Bayesian optimization

- Mainly used for optimization of "heavy" functions (computationally complex, expensive to evaluate)
- The objective function can be "black box"
- Uses approximation of the objective function
- Takes into account quality of the approximation

Optimization procedure:

1. Build approximation $\hat{f}(x)$ of function $f(x)$
2. Choose new point as an argmax of the criterion
$$x_{new} = \arg\max_x a(x)$$
3. Evaluate $f(x)$ at new point
4. Update model $\hat{f}(x)$ and go to step 2.

Expected Improvement

$$EI(x) = \mathbb{E}_{p(\hat{f})}\left[\max(0, y_{min} - \hat{f})\right]$$

where $\hat{y}, \sigma$ - mean and variance of GP model at point x, $\Phi(\cdot)$ - cdf of standard normal distribution, $\phi(\cdot)$ - pdf of standard normal distribution.

Usually logarithm of EI is used.

Task 1 (5 points)

Derive expression for EI: express it in terms of $\Phi(\cdot)$ and $\phi(\cdot)$ - cdf and pdf of $\mathcal{N}(0, 1)$.

$$EI(x) = \mathbb{E}_{p(\hat{f})}\left[\max(0, y_{min} - \hat{f})\right] = \int_{-\infty}^{y_{min}} (y_{min} - \hat{y}) \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\hat{y} - \mu)^2}{2\sigma^2}\right) d\hat{y} =$$

$$= \left| t = \frac{\hat{y} - \mu}{\sigma}, \quad z = \frac{y_{min} - \mu}{\sigma} \right| =$$

$$= \int_{-\infty}^{z} (y_{min} - \mu - \sigma t)\sigma \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{t^2}{2}\right) dt =$$

$$\int_{-\infty}^{z} (y_{min} - \mu - \sigma t)\phi(t) dt =$$

$$= (y_{min} - \mu) \int_{-\infty}^{z} \phi(t) dt - \sigma \int_{-\infty}^{z} t\phi(t) dt$$

$$= (y_{min} - \mu)\Phi(z) - \sigma \int_{-\infty}^{z} t\phi(t) dt =$$

$$= (y_{min} - \mu)\Phi(z) - \sigma \int_{-\infty}^{z} \frac{t}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) dt =$$

$$= (y_{min} - \mu)\Phi(z) - \sigma \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) d\left(\frac{t^2}{2}\right) =$$

$$= (y_{min} - \mu)\Phi(z) - \sigma - \frac{\exp\left(-\frac{t^2}{2}\right)}{\sqrt{2\pi}} \Bigg|_{-\infty}^{z} =$$

$$= (y_{min} - \mu)\Phi(z) + \sigma\phi(z) =$$

$$= (y_{min} - \mu)\Phi\left(\frac{y_{min} - \mu}{\sigma}\right) + \sigma\phi\left(\frac{y_{min} - \mu}{\sigma}\right)$$

Optimization of criterion

Any optimization algorithm could be used.

In this seminar we will use multi-start with L-BFGS optimization algorithm

Multi-start procedure:

1. Generate initial set of points $x_1, \dots, x_n$. Calculate criterion at each point to obtain $(a(x_1), \dots, a(x_n))$.
2. Choose k points with smallest values of criterion.
3. Using each point as an initial point run the optimization algorithm (L-BFGS) and obtain k optimization results.
4. From all optimization results choose the best one.

L-BFGS

It's a quasi-Newton method of optimization and it is based on second order Taylor expansion

$$f(x_k + p) \approx f(x_k) + \nabla f^T(x_k)p + \frac{1}{2}p^T \mathbf{H} p$$

$$p = -\mathbf{H}^{-1} \nabla f^T(x_k) \approx -\mathbf{B}_k^{-1} \nabla f^T(x_k),$$

where $\mathbf{B}_k$ is an approximation of hessian $\mathbf{H}$.

Approximation $\mathbf{B}_k$ is updated at every step by the following rule:

$$\mathbf{B}_{k+1} = \mathbf{B}_k - \frac{\mathbf{B}_k s_k s_k^T \mathbf{B}_k}{s_k^T \mathbf{B}_k s_k} + \frac{y_k y_k^T}{y_k^T s_k},$$

where $s_k = x_{k+1} - x_k$, $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$.

In [1]:

```
%matplotlib inline

from __future__ import print_function

import numpy as np
from matplotlib import pyplot
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm
from scipy.optimize import minimize


import GPy

import bayes_opt


def f(x):
    return (6 * x - 2)**2 * np.sin(12 * x - 4)

def get_1d_data():
    np.random.seed(239)
    x_train = np.array([0.0, 0.58, 0.38, 0.95]).reshape(-1, 1)
    y_train = f(x_train)
    return x_train, y_train
```

In [2]:

```
x_train, y_train = get_1d_data()
kernel = GPy.kern.RBF(1, variance=0.5, lengthscale=0.2)
model = GPy.models.GPRegression(x_train, y_train, kernel)
model.optimize()
```

Out[2]:

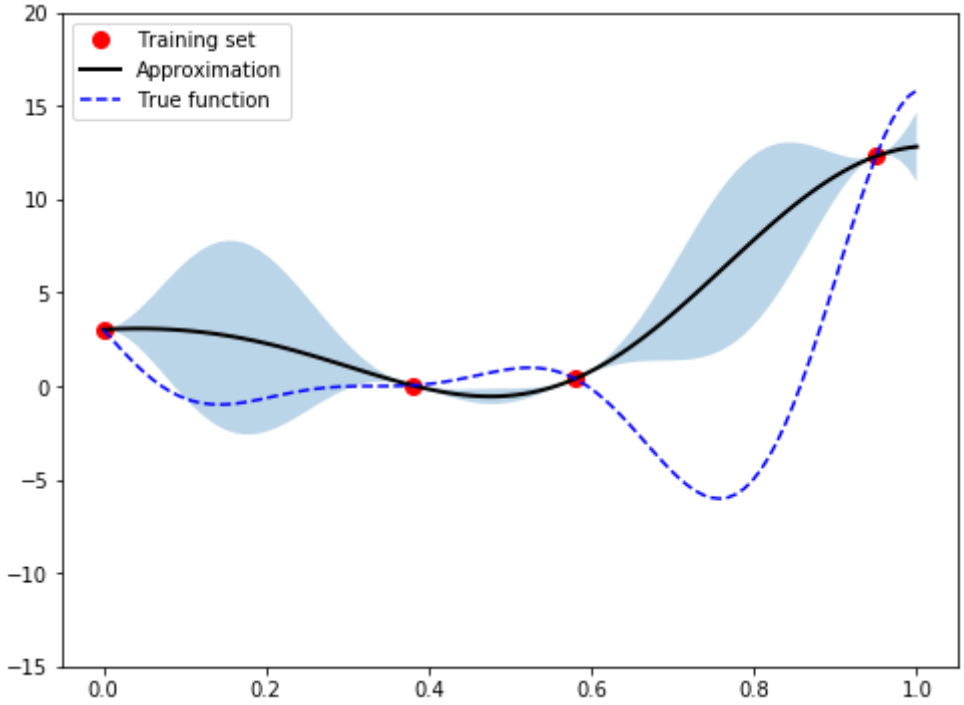
```
<paramz.optimization.optimization.opt_lbfgsb at 0x7f85bc263c88>
```

In [3]:

```
x_grid = np.linspace(0, 1, 100).reshape(-1, 1)
y_grid = f(x_grid)
prediction, std = model.predict(x_grid)
prediction = prediction.ravel()
std = std.ravel()
pyplot.figure(figsize=(8, 6))
pyplot.plot(x_train, y_train, 'or', markersize=8, label='Training set')
pyplot.plot(x_grid, prediction, '-k', linewidth=2, label='Approximation')
pyplot.fill_between(x_grid.ravel(), prediction - 2 * std, prediction + 2 * std, alp
pyplot.plot(x_grid, y_grid, '--b', label='True function')
pyplot.ylim([-15, 20])
pyplot.legend(loc='best')
```

Out[3]:

```
<matplotlib.legend.Legend at 0x7f8593813ac8>
```



Task 2 (5 points)

Implement multi-start optimization procedure

In [4]:

```
def get_new_point(model, lb, ub, data=None, multistart=10, criterion='ei', k=1, ran
    """
    Parameters:
        model - GP model of the objective function
        lb, ub - array-like, lower and upper bounds of x
        data - tuple(x_train, y_train)
        multistart - number of multistart runs
        criterion - aqcuisition function, by default EI
        k - parameter of the LowerConfidenceBound function
        random_state - np.random.RandomState
    Returns
        tuple - argmin of the objective function and min value of the objective
    """
    if random_state is None:
        random_state = np.random.RandomState()

    lb = np.array(lb).reshape(1, -1)
    ub = np.array(ub).reshape(1, -1)

    # 1. Generate inital X points (number of points == multistart) in [lb, ub]


    x_random = random_state.uniform(lb, ub, size=(multistart, lb.shape[1]))


    ######## ########
    def objective(x):
        if x.ndim == 1:
            x = x.reshape(1, -1)
        mean_values, variance = model.predict(x)
        std_values = np.sqrt(variance)
        if criterion == 'ei':
            return -bayes_opt.log_expected_improvement(mean_values, std_values, dat
        elif criterion == 'lcb':
            return lcb(mean_values, std_values, params)
        else:
            raise NotImplementedError('Criterion is not implemented!')

    criterion_value = objective(x_random)

    # 2. From each points from x_random run L-BFGS optimization algorithm,
    #    choose the best result and return it
    #    Use function minimize: minimize(objective, x_init, method='L-BFGS-B',
    #                                    bounds=np.vstack((lb, ub)).T)
    #    it returns object with fields 'fun' - optimum function value, 'x' - argmin

    best_result = None
    best_value = np.inf

    for i in x_random:
        res = minimize(objective, i, method='L-BFGS-B', bounds=np.vstack((lb, ub)).
        if res['fun'] < best_value:
            best_result, best_value = res, res['fun']

    return best_result.x, best_result.fun
```

In [5]:

```
# Check your code
lb = [0]
ub = [1]
kernel = GPy.kern.RBF(1, variance=0.5, lengthscale=0.1)
model = GPy.models.GPRegression(x_train, y_train, kernel)
x_new, f_new = get_new_point(model, lb, ub, data=(x_train, y_train), random_state=n

assert(np.isclose(x_new, 0.29985639))
assert(np.isclose(f_new, 0.86480674))
print('Correct!')
```

```
Correct!
```

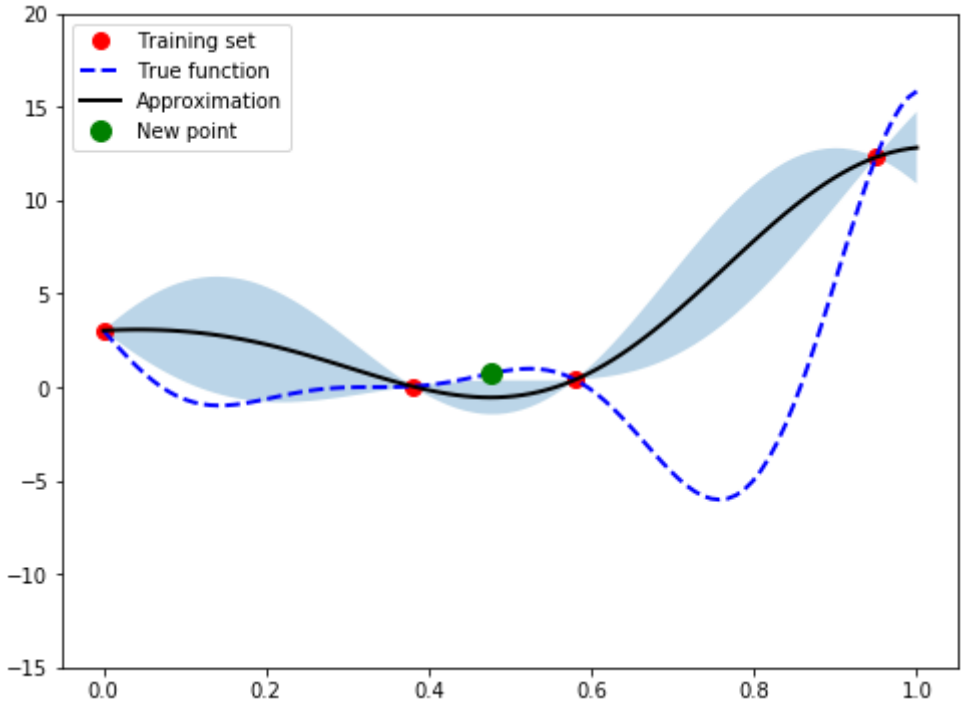
In [6]:

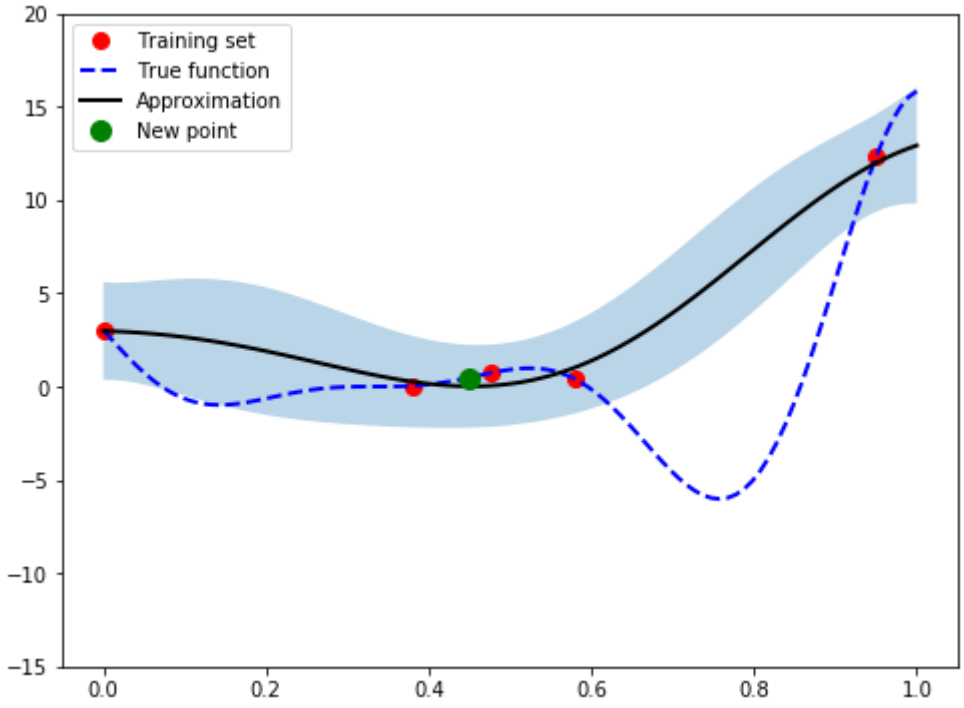
```
def optimization_step(x_train, y_train, kernel, objective, lb=None, ub=None, criter
    model = GPy.models.GPRegression(x_train, y_train, kernel)
    model.optimize_restarts(num_restarts=10, verbose=False)

    x_new, criterion_value = get_new_point(model, data=(x_train, y_train), lb=lb, u
    if plot:
        bayes_opt.plot1d(x_train, y_train, model, objective, x_new, criterion_value
        pyplot.show()

    x_new = x_new.reshape(1, -1)
    x_train = np.vstack([x_train, x_new])
    y_train = np.vstack([y_train, np.asarray(objective(x_new)).reshape(1, -1)])
    return x_train, y_train, model
```

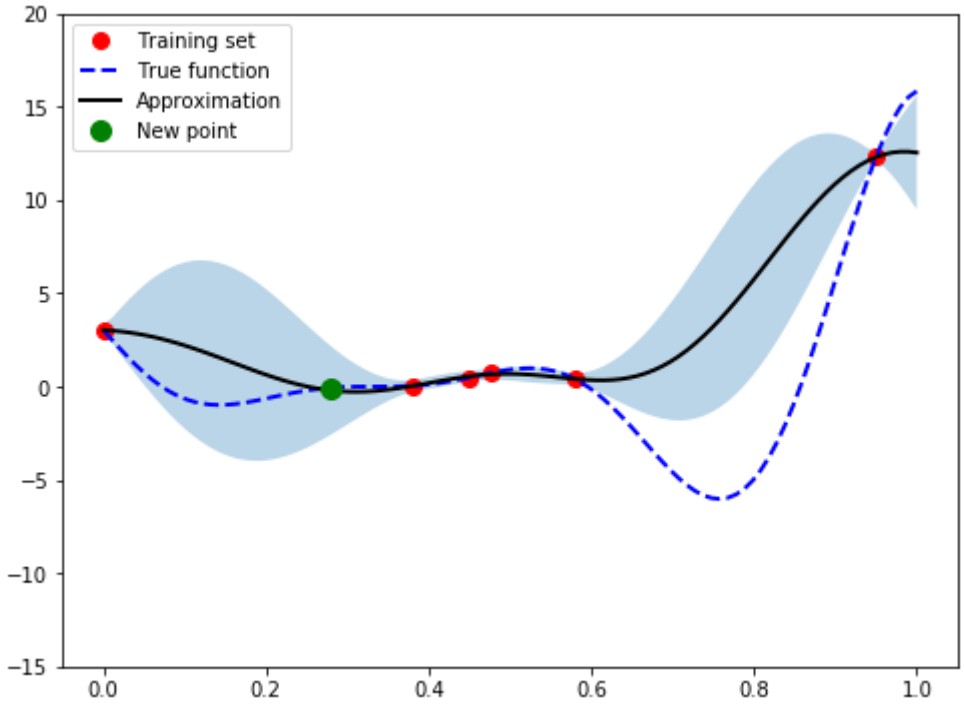
1D example

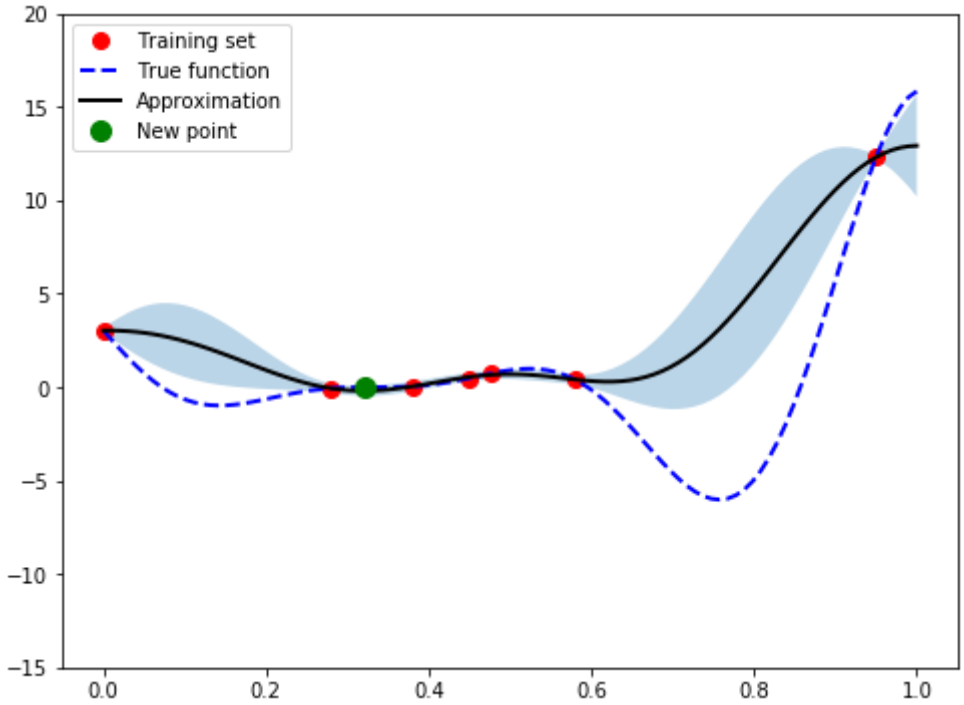
In [7]:

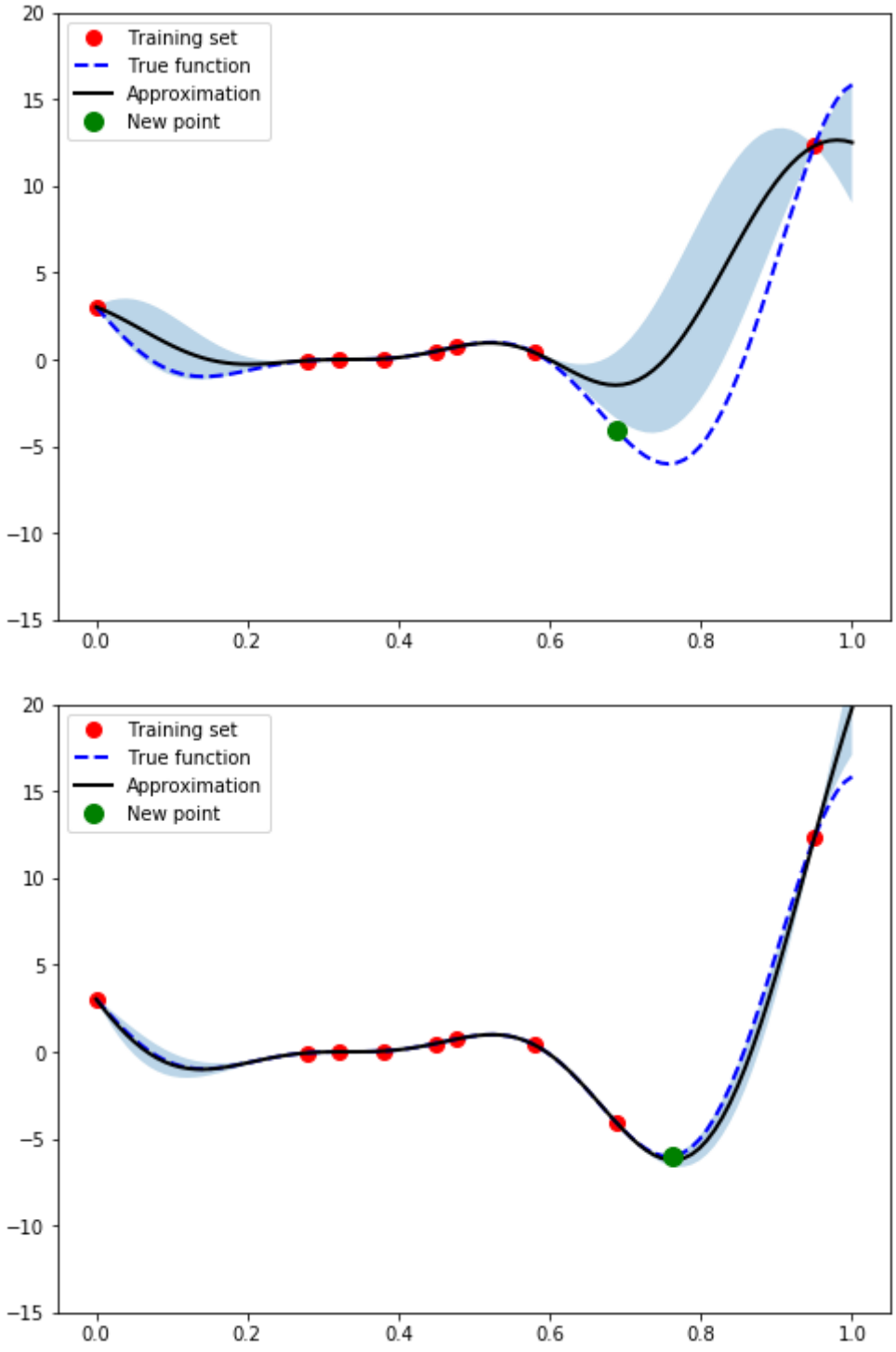
```
x_train, y_train = get_1d_data()
kernel = GPy.kern.RBF(1, variance=0.5, lengthscale=0.2)
model = GPy.models.GPRegression(x_train, y_train, kernel)
for i in range(6):
    x_train, y_train, model = bayes_opt.optimization_step(x_train, y_train, kernel,
```






Training set
True function
Approximation
New point
20
15
10
5
0
−5
−10
−15
0.0
0.2
0.4
0.6
0.8
1.0


Training set
True function
Approximation
New point
20
15
10
5
0
−5
−10
−15
0.0
0.2
0.4
0.6
0.8
1.0



Hyperparmeters tuning

- Almost all machine learning have hyperparameters
- Quality of the model depends on the hyperparameters
- Quality estimation for one set of hyperparameters can take long time
- => Bayesian optimization can be used for hyperparameters tuning.

Bayesian optimization for hyperparameter tuning

Objective function to optimize

- Takes hyperparameters as input

- Builds a model (maybe several times in case of cross-validation)
- Calculates and returns model quality

In [8]:

```
from sklearn.ensemble import RandomForestRegressor
from sklearn.model_selection import train_test_split, cross_val_score
from sklearn.preprocessing import StandardScaler

from IPython import display
```

Task 3 (5 points)

House pricing dataset

In this task you need to predict House Sale Price. There are 25 numerical input features like lot area, overall condition rating, house quality, number of kitchens and so on (there were a lot of categorical variables which we removed in this example for simplicity).

We are going to tune XGBoost parameters using Bayesian Optimization to obtain more accurate model. Also, visualize quality of prediction with parameter changing over iterations.

In [9]:

```
data = np.loadtxt('house_pricing.csv')

X = data[:, :-1]
y = data[:, -1:]

X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.8, random_st
```

```
 /usr/lib/python3.6/site-packages/sklearn/model_selection/_split.py:20
10: FutureWarning:From version 0.21, test_size will always complement
train_size unless both are specified.
```

We implement `model_error_cv()` function that will be our objective function.
We are going to use RBF kernel in our Bayesian Optimization, the result of optimization will be continuous variables, so we need to preprocess parameters - cast integer parameters to int.

In [12]:

```
import xgboost

def wrap_parameters(parameters, scaler=None):
    if scaler:
        parameters = scaler.transform(parameters)
    return parameters


def unwrap_parameters(parameters, scaler=None):
    if scaler:
        parameters = scaler.inverse_transform(parameters)
    p = [int(parameters[0]), parameters[1], int(parameters[2]),
         max(0, min(parameters[3], 1))]
    return p


def model_error_cv(parameters, X, y, scaler=None):
    errors = []
    for p in parameters:
        p = unwrap_parameters(p, scaler)
        model = xgboost.XGBRegressor(max_depth=p[0],
                                     learning_rate=p[1],
                                     n_estimators=p[2],
                                     subsample=p[3],
                                     )

        score = cross_val_score(model, X, y, cv=3).mean()
        errors.append(score)
    return np.array(errors).reshape(-1, 1)
```

We scale the parameters using StandardScaler() from sklearn - it is nice to have all the parameters with unit variance and mean zero when using RBF kernel as it is easier to tune lengthscale parameters, because these parameters depend on the range of input variables.

In [14]:

```
# xgboost params: max_depth, learning_rate, n_estimators, subsample
lower_bound = np.array([1, 0.001, 100, 0.2])
upper_bound = np.array([6, 0.1, 1000, 1])

np.random.seed(42)
n_init_points = 10
initial_parameters = np.random.rand(n_init_points, len(lower_bound)) * (upper_bound
initial_errors = -model_error_cv(initial_parameters, X, y)

scaler = StandardScaler()
scaler.fit(initial_parameters)
lower_bound = scaler.transform(lower_bound[np.newaxis,:])
upper_bound = scaler.transform(upper_bound[np.newaxis,:])
initial_parameters = wrap_parameters(initial_parameters, scaler)
```

It is also nice idea to explicitly constrain lengthscale parameter - it shouldn't be much larger than distance between points in the training set, it shouldn't be much smaller than the distance between points in the training set.

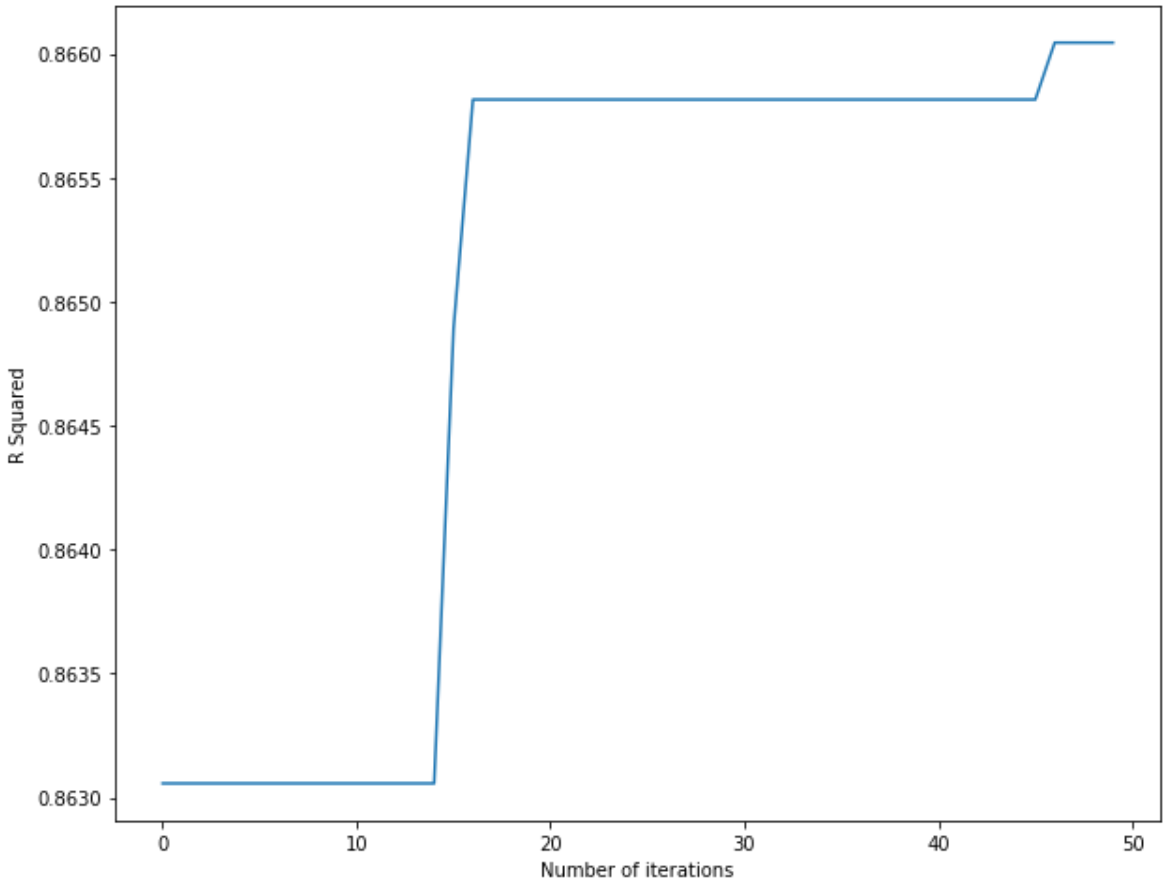
In [15]:

```
kernel = GPy.kern.RBF(lower_bound.shape[1], lengthscale=(upper_bound - lower_bound)
gp_model = GPy.models.GPRegression(initial_parameters, initial_errors, kernel=kerne
gp_model.rbf.lengthscale.constrain_bounded(0.001, 10)
gp_model.optimize()
print(gp_model)
print(gp_model.rbf.lengthscale)
```

```
WARNING:lengthscale:reconstraining parameters GP_regression.rbf.length
scale


Name : GP regression
Objective : -9.158296854171393
Number of Parameters : 3
Number of Optimization Parameters : 3
Updates : True
Parameters:
  GP_regression.           |             value  |  constraints  |  pri
ors
  rbf.variance             |    0.249762828356  |      +ve      |

  rbf.lengthscale          |              10.0  |  0.001,10.0   |

  Gaussian_noise.variance  |  0.00152782438335  |      +ve      |

  index  |  GP_regression.rbf.lengthscale  |  constraints  |  priors
  [0]    |                    10.00000000  |  0.001,10.0   |
```

In [16]:

```
budget = 40

hyperparameters = initial_parameters
errors = initial_errors
error_history = [-initial_errors[:i].min() for i in range(1, n_init_points + 1)]
objective = lambda x: -model_error_cv(x, X, y, scaler)
for i in range(budget):
    hyperparameters, errors, gp_model = bayes_opt.optimization_step(hyperparameters
                                                                    lb=lower_bound,
    error_history.append(-errors.min())
    # Visualize
    display.clear_output(wait=True)
    pyplot.figure(figsize=(10, 8))

    pyplot.xlabel("Number of iterations")
    pyplot.ylabel("R Squared")
    pyplot.plot(error_history)
    pyplot.show()

    print("New parameters: {}, new error:\t{}\nbest parameters: {}, best error:\t{}
        unwrap_parameters(hyperparameters[-1], scaler), -errors[-1, 0],
        unwrap_parameters(hyperparameters[errors.argmin()], scaler), -errors.min())
    print(gp_model.rbf.lengthscale)
```




```
New parameters: [4, 0.050442321832779434, 555, 0.3804927095824886], ne
w error:        0.8622658366202249
best parameters: [6, 0.068057951922992174, 477, 0.72908639131958275],
best error:     0.8660448920949825
  index  |  GP_regression.rbf.lengthscale  |  constraints  |  priors
  [0]    |                     2.38245095  |  0.001,10.0   |
```

In [ ]:

```
```