Bayesian Optimization from Scratch

...Just use a library for real-world applications, ok?

Decisions, Decisions, Decisions

Our psuedo-code is implemented in `simple_univariate_BO`

- x^* = the current candidate optimum
- while $i = 1..n_{it}$:
  - $x' = \text{argmax}_x \{g(x) \mid l \leq x \leq u, \tilde{f}(x) < f(x^*)\}$ # Find candidate
  - if no such x' exists, then return x^*
  - If $f(x') < f(x^*)$, then $x^* = x'$
  - update $\tilde{f}$ # Refine the surrogate model

In the implementation, a few key choices were made:

- How to pick the initial candidate optimum?
- Which surrogate model to use?
- How to optimize over the surrogate?
- Which acquisition function g to use?

Initial Candidate

It is common to initialize BO by sampling a few solutions

- This can be done uniformly at random
- ...Or we can use smarter approach

We sue the simplest approach, i.e.:

- (Uniform) Random sampling to obtain a few evaluations

```
X = np.random.uniform(l, u, size=(init_points, 1))
y = f(X)
```

- Then just pick the best point as a candidate optimum

```
best_idx = int(np.argmin(y))
best_x = X[best_idx]
best_y = X[best_idx]
```


Surrogate and Optimization Strategy

As a surrogate, we use a Gaussian Process

As a kernel we use a RBF + noise combination:

```
kernel = RBF(1, (1e-6, 1e0)) + WhiteKernel(1, (min_noise, 1e0))
```

- The first kernel parameters are initial guessesfor gradient descent
- The second parameters are bounds for the training process

For the optimization part, we use grid search

- ...Since we are doing only univariate optimization
- ...And evaluating the surrogate model is fast enough

In practice, we define a fixed grid of points to be be evaluated:

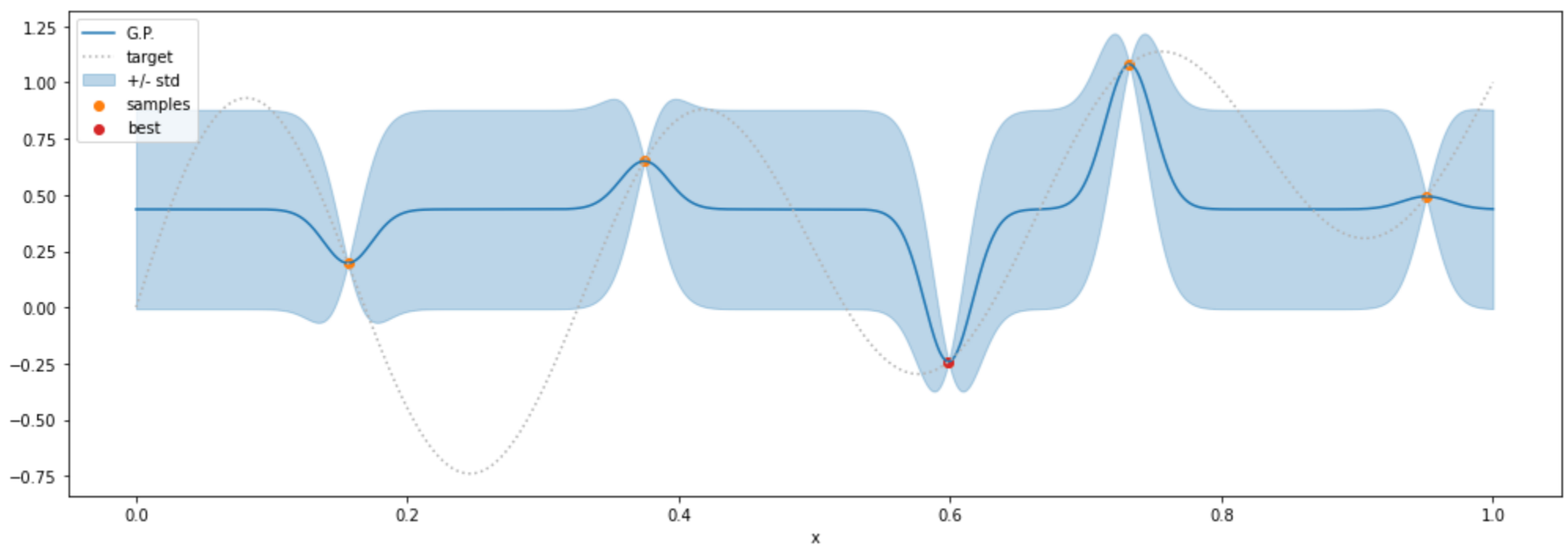
```
x = np.linspace(l, u, n_samples_gs)
```

Starting Situation

Let's start with a pool of 5 randomly sampled points

- The candidate optimum is the sample with the lower f
- The GP model estimates μ and σ for all points in our optimization grid

In [3]:
```
sol, state = util.simple_univariate_BO(f, 0, 1, init_points=5, max_it=0, seed=42, return_state=T
util.plot_series(state['mu'], samples=state['samples'], std=state['std'], target=target, samples
```



Acquisition Function

Finally, we need to pick an acquisition function

- A good acquisition function should balance exploration and exploitation
- Let's examine a few common choices

Probability of improvement

This is defined as the estimated probability of obtaining an improvement:

$$a_{PI}(x) = \mathbb{E}[\mathbb{1}_{f(x) \leq y^*}] = \int_{-\infty}^{y^*} \phi(y, \mu_{f(x)}, \sigma_{f(x)}) dy =$$

$$\Phi(y^*, \mu_{f(x)}, \sigma_{f(x)})$$

- PRO: clear interpretation
- CON: does not account for the magnitude of improvement

Acquisition Function

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Expected improvement

This is defined as the expected value of the improvement itself:

$$a_{EI}(x) = \mathbb{E}[\max(0, y^* - f(x))] = \int_{-\infty}^{y^*} (y^* - y)\phi(y, \mu_{f(x)}, \sigma_{f(x)})dy =$$

$$(y^* - \mu_{f(x)})\Phi(y^*, \mu_{f(x)}, \sigma_{f(x)}) + \sigma_{f(x)}\phi(y^*, \mu_{f(x)}, \sigma_{f(x)})$$

- PRO: accounts for exploitation (via the first term)
- PRO: accounts for exploration (via the second term)
- CON: the trade-off between the two cannot be controlled

Acquisition Function

Finally, we need to pick an acquisition function

- A good acquisition function should balance exploration and exploitation
- Let's examine a few common choices

Lower Confidence Bound

This is the lower bound of a given confidence interval

$$a_{LCB}(x) = \mu_{f(x)} - Z_{\alpha}\sigma_{f(x)}$$

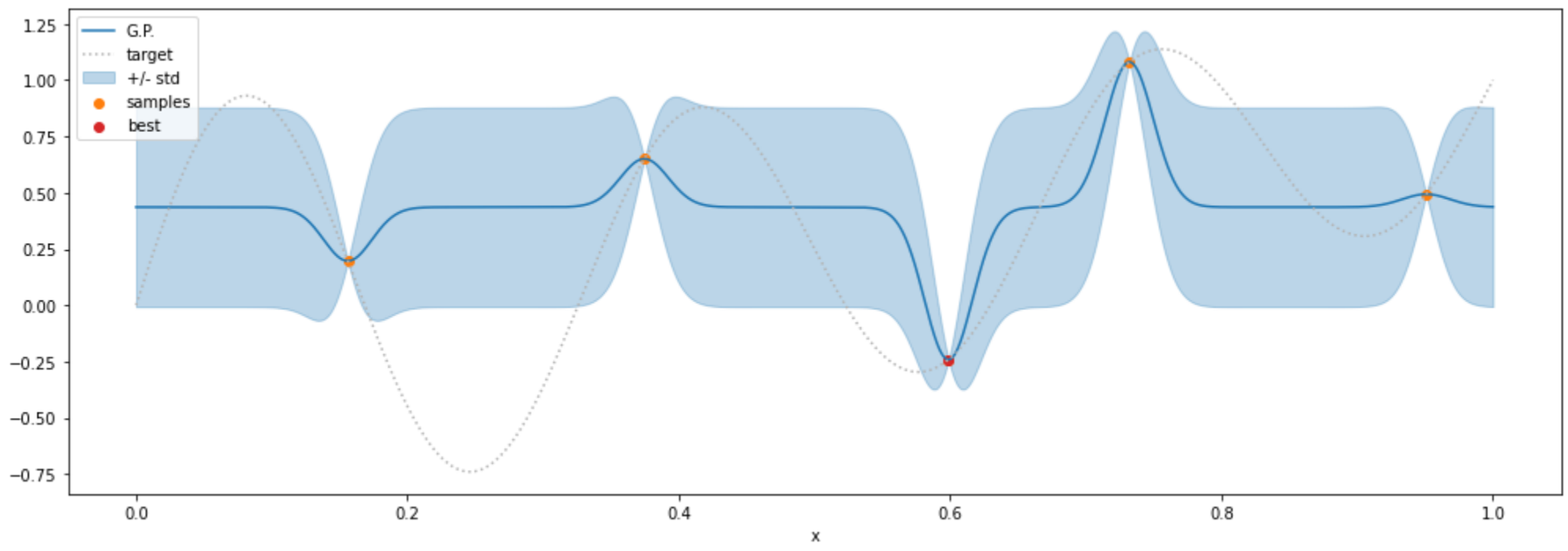
Where Z_{α} is the coefficient needed to get the $\alpha\%$ confidence interval

- PRO: accounts for exploitation and exploration
- PRO: the trade-off can be controlled
- CON: the trade-off needs to be controlled :-)

Experiments: Probability of Improvement

Let's try to iterate once using a_{PI} as acquisition function

In [4]:
```
sol, state = util.simple_univariate_BO(f, 0, 1, init_points=5, max_it=1, seed=42, ftype='pi', re
util.plot_series(state['mu'], samples=state['samples'], std=state['std'], target=target, samples
```

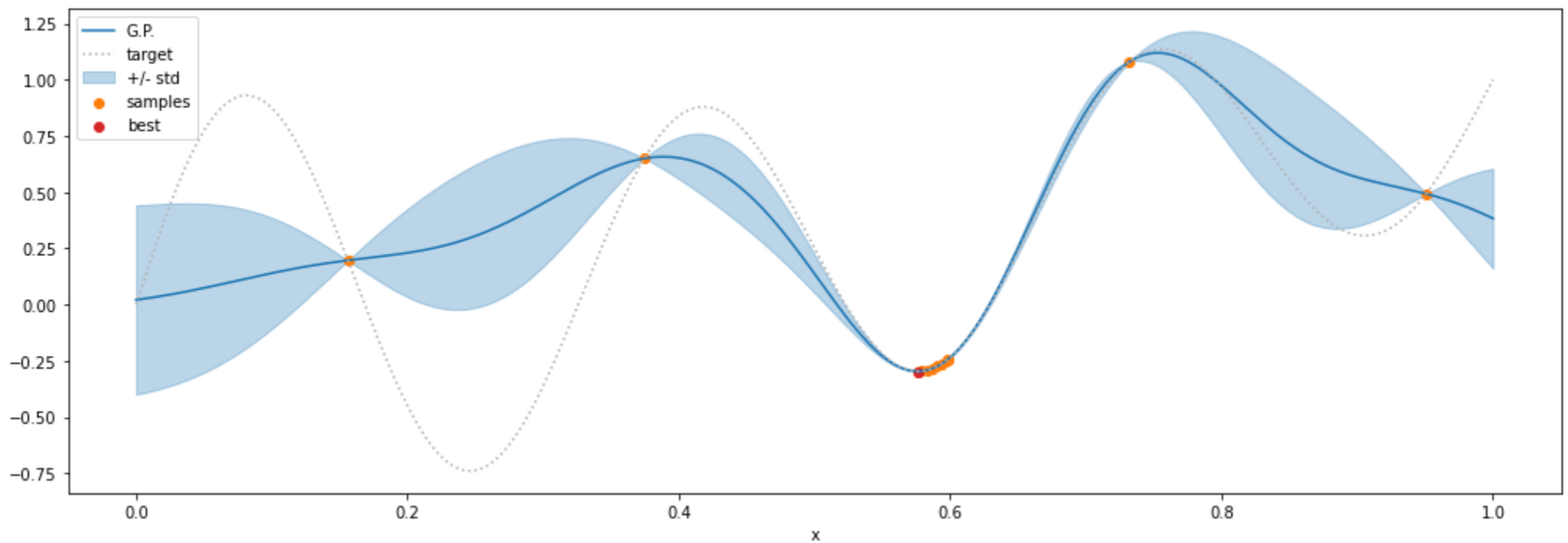


- The new points is very close to the initial candidate optimum
- ...And it also improves on its value

Experiments: Probability of Improvement

Let's try to iterate once using a_{PI} as acquisition function

In [5]:
```
sol, state = util.simple_univariate_BO(f, 0, 1, init_points=5, max_it=10, seed=42, ftype='pi', r
util.plot_series(state['mu'], samples=state['samples'], std=state['std'], target=target, samples
```

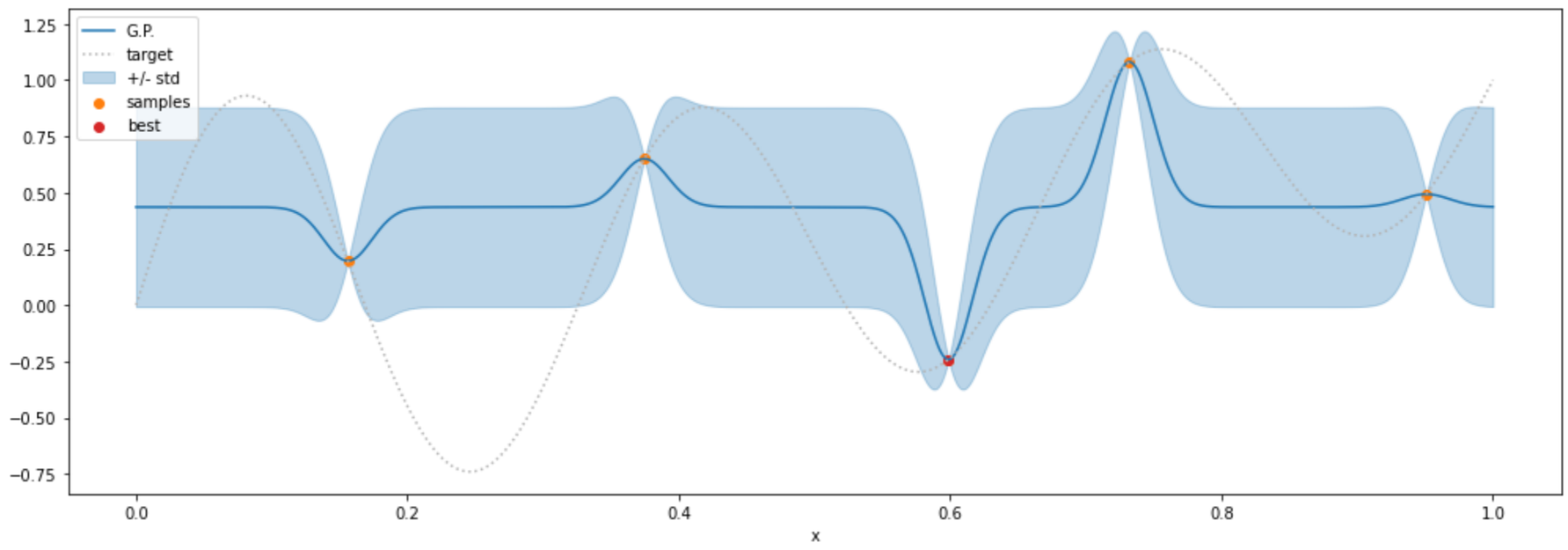


- After 10 iterations we reach a local optimum
- ...And we get stuck: this is unfortunately common for a_{PI}

Experiments: Expected Improvement

Let's try to iterate once using a_{EI} as acquisition function

In [6]:
```
sol, state = util.simple_univariate_BO(f, 0, 1, init_points=5, max_it=1, seed=42, ftype='ei', re
util.plot_series(state['mu'], samples=state['samples'], std=state['std'], target=target, samples
```

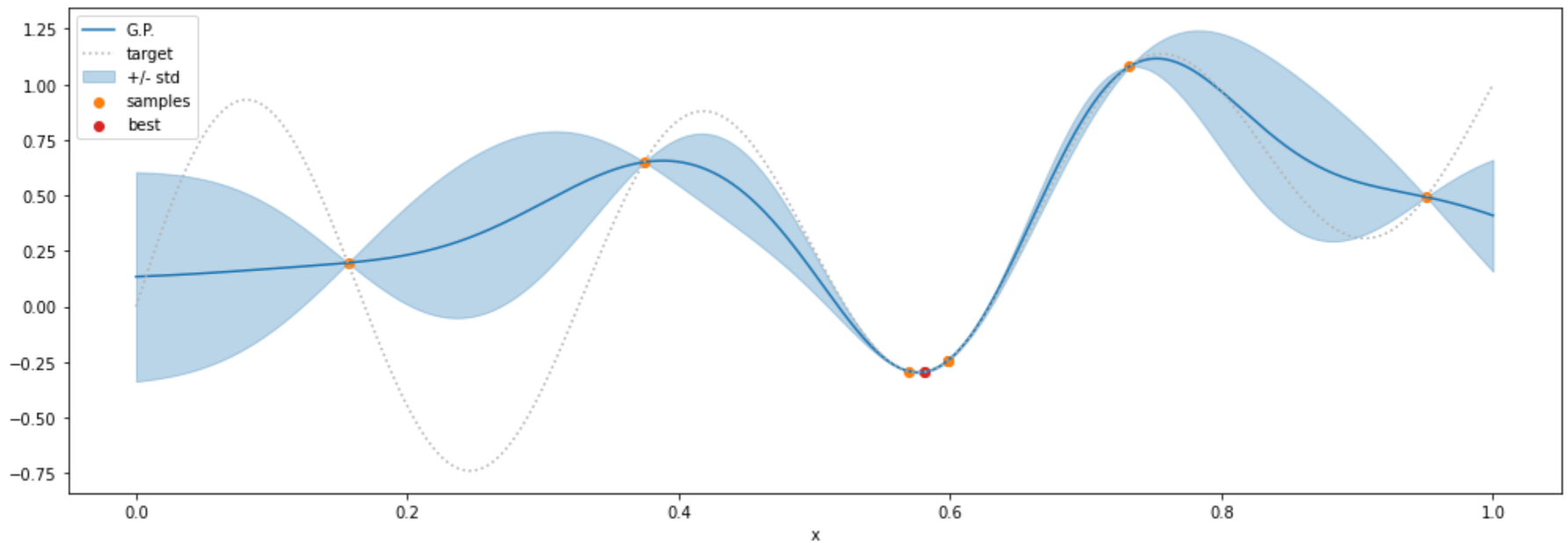


- The first point is very similar to that of a_{PI}

Experiments: Expected Improvement

Let's try to iterate once using a_{EI} as acquisition function

In [7]:
```
sol, state = util.simple_univariate_BO(f, 0, 1, init_points=5, max_it=5, seed=42, ftype='ei', re
util.plot_series(state['mu'], samples=state['samples'], std=state['std'], target=target, samples
```

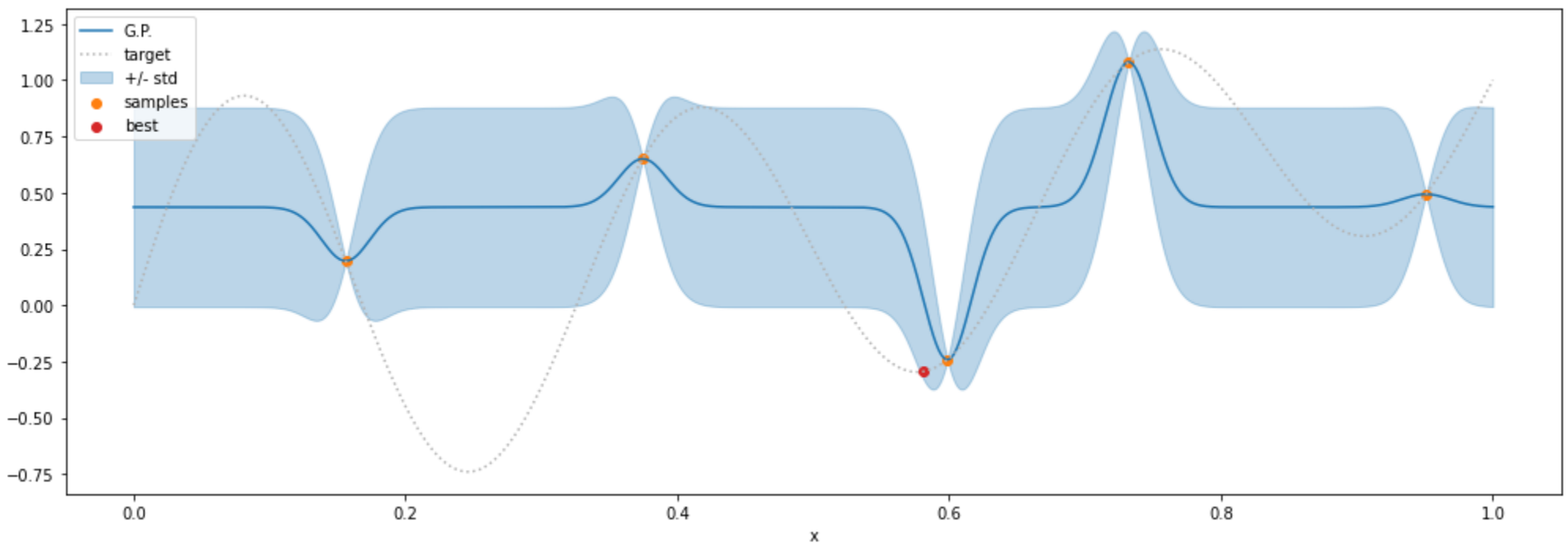


- ...But we reach a comparable solution faster (5 vs 10 iterations)

Experiments: Lower Confidence Bound

Let's try to iterate once using a_{LCB} as acquisition function

In [8]:
```
sol, state = util.simple_univariate_BO(f, 0, 1, init_points=5, max_it=1, alpha=0.95, seed=42, ft
util.plot_series(state['mu'], samples=state['samples'], std=state['std'], target=target, samples
```

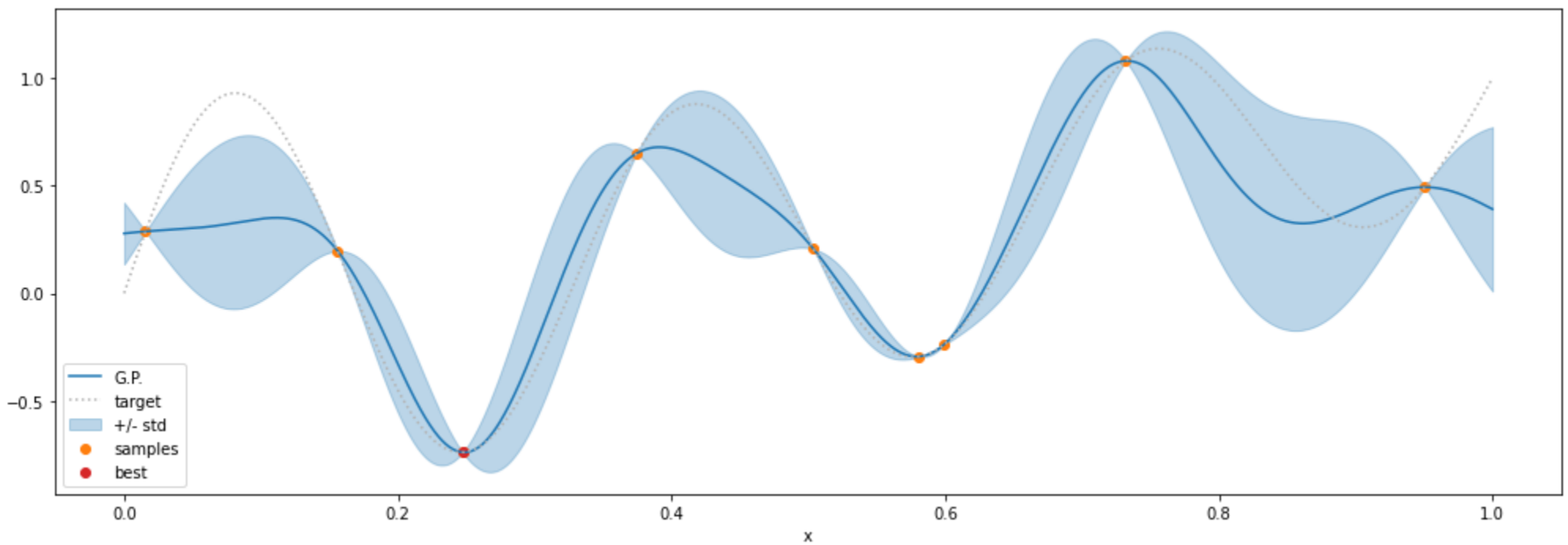


- The first point is less close to y^* than a_{PI} and a_{EI}
- This is due to the fact that we are emphasizing exploration ($\alpha = 0.95$)

Experiments: Lower Confidence Bound

Let's try to iterate once using a_{LCB} as acquisition function

In [10]:
```
sol, state = util.simple_univariate_BO(f, 0, 1, init_points=5, max_it=5, alpha=0.95, seed=42, ft
util.plot_series(state['mu'], samples=state['samples'], std=state['std'], target=target, samples
```



- After 5 iterations we have basically found the global optimum
- In fact, under some assumptions, a_{LCB} has global convergence guarantees

Bayesian Optimization for Policy Definition

Back to where we started

Back to Our Motivating Problem

We will use BO to tackle our policy definition problem

$$\text{argmin}_\theta \sum_{k \in K} cost(f(x_k\ \omega^*), 0.5)$$

$$\text{with: } \omega^* = \text{argmin}_\omega \{ L(y, \mathbb{1}_{\hat{y} \geq \theta}) \mid y = f(x, \omega) \}$$

We need to optimize over θ

- But since we have now access to a powerful new tool
- ...We will throw in an extra parameter, i.e. the class weights

The reason is that we have an imbalanced dataset

...But the usual balancing rule does not work well

- Making the classes equally important (i.e. inverse frequencies as weights)
- ...Leads to mistakes early on, and hence to suboptimal policies

Our Chosen Optimizer

We will use the scikit-optimize python module

...Which provides a somewhat rough (but fast) implementation of BO

- We start by defining our cost function

```
def f(thr, c0_weight):
    tr_lbl = (y >= thr) # Labels
    mdl.set_weights(init_wgt)
    sample_weight = np.where(tr_lbl, 1, c0_weight) # Sample weights
    train_ml_model(mdl, X, tr_lbl, epochs=epochs_per_it, # Train
            validation_split=validation_split,
            sample_weight=sample_weight, loss='binary_crossentropy')
    tr_pred = np.round(mdl.predict(X).ravel()) # Predictions
    tr_cost = cmodel.cost(machines, tr_pred, 0.5) # Cost
    return -tr_cost
```

Our Chosen Optimizer

We will use the scikit-optimize python module

...Which provides a somewhat rough (but fast) implementation of BO

- Then we specify the bounds for the two parameters

```
box = {'thr': (0.0, 0.05), 'c0_weight': (1., 5.)}
```

- ...And finally we start the optimization process

```
res = skopt.gp_minimize(f, [box[k] for k in ('thr', 'c0_weight')],
        acq_func='gp_hedge', n_calls=n_iter, n_random_starts=init_points,
        random_state=seed)
```

- `skopt` relies on a GP with a Matern Kernel as a surrogate model
- The `gp_hedge` function is a probabilistic combination of a_{PI}, a_{EI}, a_{LCB}

Optimizing the Policy

Let's use the approach to optimize our policy

We will use BO to fine-tune the our earlier classifier

In [11]:
```
nn2 = keras.models.clone_model(nn)
nn2.set_weights(nn.get_weights())
res = util.opt_classifier_policy(nn2, tr_s[dt_in], tr_s['rul'], tr_s['machine'], cmodel=cmodel,
                                 epochs_per_it=3, seed=42, verbose=1)
```

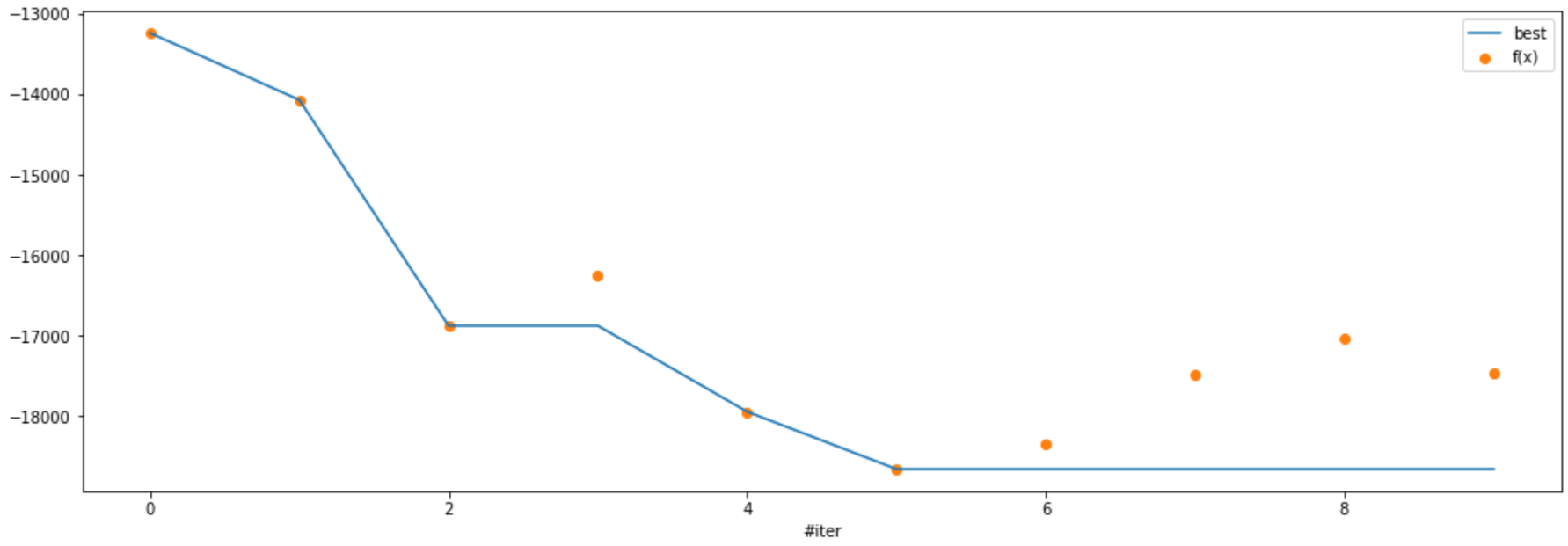
```
thr: 0.040, w0: 1.734, cost: -13245, time: 7.81
thr: 0.039, w0: 3.387, cost: -14075, time: 7.87
thr: 0.022, w0: 1.400, cost: -16876, time: 7.83
thr: 0.023, w0: 2.335, cost: -16248, time: 7.71
thr: 0.007, w0: 3.604, cost: -17942, time: 7.79
thr: 0.007, w0: 3.595, cost: -18654, time: 7.71
thr: 0.007, w0: 3.595, cost: -18344, time: 7.71
thr: 0.023, w0: 1.462, cost: -17491, time: 7.65
thr: 0.023, w0: 1.433, cost: -17041, time: 7.75
thr: 0.023, w0: 1.504, cost: -17462, time: 7.86
```

- Starting from a pre-trained model enables using few epochs per iteration
- The results may vary slighly since training is stochastic

Optimizing the Policy

We can inspect the cost values obtained during search

In [12]:
```
samples = pd.Series(res.func_vals)
best = pd.Series([np.min(samples.iloc[:i]) for i in range(1, len(samples)+1)])
util.plot_series(best, samples=samples, figsize=figsize, xlabel='#iter', ylabel='best', samples_
```



Evaluation

Finally, we can evaluate the optimized model

In [13]:
```
tr_pred2 = np.round(nn2.predict(tr_s[dt_in]).ravel())
ts_pred2 = np.round(nn2.predict(ts_s[dt_in]).ravel())
tr_c2, tr_f2, tr_sl2 = cmodel.cost(tr['machine'].values, tr_pred2, 0.5, return_margin=True)
ts_c2, ts_f2, ts_sl2 = cmodel.cost(ts['machine'].values, ts_pred2, 0.5, return_margin=True)
print(f'Cost: {tr_c2} (training), {ts_c2} (test)')
print(f'Avg. fails: {tr_f2/len(tr_mcn)} (training), {ts_f2/len(ts_mcn)} (test)')
print(f'Avg. slack: {tr_sl2/len(tr_mcn):.2f} (training), {ts_sl2/len(ts_mcn):.2f} (test)')
```

```
Cost: -18654 (training), -6947 (test)
Avg. fails: 0.0 (training), 0.0 (test)
Avg. slack: 15.80 (training), 13.54 (test)
```

The results are significantly better than the old classifier

In [14]:
```
print(f'Cost: {tr_c} (training), {ts_c} (test)')
print(f'Avg. fails: {tr_f/len(tr_mcn)} (training), {ts_f/len(ts_mcn)} (test)')
print(f'Avg. slack: {tr_sl/len(tr_mcn):.2f} (training), {ts_sl/len(ts_mcn):.2f} (test)')
```

```
Cost: -16760 (training), -6356 (test)
Avg. fails: 0.0 (training), 0.0 (test)
Avg. slack: 26.31 (training), 23.05 (test)
```