *inv_cov_X_X*, and *hyps* are given.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **cov_X_X** (*numpy.ndarray*) – kernel matrix over *X_train*. Shape: (n, n).
- **inv_cov_X_X** (*numpy.ndarray*) – kernel matrix inverse over *X_train*. Shape: (n, n).
- **hyps** (*dict.*) – dictionary of hyperparameters.

Returns acquisition function values over *X*. Shape: (l,).

Return type numpy.ndarray

Raises AssertionError

compute_posteriors(*X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *X_test: numpy.ndarray*, *cov_X_X: numpy.ndarray*, *inv_cov_X_X: numpy.ndarray*, *hyps: dict*) → numpy.ndarray

It returns posterior mean and standard deviation over *X_test*.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).
- **cov_X_X** (*numpy.ndarray*) – kernel matrix over *X_train*. Shape: (n, n).
- **inv_cov_X_X** (*numpy.ndarray*) – kernel matrix inverse over *X_train*. Shape: (n, n).
- **hyps** (*dict.*) – dictionary of hyperparameters for Gaussian process.

Returns posterior mean and standard deviation over *X_test*. Shape: ((l,), (l,)).

Return type (numpy.ndarray, numpy.ndarray)

Raises AssertionError

optimize(*X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *str_sampling_method: str = 'sobol'*, *num_samples: int = 100*) → Tuple[numpy.ndarray, dict]

It computes acquired example, candidates of acquired examples, acquisition function values for the candidates, covariance matrix, inverse matrix of the covariance matrix, hyperparameters optimized, and execution times.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **str_sampling_method** (*str., optional*) – the name of sampling method for acquisition function optimization.
- **num_samples** (*int., optional*) – the number of samples.

Returns acquired example and dictionary of information. Shape: ((d,), dict.).

Return type (numpy.ndarray, dict.)

Raises AssertionError

9.4 bayeso.bo.bo_w_trees

It defines a class of Bayesian optimization with tree-based surrogate models.

class bayeso.bo.bo_w_trees.**BOwTrees**(*range_X: numpy.ndarray, str_surrogate: str = 'rf', str_acq: str = 'ei', normalize_Y: bool = True, str_optimizer_method_bo: str = 'random_search', debug: bool = False*)

Bases: *bayeso.bo.base_bo.BaseBO*

It is a Bayesian optimization class with tree-based surrogate models.

Parameters

- **range_X** (*numpy.ndarray*) – a search space. Shape: (d, 2).
- **str_surrogate** (*str., optional*) – the name of surrogate model.
- **str_acq** (*str., optional*) – the name of acquisition function.
- **normalize_Y** (*bool., optional*) – flag for normalizing outputs.
- **str_optimizer_method_bo** (*str., optional*) – the name of optimization method for Bayesian optimization.
- **debug** (*bool., optional*) – flag for printing log messages.

_abc_impl = <_abc_data object>

compute_acquisitions(*X: numpy.ndarray, X_train: numpy.ndarray, Y_train: numpy.ndarray, trees: List[T]*) → numpy.ndarray

It computes acquisition function values over 'X', where *X_train* and *Y_train* are given.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (l, d).
- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **trees** (*list*) – list of trees.

Returns acquisition function values over *X*. Shape: (l,).

Return type numpy.ndarray

Raises AssertionError

compute_posteriors(*X: numpy.ndarray, trees: List[T]*) → numpy.ndarray

It returns posterior mean and standard deviation functions over *X*.

Parameters

- **X** (*numpy.ndarray*) – inputs to test. Shape: (l, d).
- **trees** (*list*) – list of trees.

Returns posterior mean and standard deviation functions over *X*. Shape: ((l,), (l,)).

Return type (numpy.ndarray, numpy.ndarray)

Raises AssertionError

get_trees(*X_train, Y_train, num_trees=100, depth_max=5, size_min_leaf=1*)

It returns a list of trees.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **num_trees** (*int., optional*) – the number of trees.
- **depth_max** (*int., optional*) – maximum depth.
- **size_min_leaf** (*int., optional*) – minimum size of leaves.

Returns list of trees.

Return type list

Raises AssertionError

optimize(*X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *str_sampling_method: str = 'uniform'*, *num_samples: int = 5000*) → Tuple[numpy.ndarray, dict]

It computes acquired example, candidates of acquired examples, acquisition function values for the candidates, covariance matrix, inverse matrix of the covariance matrix, hyperparameters optimized, and execution times.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **str_sampling_method** (*str., optional*) – the name of sampling method for acquisition function optimization.
- **num_samples** (*int., optional*) – the number of samples.

Returns acquired example and dictionary of information. Shape: ((d,), dict.).

Return type (numpy.ndarray, dict.)

Raises AssertionError

CHAPTER 10

bayeso.gp

These files are for implementing Gaussian process regression. It is implemented, based on the following article:

(i) Rasmussen, C. E., & Williams, C. K. (2006). Gaussian Process Regression for Machine Learning. MIT Press.

10.1 bayeso.gp.gp

It defines Gaussian process regression.

`bayeso.gp.gp.`**`predict_with_cov`**(*X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *X_test: numpy.ndarray*, *cov_X_X: numpy.ndarray*, *inv_cov_X_X: numpy.ndarray*, *hyps: dict*, *str_cov: str = 'matern52'*, *prior_mu: Optional[Callable] = None*, *debug: bool = False*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]

This function returns posterior mean and posterior standard deviation functions over *X_test*, computed by Gaussian process regression with *X_train*, *Y_train*, *cov_X_X*, *inv_cov_X_X*, and *hyps*.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).
- **cov_X_X** (*numpy.ndarray*) – kernel matrix over *X_train*. Shape: (n, n).
- **inv_cov_X_X** (*numpy.ndarray*) – kernel matrix inverse over *X_train*. Shape: (n, n).
- **hyps** (*dict.*) – dictionary of hyperparameters for Gaussian process.
- **str_cov** (*str., optional*) – the name of covariance function.
- **prior_mu** (*NoneType, or callable, optional*) – None, or prior mean function.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of posterior mean function over *X_test*, posterior standard deviation function over *X_test*, and posterior covariance matrix over *X_test*. Shape: ((l, 1), (l, 1), (l, l)).

Return type tuple of (numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

`bayeso.gp.gp.`**`predict_with_hyps`**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, X_test: numpy.ndarray, hyps: dict, str_cov: str = 'matern52', prior_mu: Optional[Callable] = None, debug: bool = False*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]

This function returns posterior mean and posterior standard deviation functions over *X_test*, computed by Gaussian process regression with *X_train*, *Y_train*, and *hyps*.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).
- **hyps** (*dict.*) – dictionary of hyperparameters for Gaussian process.
- **str_cov** (*str., optional*) – the name of covariance function.
- **prior_mu** (*NoneType, or callable, optional*) – None, or prior mean function.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of posterior mean function over *X_test*, posterior standard deviation function over *X_test*, and posterior covariance matrix over *X_test*. Shape: ((l, 1), (l, 1), (l, l)).

Return type tuple of (numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

`bayeso.gp.gp.`**`predict_with_optimized_hyps`**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, X_test: numpy.ndarray, str_cov: str = 'matern52', str_optimizer_method: str = 'BFGS', prior_mu: Optional[Callable] = None, fix_noise: float = True, debug: bool = False*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]

This function returns posterior mean and posterior standard deviation functions over *X_test*, computed by the Gaussian process regression optimized with *X_train* and *Y_train*.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).
- **str_cov** (*str., optional*) – the name of covariance function.
- **str_optimizer_method** (*str., optional*) – the name of optimization method.
- **prior_mu** (*NoneType, or callable, optional*) – None, or prior mean function.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of posterior mean function over *X_test*, posterior standard deviation function over *X_test*, and posterior covariance matrix over *X_test*. Shape: ((l, 1), (l, 1), (l, l)).

Return type tuple of (numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

`bayeso.gp.gp.`**`sample_functions`**(*mu: numpy.ndarray*, *Sigma: numpy.ndarray*, *num_samples: int = 1*) → numpy.ndarray

It samples *num_samples* functions from multivariate Gaussian distribution (mu, Sigma).

Parameters

- **mu** (*numpy.ndarray*) – mean vector. Shape: (n,).
- **Sigma** (*numpy.ndarray*) – covariance matrix. Shape: (n, n).
- **num_samples** (*int., optional*) – the number of sampled functions

Returns sampled functions. Shape: (num_samples, n).

Return type numpy.ndarray

Raises AssertionError

10.2 bayeso.gp.gp_likelihood

It defines the functions related to likelihood for Gaussian process regression.

`bayeso.gp.gp_likelihood.`**`neg_log_ml`**(*X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *hyps: numpy.ndarray*, *str_cov: str*, *prior_mu_train: numpy.ndarray*, *use_ard: bool = True*, *fix_noise: bool = True*, *use_cholesky: bool = True*, *use_gradient: bool = True*, *debug: bool = False*) → Union[float, Tuple[float, numpy.ndarray]]

This function computes a negative log marginal likelihood.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **hyps** (*numpy.ndarray*) – hyperparameters for Gaussian process. Shape: (h,).
- **str_cov** (*str.*) – the name of covariance function.
- **prior_mu_train** (*numpy.ndarray*) – the prior values computed by get_prior_mu(). Shape: (n, 1).
- **use_ard** (*bool., optional*) – flag for automatic relevance determination.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.
- **use_cholesky** (*bool., optional*) – flag for using a cholesky decomposition.
- **use_gradient** (*bool., optional*) – flag for computing and returning gradients of negative log marginal likelihood.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns negative log marginal likelihood, or (negative log marginal likelihood, gradients of the likelihood).

Return type float, or tuple of (float, np.ndarray)

Raises AssertionError

`bayeso.gp.gp_likelihood.`**`neg_log_pseudo_l_loocv`**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, hyps: numpy.ndarray, str_cov: str, prior_mu_train: numpy.ndarray, fix_noise: bool = True, debug: bool = False*) → float

It computes a negative log pseudo-likelihood using leave-one-out cross-validation.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **hyps** (*numpy.ndarray*) – hyperparameters for Gaussian process. Shape: (h,).
- **str_cov** (*str.*) – the name of covariance function.
- **prior_mu_train** (*numpy.ndarray*) – the prior values computed by get_prior_mu(). Shape: (n, 1).
- **fix_noise** (*bool., optional*) – flag for fixing a noise.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns negative log pseudo-likelihood.

Return type float

Raises AssertionError

10.3 bayeso.gp.gp_kernel

It defines the functions related to kernels for Gaussian process regression.

`bayeso.gp.gp_kernel.`**`get_optimized_kernel`**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, prior_mu: Optional[Callable], str_cov: str, str_optimizer_method: str = 'BFGS', str_modelselection_method: str = 'ml', use_ard: bool = True, fix_noise: bool = True, debug: bool = False*) → Tuple[numpy.ndarray, numpy.ndarray, dict]

This function computes the kernel matrix optimized by optimization method specified, its inverse matrix, and the optimized hyperparameters.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **prior_mu** (*callable or NoneType*) – prior mean function or None.
- **str_cov** (*str.*) – the name of covariance function.
- **str_optimizer_method** (*str., optional*) – the name of optimization method.
- **str_modelselection_method** (*str., optional*) – the name of model selection method.
- **use_ard** (*bool., optional*) – flag for using automatic relevance determination.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.

- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of kernel matrix over *X_train*, kernel matrix inverse, and dictionary of hyperparameters.

Return type tuple of (numpy.ndarray, numpy.ndarray, dict.)

Raises AssertionError, ValueError

CHAPTER 11

bayeso.tp

These files are for implementing Student-t process regression. It is implemented, based on the following article:

(i) Rasmussen, C. E., & Williams, C. K. (2006). Gaussian Process Regression for Machine Learning. MIT Press.

(ii) Shah, A., Wilson, A. G., & Ghahramani, Z. (2014). Student-t Processes as Alternatives to Gaussian Processes. In Proceedings of the 17th International Conference on Artificial Intelligence and Statistics (pp. 877-885).

11.1 bayeso.tp.tp

It defines Student-t process regression.

`bayeso.tp.tp.`**`predict_with_cov`**(*X_train: numpy.ndarray*, *Y_train: numpy.ndarray*, *X_test: numpy.ndarray*, *cov_X_X: numpy.ndarray*, *inv_cov_X_X: numpy.ndarray*, *hyps: dict*, *str_cov: str = 'matern52'*, *prior_mu: Optional[Callable] = None*, *debug: bool = False*) → Tuple[float, numpy.ndarray, numpy.ndarray, numpy.ndarray]

This function returns degree of freedom, posterior mean, posterior standard variance, and posterior covariance functions over *X_test*, computed by Student-t process regression with *X_train*, *Y_train*, *cov_X_X*, *inv_cov_X_X*, and *hyps*.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).
- **cov_X_X** (*numpy.ndarray*) – kernel matrix over *X_train*. Shape: (n, n).
- **inv_cov_X_X** (*numpy.ndarray*) – kernel matrix inverse over *X_train*. Shape: (n, n).
- **hyps** (*dict.*) – dictionary of hyperparameters for Student-t process.
- **str_cov** (*str., optional*) – the name of covariance function.

- **prior_mu** (*NoneType, or callable, optional*) – None, or prior mean function.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of degree of freedom, posterior mean function over *X_test*, posterior standrad variance function over *X_test*, and posterior covariance matrix over *X_test*. Shape: (((), (l, 1), (l, 1), (l, l)).

Return type tuple of (float, numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

bayeso.tp.tp.**predict_with_hyps**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, X_test: numpy.ndarray, hyps: dict, str_cov: str = 'matern52', prior_mu: Optional[Callable] = None, debug: bool = False*) → Tuple[float, numpy.ndarray, numpy.ndarray, numpy.ndarray]

This function returns degree of freedom, posterior mean, posterior standard variance, and posterior covariance functions over *X_test*, computed by Student-t process regression with *X_train*, *Y_train*, and *hyps*.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).
- **hyps** (*dict.*) – dictionary of hyperparameters for Student-t process.
- **str_cov** (*str., optional*) – the name of covariance function.
- **prior_mu** (*NoneType, or callable, optional*) – None, or prior mean function.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of degree of freedom, posterior mean function over *X_test*, posterior standrad variance function over *X_test*, and posterior covariance matrix over *X_test*. Shape: (((), (l, 1), (l, 1), (l, l)).

Return type tuple of (float, numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

bayeso.tp.tp.**predict_with_optimized_hyps**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, X_test: numpy.ndarray, str_cov: str = 'matern52', str_optimizer_method: str = 'SLSQP', prior_mu: Optional[Callable] = None, fix_noise: float = True, debug: bool = False*) → Tuple[float, numpy.ndarray, numpy.ndarray, numpy.ndarray]

This function returns degree of freedom, posterior mean, posterior standard variance, and posterior covariance functions over *X_test*, computed by the Student-t process regression optimized with *X_train* and *Y_train*.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – inputs. Shape: (l, d) or (l, m, d).
- **str_cov** (*str., optional*) – the name of covariance function.
- **str_optimizer_method** (*str., optional*) – the name of optimization method.

- **prior_mu** (*NoneType, or callable, optional*) – None, or prior mean function.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of degree of freedom, posterior mean function over *X_test*, posterior standrad variance function over *X_test*, and posterior covariance matrix over *X_test*. Shape: ((), (l, 1), (l, 1), (l, l)).

Return type tuple of (float, numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

`bayeso.tp.tp.`**`sample_functions`**(*nu: float, mu: numpy.ndarray, Sigma: numpy.ndarray, num_samples: int = 1*) → numpy.ndarray

It samples *num_samples* functions from multivariate Student-t distribution (nu, mu, Sigma).

Parameters

- **mu** (*numpy.ndarray*) – mean vector. Shape: (n,).
- **Sigma** (*numpy.ndarray*) – covariance matrix. Shape: (n, n).
- **num_samples** (*int., optional*) – the number of sampled functions

Returns sampled functions. Shape: (num_samples, n).

Return type numpy.ndarray

Raises AssertionError

11.2 bayeso.tp.tp_likelihood

It defines the functions related to likelihood for Student-*t* process regression.

`bayeso.tp.tp_likelihood.`**`neg_log_ml`**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, hyps: numpy.ndarray, str_cov: str, prior_mu_train: numpy.ndarray, use_ard: bool = True, fix_noise: bool = True, use_gradient: bool = True, debug: bool = False*) → Union[float, Tuple[float, numpy.ndarray]]

This function computes a negative log marginal likelihood.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **hyps** (*numpy.ndarray*) – hyperparameters for Gaussian process. Shape: (h,).
- **str_cov** (*str.*) – the name of covariance function.
- **prior_mu_train** (*numpy.ndarray*) – the prior values computed by get_prior_mu(). Shape: (n, 1).
- **use_ard** (*bool., optional*) – flag for automatic relevance determination.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.
- **use_gradient** (*bool., optional*) – flag for computing and returning gradients of negative log marginal likelihood.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns negative log marginal likelihood, or (negative log marginal likelihood, gradients of the likelihood).

Return type float, or tuple of (float, np.ndarray)

Raises AssertionError

11.3 bayeso.tp.tp_kernel

It defines the functions related to kernels for Student-t process regression.

`bayeso.tp.tp_kernel.`**`get_optimized_kernel`**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, prior_mu: Optional[Callable], str_cov: str, str_optimizer_method: str = 'SLSQP', use_ard: bool = True, fix_noise: bool = True, debug: bool = False*) → Tuple[numpy.ndarray, numpy.ndarray, dict]

This function computes the kernel matrix optimized by optimization method specified, its inverse matrix, and the optimized hyperparameters.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **prior_mu** (*callable or NoneType*) – prior mean function or None.
- **str_cov** (*str.*) – the name of covariance function.
- **str_optimizer_method** (*str., optional*) – the name of optimization method.
- **use_ard** (*bool., optional*) – flag for using automatic relevance determination.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.
- **debug** (*bool., optional*) – flag for printing log messages.

Returns a tuple of kernel matrix over *X_train*, kernel matrix inverse, and dictionary of hyperparameters.

Return type tuple of (numpy.ndarray, numpy.ndarray, dict.)

Raises AssertionError, ValueError

CHAPTER 12

bayeso.trees

These files are written to implement tree-based regression models.

12.1 bayeso.trees.trees_common

It defines a common function for tree-based surrogates.

`bayeso.trees.trees_common.`**`_mse`**(*Y: numpy.ndarray*) → float

It returns a mean squared loss over *Y*.

Parameters **Y** (*numpy.ndarray*) – outputs in a leaf.

Returns a loss value.

Return type float

Raises AssertionError

`bayeso.trees.trees_common.`**`_predict_by_tree`**(*bx: numpy.ndarray*, *tree: dict*) → Tuple[float, float]

It predicts a posterior distribution over *bx*, given *tree*.

Parameters

- **bx** (*numpy.ndarray*) – an input. Shape: (d,).
- **tree** (*dict.*) – a decision tree.

Returns posterior mean and standard devitation estimates.

Return type (float, float)

Raises AssertionError

`bayeso.trees.trees_common.`**`_predict_by_trees`**(*bx: numpy.ndarray*, *list_trees: list*) → Tuple[float, float]

It predicts a posterior distribution over *bx*, given *list_trees*.

Parameters

- **bx** (*numpy.ndarray*) – an input. Shape: (d,).
- **list_trees** (*list*) – a list of decision trees.

Returns posterior mean and standard devitation estimates.

Return type (float, float)

Raises AssertionError

bayeso.trees.trees_common.**_split**(*X: numpy.ndarray*, *Y: numpy.ndarray*, *num_features: int*, *split_random_location: bool*) → dict

It splits *X* and *Y* to left and right leaves as a dictionary including split dimension and split location.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **Y** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **num_features** (*int.*) – the number of features to split.
- **split_random_location** (*bool.*) – flag for setting a split location randomly or not.

Returns a dictionary of left and right leaves, spilt dimension, and split location.

Return type dict.

Raises AssertionError

bayeso.trees.trees_common.**_split_left_right**(*X: numpy.ndarray*, *Y: numpy.ndarray*, *dim_to_split: int*, *val_to_split: float*) → tuple

It splits *X* and *Y* to left and right leaves.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **Y** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **dim_to_split** (*int.*) – a dimension to split.
- **val_to_split** (*float*) – a value to split.

Returns a tuple of left and right leaves.

Return type tuple

Raises AssertionError

bayeso.trees.trees_common.**compute_sigma**(*preds_mu_leaf: numpy.ndarray*, *preds_sigma_leaf: numpy.ndarray*, *min_sigma: float = 0.0*) → numpy.ndarray

It computes predictive standard deviation estimates.

Parameters

- **preds_mu_leaf** (*numpy.ndarray*) – predictive mean estimates of leaf. Shape: (n,).
- **preds_sigma_leaf** (*numpy.ndarray*) – predictive standard deviation estimates of leaf. Shape: (n,).
- **min_sigma** (*float*) – threshold for minimum standard deviation.

Returns predictive standard deviation estimates. Shape: (n,).

Return type numpy.ndarray

Raises AssertionError

`bayeso.trees.trees_common.`**`get_inputs_from_leaf`**(*leaf: list*) → numpy.ndarray

It returns an input from a leaf.

Parameters **`leaf`** (*`list`*) – pairs of input and output in a leaf.

Returns an input. Shape: (n, d).

Return type numpy.ndarray

Raises AssertionError

`bayeso.trees.trees_common.`**`get_outputs_from_leaf`**(*leaf: list*) → numpy.ndarray

It returns an output from a leaf.

Parameters **`leaf`** (*`list`*) – pairs of input and output in a leaf.

Returns an output. Shape: (n, 1).

Return type numpy.ndarray

Raises AssertionError

`bayeso.trees.trees_common.`**`mse`**(*left_right: tuple*) → float

It returns a mean squared loss over *left_right*.

Parameters **`left_right`** (*`tuple`*) – a tuple of left and right leaves.

Returns a loss value.

Return type float

Raises AssertionError

`bayeso.trees.trees_common.`**`predict_by_trees`**(*X: numpy.ndarray*, *list_trees: list*) → Tuple[numpy.ndarray, numpy.ndarray]

It predicts a posterior distribution over *X*, given *list_trees*, using *multiprocessing*.

Parameters

- **`X`** (*`numpy.ndarray`*) – inputs. Shape: (n, d).
- **`list_trees`** (*`list`*) – a list of decision trees.

Returns posterior mean and standard devitation estimates. Shape: ((n, 1), (n, 1)).

Return type (numpy.ndarray, numpy.ndarray)

Raises AssertionError

`bayeso.trees.trees_common.`**`split`**(*node: dict*, *depth_max: int*, *size_min_leaf: int*, *num_features: int*, *split_random_location: bool*, *cur_depth: int*) → None

It splits a root node to construct a tree.

Parameters

- **`node`** (*`dict.`*) – a root node.
- **`depth_max`** (*`int.`*) – maximum depth of tree.
- **`size_min_leaf`** (*`int.`*) – minimum size of leaf.
- **`num_features`** (*`int.`*) – the number of split features.
- **`split_random_location`** (*`bool.`*) – flag for setting a split location randomly or not.
- **`cur_depth`** (*`int.`*) – depth of the current node.

Returns None.

Return type NoneType

Raises AssertionError

`bayeso.trees.trees_common.`**`subsample`**(*X: numpy.ndarray*, *Y: numpy.ndarray*, *ratio_sampling: float*, *replace_samples: bool*) → Tuple[numpy.ndarray, numpy.ndarray]

It subsamples a bootstrap sample.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **Y** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **ratio_sampling** (*float*) – ratio of sampling.
- **replace_samples** (*bool.*) – a flag for sampling with replacement or without replacement.

Returns a tuple of bootstrap sample. Shape: ((m, d), (m, 1)).

Return type (numpy.ndarray, numpy.ndarray)

Raises AssertionError

`bayeso.trees.trees_common.`**`unit_predict_by_trees`**(*X: numpy.ndarray*, *list_trees: list*) → Tuple[numpy.ndarray, numpy.ndarray]

It predicts a posterior distribution over *X*, given *list_trees*.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **list_trees** (*list*) – a list of decision trees.

Returns posterior mean and standard devitation estimates. Shape: ((n, 1), (n, 1)).

Return type (numpy.ndarray, numpy.ndarray)

Raises AssertionError

12.2 bayeso.trees.trees_generic_trees

It defines generic trees.

`bayeso.trees.trees_generic_trees.`**`get_generic_trees`**(*X: numpy.ndarray*, *Y: numpy.ndarray*, *num_trees: int*, *depth_max: int*, *size_min_leaf: int*, *ratio_sampling: float*, *replace_samples: bool*, *num_features: int*, *split_random_location: bool*) → list

It returns a list of generic trees.

Parameters

- **X** (*np.ndarray*) – inputs. Shape: (N, d).
- **Y** (*str.*) – outputs. Shape: (N, 1).
- **num_trees** (*int.*) – the number of trees.

- **depth_max** (*int.*) – maximum depth of tree.
- **size_min_leaf** (*int.*) – minimum size of leaf.
- **ratio_sampling** (*float*) – ratio of dataset subsampling.
- **replace_samples** (*bool.*) – flag for replacement.
- **num_features** (*int.*) – the number of split features.
- **split_random_location** (*bool.*) – flag for random split location.

Returns list of trees

Return type list

Raises AssertionError

12.3 bayeso.trees.trees_random_forest

It defines a random forest.

`bayeso.trees.trees_random_forest.`**`get_random_forest`**(*X: numpy.ndarray, Y: numpy.ndarray, num_trees: int, depth_max: int, size_min_leaf: int, num_features: int*) → list

It returns a random forest.

Parameters

- **X** (*np.ndarray*) – inputs. Shape: (N, d).
- **Y** (*str.*) – outputs. Shape: (N, 1).
- **num_trees** (*int.*) – the number of trees.
- **depth_max** (*int.*) – maximum depth of tree.
- **size_min_leaf** (*int.*) – minimum size of leaf.
- **num_features** (*int.*) – the number of split features.

Returns list of trees

Return type list

Raises AssertionError

CHAPTER 13

bayeso.utils

These files are for implementing utilities for various features.

13.1 bayeso.utils.utils_bo

It is utilities for Bayesian optimization.

`bayeso.utils.utils_bo.`**`check_hyps_convergence`**(*list_hyps: List[dict], hyps: dict, str_cov: str, fix_noise: bool, ratio_threshold: float = 0.05*) → bool

It checks convergence of hyperparameters for Gaussian process regression.

Parameters

- **`list_hyps`** (*`list`*) – list of historical hyperparameters for Gaussian process regression.
- **`hyps`** (*`dict.`*) – dictionary of hyperparameters for acquisition function.
- **`str_cov`** (*`str.`*) – the name of covariance function.
- **`fix_noise`** (*`bool.`*) – flag for fixing a noise.
- **`ratio_threshold`** (*`float, optional`*) – ratio of threshold for checking convergence.

Returns flag for checking convergence. If converged, it is True.

Return type bool.

Raises AssertionError

`bayeso.utils.utils_bo.`**`check_optimizer_method_bo`**(*str_optimizer_method_bo: str, dim: int, debug: bool*) → str

It checks the availability of optimization methods. It helps to run Bayesian optimization, even though additional optimization methods are not installed or there exist the conditions some of optimization methods cannot be run.

Parameters

- **str_optimizer_method_bo** (*str.*) – the name of optimization method for Bayesian optimization.
- **dim** (*int.*) – dimensionality of the problem we solve.
- **debug** (*bool.*) – flag for printing log messages.

Returns available *str_optimizer_method_bo*.

Return type str.

Raises AssertionError

bayeso.utils.utils_bo.**choose_fun_acquisition**(*str_acq: str, noise: Optional[float] = None*) → Callable

It chooses and returns an acquisition function.

Parameters

- **str_acq** (*str.*) – the name of acquisition function.
- **hyps** (*dict.*) – dictionary of hyperparameters for acquisition function.

Returns acquisition function.

Return type callable

Raises AssertionError

bayeso.utils.utils_bo.**get_best_acquisition_by_evaluation**(*initials: numpy.ndarray, fun_objective: Callable*) → numpy.ndarray

It returns the best acquisition with respect to values of *fun_objective*. Here, the best acquisition is a minimizer of *fun_objective*.

Parameters

- **initials** (*numpy.ndarray*) – inputs. Shape: (n, d).
- **fun_objective** (*callable*) – an objective function.

Returns the best example of *initials*. Shape: (1, d).

Return type numpy.ndarray

Raises AssertionError

bayeso.utils.utils_bo.**get_best_acquisition_by_history**(*X: numpy.ndarray, Y: numpy.ndarray*) → Tuple[numpy.ndarray, float]

It returns the best acquisition that has shown minimum result, and its minimum result.

Parameters

- **X** (*numpy.ndarray*) – historical queries. Shape: (n, d).
- **Y** (*numpy.ndarray*) – the observations of *X*. Shape: (n, 1).

Returns a tuple of the best query and its result.

Return type (numpy.ndarray, float)

Raises AssertionError

bayeso.utils.utils_bo.**get_next_best_acquisition**(*points: numpy.ndarray, acquisitions: numpy.ndarray, points_evaluated: numpy.ndarray*) → numpy.ndarray

It returns the next best acquired sample.

Parameters

- **points** (*numpy.ndarray*) – inputs for acquisition function. Shape: (n, d).
- **acquisitions** (*numpy.ndarray*) – acquisition function values over *points*. Shape: (n,).
- **points_evaluated** (*numpy.ndarray*) – the samples evaluated so far. Shape: (m, d).

Returns next best acquired point. Shape: (d,).

Return type numpy.ndarray

Raises AssertionError

13.2 bayeso.utils.utils_common

It is utilities for common features.

`bayeso.utils.utils_common.`**`get_grids`**(*ranges: numpy.ndarray, num_grids: int*) → numpy.ndarray

It returns grids of given *ranges*, where each of dimension has *num_grids* partitions.

Parameters

- **ranges** (*numpy.ndarray*) – ranges. Shape: (d, 2).
- **num_grids** (*int.*) – the number of partitions per dimension.

Returns grids of given *ranges*. Shape: (num_grids^d, d).

Return type numpy.ndarray

Raises AssertionError

`bayeso.utils.utils_common.`**`get_minimum`**(*Y_all: numpy.ndarray, num_init: int*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]

It returns accumulated minima at each iteration, their arithmetic means over rounds, and their standard deviations over rounds, which is widely used in Bayesian optimization community.

Parameters

- **Y_all** (*numpy.ndarray*) – historical function values. Shape: (r, t) where r is the number of Bayesian optimization rounds and t is the number of iterations including initial points for each round. For example, if we run 50 iterations with 5 initial examples and repeat this procedure 3 times, r would be 3 and t would be 55 (= 50 + 5).
- **num_init** (*int.*) – the number of initial points.

Returns tuple of accumulated minima, their arithmetic means over rounds, and their standard deviations over rounds. Shape: ((r, t - *num_init* + 1), (t - *num_init* + 1,), (t - *num_init* + 1,)).

Return type (numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

`bayeso.utils.utils_common.`**`get_time`**(*time_all: numpy.ndarray, num_init: int, include_init: bool*) → numpy.ndarray

It returns the means of accumulated execution times over rounds.

Parameters

- **time_all** (*numpy.ndarray*) – execution times for all Bayesian optimization rounds. Shape: (r, t) where r is the number of Bayesian optimization rounds and t is the number of iterations (including initial points if *include_init* is True, or excluding them if *include_init* is False) for each round.
- **num_init** (*int.*) – the number of initial points. If *include_init* is False, it is ignored even if it is provided.
- **include_init** (*bool.*) – flag for describing whether execution times to observe initial examples have been included or not.

Returns arithmetic means of accumulated execution times over rounds. Shape: (t - *num_init*,) if *include_init* is True. (t,), otherwise.

Return type numpy.ndarray

Raises AssertionError

bayeso.utils.utils_common.**validate_types**(*func: Callable*) → Callable

It is a decorator for validating the number of types, which are declared for typing.

Parameters **func** (*callable*) – an original function.

Returns a callable decorator.

Return type callable

Raises AssertionError

13.3 bayeso.utils.utils_covariance

It is utilities for covariance functions.

bayeso.utils.utils_covariance.**_get_list_first**() → List[str]

It provides list of strings. The strings in that list require two hyperparameters, *signal* and *lengthscales*. We simply call it as *list_first*.

Returns list of strings, which satisfy some requirements we mentioned above.

Return type list

bayeso.utils.utils_covariance.**check_str_cov**(*str_fun: str*, *str_cov: str*, *shape_X1: tuple*, *shape_X2: tuple = None*) → None

It is for validating the shape of X1 (and optionally the shape of X2).

Parameters

- **str_fun** (*str.*) – the name of function.
- **str_cov** (*str.*) – the name of covariance function.
- **shape_X1** (*tuple*) – the shape of X1.
- **shape_X2** (*NoneType or tuple, optional*) – None, or the shape of X2.

Returns None, if it is valid. Raise an error, otherwise.

Return type NoneType

Raises AssertionError, ValueError

bayeso.utils.utils_covariance.**convert_hyps**(*str_cov: str*, *hyps: dict*, *use_gp: bool = True*, *fix_noise: bool = False*) → numpy.ndarray

It converts hyperparameters dictionary, *hyps* to numpy array.

Parameters

- **str_cov** (*str.*) – the name of covariance function.
- **hyps** (*dict.*) – dictionary of hyperparameters for covariance function.
- **use_gp** (*bool., optional*) – flag for Gaussian process or Student-t process.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.

Returns converted array of the hyperparameters given by *hyps*.

Return type numpy.ndarray

Raises AssertionError

bayeso.utils.utils_covariance.**get_hyps**(*str_cov: str*, *dim: int*, *use_gp: bool = True*, *use_ard: bool = True*) → dict

It returns a dictionary of default hyperparameters for covariance function, where *str_cov* and *dim* are given. If *use_ard* is True, the length scales would be *dim*-dimensional vector.

Parameters

- **str_cov** (*str.*) – the name of covariance function.
- **dim** (*int.*) – dimensionality of the problem we are solving.
- **use_gp** (*bool., optional*) – flag for Gaussian process or Student-t process.
- **use_ard** (*bool., optional*) – flag for automatic relevance determination.

Returns dictionary of default hyperparameters for covariance function.

Return type dict.

Raises AssertionError

bayeso.utils.utils_covariance.**get_range_hyps**(*str_cov: str*, *dim: int*, *use_gp: bool = True*, *use_ard: bool = True*, *fix_noise: bool = False*) → List[list]

It returns default optimization ranges of hyperparameters for Gaussian process regression.

Parameters

- **str_cov** (*str.*) – the name of covariance function.
- **dim** (*int.*) – dimensionality of the problem we are solving.
- **use_gp** (*bool., optional*) – flag for Gaussian process or Student-t process.
- **use_ard** (*bool., optional*) – flag for automatic relevance determination.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.

Returns list of default optimization ranges for hyperparameters.

Return type list

Raises AssertionError

bayeso.utils.utils_covariance.**restore_hyps**(*str_cov: str*, *hyps: numpy.ndarray*, *use_gp: bool = True*, *use_ard: bool = True*, *fix_noise: bool = False*, *noise: float = 0.01*) → dict

It restores hyperparameters array, *hyps* to dictionary.

Parameters

- **str_cov** (*str.*) – the name of covariance function.
- **hyps** (*numpy.ndarray*) – array of hyperparameters for covariance function.

- **use_gp** (*bool., optional*) – flag for Gaussian process or Student-t process.
- **use_ard** (*bool., optional*) – flag for using automatic relevance determination.
- **fix_noise** (*bool., optional*) – flag for fixing a noise.
- **noise** (*float, optional*) – fixed noise value.

Returns restored dictionary of the hyperparameters given by *hyps*.

Return type dict.

Raises AssertionError

bayeso.utils.utils_covariance.**validate_hyps_arr**(*hyps: numpy.ndarray, str_cov: str, dim: int, use_gp: bool = True*) → Tuple[numpy.ndarray, bool]

It validates hyperparameters array, *hyps*.

Parameters

- **hyps** (*numpy.ndarray*) – array of hyperparameters for covariance function.
- **str_cov** (*str.*) – the name of covariance function.
- **dim** (*int.*) – dimensionality of the problem we are solving.
- **use_gp** (*bool., optional*) – flag for Gaussian process or Student-t process.

Returns a tuple of valid hyperparameters and validity flag.

Return type (numpy.ndarray, bool.)

Raises AssertionError

bayeso.utils.utils_covariance.**validate_hyps_dict**(*hyps: dict, str_cov: str, dim: int, use_gp: bool = True*) → Tuple[dict, bool]

It validates hyperparameters dictionary, *hyps*.

Parameters

- **hyps** (*dict.*) – dictionary of hyperparameters for covariance function.
- **str_cov** (*str.*) – the name of covariance function.
- **dim** (*int.*) – dimensionality of the problem we are solving.
- **use_gp** (*bool., optional*) – flag for Gaussian process or Student-t process.

Returns a tuple of valid hyperparameters and validity flag.

Return type (dict., bool.)

Raises AssertionError

13.4 bayeso.utils.utils_gp

It is utilities for Gaussian process regression and Student-t process regression.

bayeso.utils.utils_gp.**get_prior_mu**(*prior_mu: Optional[Callable], X: numpy.ndarray*) → numpy.ndarray

It computes the prior mean function values over inputs X.

Parameters

- **prior_mu** (*function or NoneType*) – prior mean function or None.
- **X** (*numpy.ndarray*) – inputs for prior mean function. Shape: (n, d) or (n, m, d).

Returns zero array, or array of prior mean function values. Shape: (n, 1).

Return type numpy.ndarray

Raises AssertionError

bayeso.utils.utils_gp.**validate_common_args**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, str_cov: str, prior_mu: Optional[Callable], debug: bool, X_test: Optional[numpy.ndarray] = None*) → None

It validates the common arguments for various functions.

Parameters

- **X_train** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – outputs. Shape: (n, 1).
- **str_cov** (*str.*) – the name of covariance function.
- **prior_mu** (*NoneType, or function*) – None, or prior mean function.
- **debug** (*bool.*) – flag for printing log messages.
- **X_test** (*numpy.ndarray, or NoneType, optional*) – inputs or None. Shape: (l, d) or (l, m, d).

Returns None.

Return type NoneType

Raises AssertionError

13.5 bayeso.utils.utils_logger

It is utilities for loggers.

bayeso.utils.utils_logger.**get_logger**(*str_name: str*) → logging.Logger

It returns a logger to record the messages generated in our package.

Parameters **str_name** (*str.*) – a logger name.

Returns a logger.

Return type logging.Logger

Raises AssertionError

bayeso.utils.utils_logger.**get_str_array**(*arr: numpy.ndarray*) → str

It converts an array into string. It can take one-dimensional, two-dimensional, and three-dimensional arrays.

Parameters **arr** (*numpy.ndarray*) – an array to be converted.

Returns a string.

Return type str.

Raises AssertionError

bayeso.utils.utils_logger.**get_str_array_1d**(*arr: numpy.ndarray*) → str

It converts a one-dimensional array into string.

Parameters **arr** (*numpy.ndarray*) – an array to be converted.

Returns a string.

Return type str.

Raises AssertionError

`bayeso.utils.utils_logger.`**`get_str_array_2d`**(*arr: numpy.ndarray*) → str

It converts a two-dimensional array into string.

Parameters **arr** (*numpy.ndarray*) – an array to be converted.

Returns a string.

Return type str.

Raises AssertionError

`bayeso.utils.utils_logger.`**`get_str_array_3d`**(*arr: numpy.ndarray*) → str

It converts a three-dimensional array into string.

Parameters **arr** (*numpy.ndarray*) – an array to be converted.

Returns a string.

Return type str.

Raises AssertionError

`bayeso.utils.utils_logger.`**`get_str_hyps`**(*hyps: dict*) → str

It converts a dictionary of hyperparameters into string.

Parameters **hyps** (*dict.*) – a hyperparameter dictionary to be converted.

Returns a string.

Return type str.

Raises AssertionError

13.6 bayeso.utils.utils_plotting

It is utilities for plotting figures.

`bayeso.utils.utils_plotting.`**`_save_figure`**(*path_save: str*, *str_postfix: str*, *str_prefix: str = ''*) → None

It saves a figure.

Parameters

- **path_save** (*str.*) – path for saving a figure.
- **str_postfix** (*str.*) – the name of postfix.
- **str_prefix** (*str., optional*) – the name of prefix.

Returns None.

Return type NoneType

`bayeso.utils.utils_plotting.`**`_set_ax_config`**(*ax: matplotlib.axes._subplots.AxesSubplot, str_x_axis: str, str_y_axis: str, size_labels: int = 32, size_ticks: int = 22, xlim_min: Optional[float] = None, xlim_max: Optional[float] = None, draw_box: bool = True, draw_zero_axis: bool = False, draw_grid: bool = True*) → None

It sets an axis configuration.

Parameters

- **ax** (*matplotlib.axes._subplots.AxesSubplot*) – inputs for acquisition function. Shape: (n, d).
- **str_x_axis** (*str.*) – the name of x axis.
- **str_y_axis** (*str.*) – the name of y axis.
- **size_labels** (*int., optional*) – label size.
- **size_ticks** (*int., optional*) – tick size.
- **xlim_min** (*NoneType or float, optional*) – None, or minimum for x limit.
- **xlim_max** (*NoneType or float, optional*) – None, or maximum for x limit.
- **draw_box** (*bool., optional*) – flag for drawing a box.
- **draw_zero_axis** (*bool., optional*) – flag for drawing a zero axis.
- **draw_grid** (*bool., optional*) – flag for drawing grids.

Returns None.

Return type NoneType

`bayeso.utils.utils_plotting.`**`_set_font_config`**(*use_tex: bool*) → None

It sets a font configuration.

Parameters **use_tex** (*bool.*) – flag for using latex.

Returns None.

Return type NoneType

`bayeso.utils.utils_plotting.`**`_show_figure`**(*pause_figure: bool, time_pause: Union[int, float]*) → None

It shows a figure.

Parameters

- **pause_figure** (*bool.*) – flag for pausing before closing a figure.
- **time_pause** (*int. or float*) – pausing time.

Returns None.

Return type NoneType

`bayeso.utils.utils_plotting.`**`plot_bo_step`**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, X_test: numpy.ndarray, Y_test: numpy.ndarray, mean_test: numpy.ndarray, std_test: numpy.ndarray, path_save: Optional[str] = None, str_postfix: Optional[str] = None, str_x_axis: str = 'x', str_y_axis: str = 'y', num_init: Optional[int] = None, use_tex: bool = False, draw_zero_axis: bool = False, pause_figure: bool = True, time_pause: Union[int, float] = 2.0, range_shade: float = 1.96*) → None

It is for plotting Bayesian optimization results step by step.

Parameters

- **X_train** (*numpy.ndarray*) – training inputs. Shape: (n, 1).
- **Y_train** (*numpy.ndarray*) – training outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – test inputs. Shape: (m, 1).
- **Y_test** (*numpy.ndarray*) – true test outputs. Shape: (m, 1).
- **mean_test** (*numpy.ndarray*) – posterior predictive mean function values over *X_test*. Shape: (m, 1).
- **std_test** (*numpy.ndarray*) – posterior predictive standard deviation function values over *X_test*. Shape: (m, 1).
- **path_save** (*NoneType or str., optional*) – None, or path for saving a figure.
- **str_postfix** (*NoneType or str., optional*) – None, or the name of postfix.
- **str_x_axis** (*str., optional*) – the name of x axis.
- **str_y_axis** (*str., optional*) – the name of y axis.
- **num_init** (*NoneType or int., optional*) – None, or the number of initial examples.
- **use_tex** (*bool., optional*) – flag for using latex.
- **draw_zero_axis** (*bool., optional*) – flag for drawing a zero axis.
- **pause_figure** (*bool., optional*) – flag for pausing before closing a figure.
- **time_pause** (*int. or float, optional*) – pausing time.
- **range_shade** (*float, optional*) – shade range for standard deviation.

Returns None.

Return type NoneType

Raises AssertionError

bayeso.utils.utils_plotting.**plot_bo_step_with_acq**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, X_test: numpy.ndarray, Y_test: numpy.ndarray, mean_test: numpy.ndarray, std_test: numpy.ndarray, acq_test: numpy.ndarray, path_save: Optional[str] = None, str_postfix: Optional[str] = None, str_x_axis: str = 'x', str_y_axis: str = 'y', str_acq_axis: str = 'acq.', num_init: Optional[int] = None, use_tex: bool = False, draw_zero_axis: bool = False, pause_figure: bool = True, time_pause: Union[int, float] = 2.0, range_shade: float = 1.96*) → None

It is for plotting Bayesian optimization results step by step.

Parameters

- **X_train** (*numpy.ndarray*) – training inputs. Shape: (n, 1).
- **Y_train** (*numpy.ndarray*) – training outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – test inputs. Shape: (m, 1).
- **Y_test** (*numpy.ndarray*) – true test outputs. Shape: (m, 1).
- **mean_test** (*numpy.ndarray*) – posterior predictive mean function values over *X_test*. Shape: (m, 1).
- **std_test** (*numpy.ndarray*) – posterior predictive standard deviation function values over *X_test*. Shape: (m, 1).
- **acq_test** (*numpy.ndarray*) – acquisition funcion values over *X_test*. Shape: (m, 1).
- **path_save** (*NoneType or str., optional*) – None, or path for saving a figure.
- **str_postfix** (*NoneType or str., optional*) – None, or the name of postfix.
- **str_x_axis** (*str., optional*) – the name of x axis.
- **str_y_axis** (*str., optional*) – the name of y axis.
- **str_acq_axis** (*str., optional*) – the name of acquisition function axis.
- **num_init** (*NoneType or int., optional*) – None, or the number of initial examples.
- **use_tex** (*bool., optional*) – flag for using latex.
- **draw_zero_axis** (*bool., optional*) – flag for drawing a zero axis.
- **pause_figure** (*bool., optional*) – flag for pausing before closing a figure.
- **time_pause** (*int. or float, optional*) – pausing time.
- **range_shade** (*float, optional*) – shade range for standard deviation.

Returns None.

Return type NoneType

Raises AssertionError

bayeso.utils.utils_plotting.**plot_gp_via_distribution**(*X_train: numpy.ndarray, Y_train: numpy.ndarray, X_test: numpy.ndarray, mean_test: numpy.ndarray, std_test: numpy.ndarray, Y_test: Optional[numpy.ndarray] = None, path_save: Optional[str] = None, str_postfix: Optional[str] = None, str_x_axis: str = 'x', str_y_axis: str = 'y', use_tex: bool = False, draw_zero_axis: bool = False, pause_figure: bool = True, time_pause: Union[int, float] = 2.0, range_shade: float = 1.96, colors: numpy.ndarray = array(['red', 'green', 'blue', 'orange', 'olive', 'purple', 'darkred', 'limegreen', 'deepskyblue', 'lightsalmon', 'aquamarine', 'navy', 'rosybrown', 'darkkhaki', 'darkslategray'], dtype='<U13')*) → None

It is for plotting Gaussian process regression.

Parameters

- **X_train** (*numpy.ndarray*) – training inputs. Shape: (n, 1).
- **Y_train** (*numpy.ndarray*) – training outputs. Shape: (n, 1).
- **X_test** (*numpy.ndarray*) – test inputs. Shape: (m, 1).
- **mean_test** (*numpy.ndarray*) – posterior predictive mean function values over *X_test*. Shape: (m, 1).
- **std_test** (*numpy.ndarray*) – posterior predictive standard deviation function values over *X_test*. Shape: (m, 1).
- **Y_test** (*NoneType or numpy.ndarray, optional*) – None, or true test outputs. Shape: (m, 1).
- **path_save** (*NoneType or str., optional*) – None, or path for saving a figure.
- **str_postfix** (*NoneType or str., optional*) – None, or the name of postfix.
- **str_x_axis** (*str., optional*) – the name of x axis.
- **str_y_axis** (*str., optional*) – the name of y axis.
- **use_tex** (*bool., optional*) – flag for using latex.
- **draw_zero_axis** (*bool., optional*) – flag for drawing a zero axis.
- **pause_figure** (*bool., optional*) – flag for pausing before closing a figure.
- **time_pause** (*int. or float, optional*) – pausing time.
- **range_shade** (*float, optional*) – shade range for standard deviation.
- **colors** (*np.ndarray, optional*) – array of colors.

Returns None.

Return type NoneType

Raises AssertionError

`bayeso.utils.utils_plotting.`**`plot_gp_via_sample`**(*X: numpy.ndarray, Ys: numpy.ndarray, path_save: Optional[str] = None, str_postfix: Optional[str] = None, str_x_axis: str = 'x', str_y_axis: str = 'y', use_tex: bool = False, draw_zero_axis: bool = False, pause_figure: bool = True, time_pause: Union[int, float] = 2.0, colors: numpy.ndarray = array(['red', 'green', 'blue', 'orange', 'olive', 'purple', 'darkred', 'limegreen', 'deepskyblue', 'lightsalmon', 'aquamarine', 'navy', 'rosybrown', 'darkkhaki', 'darkslategray'], dtype='<U13')*) → None

It is for plotting sampled functions from multivariate distributions.

Parameters

- **X** (*numpy.ndarray*) – training inputs. Shape: (n, 1).
- **Ys** (*numpy.ndarray*) – training outputs. Shape: (m, n).
- **path_save** (*NoneType or str., optional*) – None, or path for saving a figure.
- **str_postfix** (*NoneType or str., optional*) – None, or the name of postfix.
- **str_x_axis** (*str., optional*) – the name of x axis.
- **str_y_axis** (*str., optional*) – the name of y axis.
- **use_tex** (*bool., optional*) – flag for using latex.
- **draw_zero_axis** (*bool., optional*) – flag for drawing a zero axis.
- **pause_figure** (*bool., optional*) – flag for pausing before closing a figure.
- **time_pause** (*int. or float, optional*) – pausing time.
- **colors** (*np.ndarray, optional*) – array of colors.

Returns None.

Return type NoneType

Raises AssertionError

`bayeso.utils.utils_plotting.`**`plot_minimum_vs_iter`**(*minima: numpy.ndarray, list_str_label: List[str], num_init: int, draw_std: bool, include_marker: bool = True, include_legend: bool = False, use_tex: bool = False, path_save: Optional[str] = None, str_postfix: Optional[str] = None, str_x_axis: str = 'Iteration', str_y_axis: str = 'Minimum function value', pause_figure: bool = True, time_pause: Union[int, float] = 2.0, range_shade: float = 1.96, markers: numpy.ndarray = array(['.', 'x', '*', '+', '^', 'v', '<', '>', 'd', ',', '8', 'h', '1', '2', '3'], dtype='<U1'), colors: numpy.ndarray = array(['red', 'green', 'blue', 'orange', 'olive', 'purple', 'darkred', 'limegreen', 'deepskyblue', 'lightsalmon', 'aquamarine', 'navy', 'rosybrown', 'darkkhaki', 'darkslategray'], dtype='<U13')*) → None

It is for plotting optimization results of Bayesian optimization, in terms of iterations.

Parameters

- **minima** (*numpy.ndarray*) – function values over acquired examples. Shape: (b, r, n) where b is the number of experiments, r is the number of rounds, and n is the number of iterations per round.
- **list_str_label** (*list*) – list of label strings. Shape: (b,).
- **num_init** (*int.*) – the number of initial examples < n.
- **draw_std** (*bool.*) – flag for drawing standard deviations.
- **include_marker** (*bool., optional*) – flag for drawing markers.
- **include_legend** (*bool., optional*) – flag for drawing a legend.
- **use_tex** (*bool., optional*) – flag for using latex.
- **path_save** (*NoneType or str., optional*) – None, or path for saving a figure.
- **str_postfix** (*NoneType or str., optional*) – None, or the name of postfix.
- **str_x_axis** (*str., optional*) – the name of x axis.
- **str_y_axis** (*str., optional*) – the name of y axis.
- **pause_figure** (*bool., optional*) – flag for pausing before closing a figure.
- **time_pause** (*int. or float, optional*) – pausing time.
- **range_shade** (*float, optional*) – shade range for standard deviation.
- **markers** (*np.ndarray, optional*) – array of markers.
- **colors** (*np.ndarray, optional*) – array of colors.

Returns None.

Return type NoneType

Raises AssertionError

`bayeso.utils.utils_plotting.`**`plot_minimum_vs_time`**(*times: numpy.ndarray, minima: numpy.ndarray, list_str_label: List[str], num_init: int, draw_std: bool, include_marker: bool = True, include_legend: bool = False, use_tex: bool = False, path_save: Optional[str] = None, str_postfix: Optional[str] = None, str_x_axis: str = 'Time (sec.)', str_y_axis: str = 'Minimum function value', pause_figure: bool = True, time_pause: Union[int, float] = 2.0, range_shade: float = 1.96, markers: numpy.ndarray = array(['.', 'x', '*', '+', '^', 'v', '<', '>', 'd', ',', '8', 'h', '1', '2', '3'], dtype='<U1'), colors: numpy.ndarray = array(['red', 'green', 'blue', 'orange', 'olive', 'purple', 'darkred', 'limegreen', 'deepskyblue', 'lightsalmon', 'aquamarine', 'navy', 'rosybrown', 'darkkhaki', 'darkslategray'], dtype='<U13')*) → None

It is for plotting optimization results of Bayesian optimization, in terms of execution time.

Parameters

- **`times`** (*`numpy.ndarray`*) – execution times. Shape: (b, r, n), or (b, r, *num_init* + n) where b is the number of experiments, r is the number of rounds, and n is the number of iterations per round.
- **`minima`** (*`numpy.ndarray`*) – function values over acquired examples. Shape: (b, r, *num_init* + n) where b is the number of experiments, r is the number of rounds, and n is the number of iterations per round.
- **`list_str_label`** (*`list`*) – list of label strings. Shape: (b,).
- **`num_init`** (*`int.`*) – the number of initial examples.
- **`draw_std`** (*`bool.`*) – flag for drawing standard deviations.
- **`include_marker`** (*`bool., optional`*) – flag for drawing markers.
- **`include_legend`** (*`bool., optional`*) – flag for drawing a legend.
- **`use_tex`** (*`bool., optional`*) – flag for using latex.
- **`path_save`** (*`NoneType or str., optional`*) – None, or path for saving a figure.
- **`str_postfix`** (*`NoneType or str., optional`*) – None, or the name of postfix.
- **`str_x_axis`** (*`str., optional`*) – the name of x axis.
- **`str_y_axis`** (*`str., optional`*) – the name of y axis.
- **`pause_figure`** (*`bool., optional`*) – flag for pausing before closing a figure.
- **`time_pause`** (*`int. or float, optional`*) – pausing time.
- **`range_shade`** (*`float, optional`*) – shade range for standard deviation.

- **markers** (*np.ndarray, optional*) – array of markers.
- **colors** (*np.ndarray, optional*) – array of colors.

Returns None.

Return type NoneType

Raises AssertionError

CHAPTER 14

bayeso.wrappers

These files are for implementing various wrappers.

14.1 bayeso.wrappers.wrappers_bo_class

It defines a wrapper class for Bayesian optimization.

class bayeso.wrappers.wrappers_bo_class.**BayesianOptimization**(*range_X: numpy.ndarray, fun_target: Callable, num_iter: int, str_surrogate: str = 'gp', str_cov: str = 'matern52', str_acq: str = 'ei', normalize_Y: bool = True, use_ard: bool = True, prior_mu: Optional[Callable] = None, str_initial_method_bo: str = 'sobol', str_sampling_method_ao: str = 'sobol', str_optimizer_method_gp: str = 'BFGS', str_optimizer_method_tp: str = 'SLSQP', str_optimizer_method_bo: str = 'L-BFGS-B', str_mlm_method: str = 'regular', str_modelselection_method: str = 'ml', num_samples_ao: int = 100, debug: bool = False*)

Bases: `object`

It is a wrapper class for Bayesian optimization. A function for optimizing *fun_target* runs a single round of Bayesian optimization with an iteration budget *num_iter*.

Parameters

- **range_X** (*numpy.ndarray*) – a search space. Shape: (d, 2).
- **fun_target** (*callable*) – a target function.
- **num_iter** (*int.*) – an iteration budget for Bayesian optimization.
- **str_surrogate** (*str., optional*) – the name of surrogate model.
- **str_cov** (*str., optional*) – the name of covariance function.
- **str_acq** (*str., optional*) – the name of acquisition function.
- **normalize_Y** (*bool., optional*) – a flag for normalizing outputs.
- **use_ard** (*bool., optional*) – a flag for automatic relevance determination.
- **prior_mu** (*NoneType, or callable, optional*) – None, or a prior mean function.
- **str_initial_method_bo** (*str., optional*) – the name of initialization method for sampling initial examples in Bayesian optimization.

- **str_sampling_method_ao** (*str., optional*) – the name of sampling method for acquisition function optimization.
- **str_optimizer_method_gp** (*str., optional*) – the name of optimization method for Gaussian process regression.
- **str_optimizer_method_bo** (*str., optional*) – the name of optimization method for Bayesian optimization.
- **str_mlm_method** (*str., optional*) – the name of marginal likelihood maximization method for Gaussian process regression.
- **str_modelselection_method** (*str., optional*) – the name of model selection method for Gaussian process regression.
- **num_samples_ao** (*int., optional*) – the number of samples for acquisition function optimization. If a local search method (e.g., L-BFGS-B) is selected for acquisition function optimization, it is employed.
- **debug** (*bool., optional*) – a flag for printing log messages.

_get_model_bo_gp()

It returns an object of *bayeso.bo.bo_w_gp.BO_w_GP*.

Returns an object of Bayesian optimization.

Return type *bayeso.bo.bo_w_gp.BOwGP*

_get_model_bo_tp()

It returns an object of *bayeso.bo.bo_w_tp.BO_w_TP*.

Returns an object of Bayesian optimization.

Return type *bayeso.bo.bo_w_tp.BOwTP*

_get_model_bo_trees()

It returns an object of *bayeso.bo.bo_w_trees.BO_w_Trees*.

Returns an object of Bayesian optimization.

Return type *bayeso.bo.bo_w_trees.BOwTrees*

_get_next_best_sample(*next_sample: numpy.ndarray, X: numpy.ndarray, next_samples: numpy.ndarray, acq_vals: numpy.ndarray*) → numpy.ndarray

It returns the next best sample in terms of acquisition function values.

Parameters

- **next_sample** (*np.ndarray*) – the next sample acquired.
- **X** (*np.ndarray*) – the samples evaluated so far.
- **next_samples** (*np.ndarray*) – the candidates of the next sample.
- **acq_vals** (*np.ndarray*) – the values of acquisition function over *next_samples*.

Returns the next best sample. Shape: (d,).

Return type numpy.ndarray

Raises AssertionError

optimize(*num_init: int, seed: Optional[int] = None*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray]

It returns the optimization results and times consumed, given the number of initial samples *num_init* and a random seed *seed*.

Parameters

- **num_init** (*int.*) – the number of initial samples.
- **seed** (*NoneType or int., optional*) – None, or a random seed.

Returns a tuple of acquired samples, their function values, overall times consumed per iteration, time consumed in modeling Gaussian process regression, and time consumed in acquisition function optimization. Shape: ((*num_init* + *num_iter*, d), (*num_init* + *num_iter*, 1), (*num_init* + *num_iter*,), (*num_iter*,), (*num_iter*,)), or ((*num_init* + *num_iter*, m, d), (*num_init* + *num_iter*, m, 1), (*num_init* + *num_iter*,), (*num_iter*,), (*num_iter*,)), where d is a dimensionality of the problem we are solving and m is a cardinality of sets.

Return type (numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

optimize_single_iteration(*X: numpy.ndarray*, *Y: numpy.ndarray*) → Tuple[numpy.ndarray, dict]

It returns the optimization result and time consumed of single iteration, given *X* and *Y*.

Parameters

- **X** (*numpy.ndarray*) – inputs. Shape: (n, d) or (n, m, d).
- **Y** (*numpy.ndarray*) – outputs. Shape: (n, 1).

Returns a tuple of the next sample and information dictionary.

Return type (numpy.ndarray, dict.)

Raises AssertionError, NotImplementedError

optimize_with_all_initial_information(*X: numpy.ndarray*, *Y: numpy.ndarray*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray]

It returns the optimization results and times consumed, given inital inputs *X* and their corresponding outputs *Y*.

Parameters

- **X** (*numpy.ndarray*) – initial inputs. Shape: (n, d) or (n, m, d).
- **Y** (*numpy.ndarray*) – initial outputs. Shape: (n, 1).

Returns a tuple of acquired samples, their function values, overall times consumed per iteration, time consumed in modeling Gaussian process regression, and time consumed in acquisition function optimization. Shape: ((n + *num_iter*, d), (n + *num_iter*, 1), (*num_iter*,), (*num_iter*,), (*num_iter*,)), or ((n + *num_iter*, m, d), (n + *num_iter*, m, 1), (*num_iter*,), (*num_iter*,), (*num_iter*,)).

Return type (numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

optimize_with_initial_inputs(*X: numpy.ndarray*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray]

It returns the optimization results and times consumed, given inital inputs *X*.

Parameters **X** (*numpy.ndarray*) – initial inputs. Shape: (n, d) or (n, m, d).

Returns a tuple of acquired samples, their function values, overall times consumed per iteration, time consumed in modeling Gaussian process regression, and time consumed in acquisition function optimization. Shape: ((n + *num_iter*, d), (n + *num_iter*, 1), (n + *num_iter*,),

(*num_iter*,), (*num_iter*,)), or ((n + *num_iter*, m, d), (n + *num_iter*, m, 1), (n + *num_iter*,), (*num_iter*,), (*num_iter*,)).

Return type (numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

print_info(*num_init*, *seed*)

14.2 bayeso.wrappers.wrappers_bo_function

It defines wrappers for Bayesian optimization.

bayeso.wrappers.wrappers_bo_function.**run_single_round**(*model_bo: bayeso.bo.bo_w_gp.BOwGP*, *fun_target: Callable*, *num_init: int*, *num_iter: int*, *str_initial_method_bo: str = 'sobol'*, *str_sampling_method_ao: str = 'sobol'*, *num_samples_ao: int = 100*, *str_mlm_method: str = 'regular'*, *seed: Optional[int] = None*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray]

It optimizes *fun_target* for *num_iter* iterations with given *model_bo* and *num_init* initial examples. Initial examples are sampled by *get_initials* method in *model_bo*. It returns the optimization results and execution times.

Parameters

- **model_bo** (*bayeso.bo.BO*) – Bayesian optimization model.
- **fun_target** (*callable*) – a target function.
- **num_init** (*int.*) – the number of initial examples for Bayesian optimization.
- **num_iter** (*int.*) – the number of iterations for Bayesian optimization.
- **str_initial_method_bo** (*str., optional*) – the name of initialization method for sampling initial examples in Bayesian optimization.
- **str_sampling_method_ao** (*str., optional*) – the name of initialization method for acquisition function optimization.
- **num_samples_ao** (*int., optional*) – the number of samples for acquisition function optimization. If L-BFGS-B is used as an acquisition function optimization method, it is employed.
- **str_mlm_method** (*str., optional*) – the name of marginal likelihood maximization method for Gaussian process regression.
- **seed** (*NoneType or int., optional*) – None, or random seed.

Returns tuple of acquired examples, their function values, overall execution times per iteration, execution time consumed in Gaussian process regression, and execution time consumed in acquisition function optimization. Shape: ((*num_init* + *num_iter*, d), (*num_init* + *num_iter*, 1),

(*num_init* + *num_iter*,), (*num_iter*,), (*num_iter*,)), or ((*num_init* + *num_iter*, m, d), (*num_init* + *num_iter*, m, 1), (*num_init* + *num_iter*,), (*num_iter*,), (*num_iter*,)), where d is a dimensionality of the problem we are solving and m is a cardinality of sets.

Return type (numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

`bayeso.wrappers.wrappers_bo_function.`**`run_single_round_with_all_initial_information`**(*model_bo: bayeso.bo.l fun_target: Callable, X_train: numpy.nda Y_train: numpy.nda num_iter: int, str_sampli str = 'sobol', num_samp int = 100, str_mlm_m str = 'regular'*) → Tuple[numpy. numpy.nda numpy.nda numpy.nda numpy.nda

It optimizes *fun_target* for *num_iter* iterations with given *model_bo*. It returns the optimization results and execution times.

Parameters

- **model_bo** (*bayeso.bo.BO*) – Bayesian optimization model.
- **fun_target** (*callable*) – a target function.
- **X_train** (*numpy.ndarray*) – initial inputs. Shape: (n, d) or (n, m, d).
- **Y_train** (*numpy.ndarray*) – initial outputs. Shape: (n, 1).
- **num_iter** (*int.*) – the number of iterations for Bayesian optimization.
- **str_sampling_method_ao** (*str., optional*) – the name of initialization method for acquisition function optimization.
- **num_samples_ao** (*int., optional*) – the number of samples for acquisition function optimization. If L-BFGS-B is used as an acquisition function optimization method, it is employed.

- **str_mlm_method** (*str., optional*) – the name of marginal likelihood maximization method for Gaussian process regression.

Returns tuple of acquired examples, their function values, overall execution times per iteration, execution time consumed in Gaussian process regression, and execution time consumed in acquisition function optimization. Shape: ((n + *num_iter*, d), (n + *num_iter*, 1), (*num_iter*,), (*num_iter*,), (*num_iter*,)), or ((n + *num_iter*, m, d), (n + *num_iter*, m, 1), (*num_iter*,), (*num_iter*,), (*num_iter*,)).

Return type (numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

bayeso.wrappers.wrappers_bo_function.**run_single_round_with_initial_inputs**(*model_bo: bayeso.bo.bo_w_gp.BOw fun_target: Callable, X_train: numpy.ndarray, num_iter: int, str_sampling_method_ao: str = 'sobol', num_samples_ao: int = 100, str_mlm_method: str = 'regular'*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray]

It optimizes *fun_target* for *num_iter* iterations with given *model_bo* and initial inputs *X_train*. It returns the optimization results and execution times.

Parameters

- **model_bo** (*bayeso.bo.BO*) – Bayesian optimization model.
- **fun_target** (*callable*) – a target function.
- **X_train** (*numpy.ndarray*) – initial inputs. Shape: (n, d) or (n, m, d).
- **num_iter** (*int.*) – the number of iterations for Bayesian optimization.
- **str_sampling_method_ao** (*str., optional*) – the name of initialization method for acquisition function optimization.
- **num_samples_ao** (*int., optional*) – the number of samples for acquisition function optimization. If L-BFGS-B is used as an acquisition function optimization method, it

is employed.

- **str_mlm_method** (*str., optional*) – the name of marginal likelihood maximization method for Gaussian process regression.

Returns tuple of acquired examples, their function values, overall execution times per iteration, execution time consumed in Gaussian process regression, and execution time consumed in acquisition function optimization. Shape: ((n + *num_iter*, d), (n + *num_iter*, 1), (n + *num_iter*,), (*num_iter*,), (*num_iter*,)), or ((n + *num_iter*, m, d), (n + *num_iter*, m, 1), (n + *num_iter*,), (*num_iter*,), (*num_iter*,)).

Return type (numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray, numpy.ndarray)

Raises AssertionError

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