Classifier-Based RUL Policies

Boring start, interesting consequences

RUL Prediction as Classification

Since we have established that RUL prediction is hard

...Why don't we got for a classification approach?

- Classification is often easier than regression
- ...And it would remove our "fake" high RUL values when the machine is healthy
- ...Since those point will all belong to the same "healthy" class

Formally, let's predict when the end of life is approaching, i.e.:

$$f(x, \omega) = \begin{cases} 0 \text{ if RUL} < \theta \\ 1 \text{ otherwise} \end{cases}$$

- f is the classifier (with parameter vector ω)
- θ is defines what we mean by "approaching"

The idea is to stop as soon as the classifier outputs a 1

Fool Me Once...

Let's not make the same mistake twice

...And start by drafting a problem formulation:

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

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

Here we assume that $f(x, \omega)$ is a neural classifier (output in $[0, 1]$)

- The $cost$ function and the $\hat{y}$ vector are the same as before
- The value 0.5 in $cost$ mimics the effect of rounding
- ...And $\mathbb{1}_{\hat{y} \geq \theta}$ is the indicator function of the condition $\hat{y} \geq \theta$

Superficially, this is similar to our regression-based approach

Fool Me Twice...

...But in fact it is a very different problem!

Let's look again at the formulation:

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

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

- When we change θ, were are changing the class labels
- ...And therefore we need to retrain the classifier

This is no longer a "predict, then optimize" scheme

- Even at deployment time, the classifier completely defines the policy
- Once we have the predictions, there is nothing left to optimize

Fool Me Twice...

...But in fact it is a very different problem!

Let's look again at the formulation:

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

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

- When we change θ, were are changing the class labels
- ...And therefore we need to retrain the classifier

However this is still a univariate optimization problem

...Meaning that we can still solve it with grid search

- The catch is that every cost function evaluation will be slower
- ...Since it will require to perform training

Classifier Implementation

How slow are we talking about? Only one way to know...

Classifier Implementation

We start by building a neural classifier

In [2]:
```
hidden = [16, 16]
nn = util.build_ml_model(input_size=len(dt_in), output_size=1, hidden=hidden,
                         output_activation='sigmoid')
```

- The input values are the same as before
- ...But we need to define the classes

For now, we choose θ based on the slack in the regression experiments

In [3]:
```
thr = 20
tr_lbl = (tr['rul'] >= thr)
ts_lbl = (ts['rul'] >= thr)
```

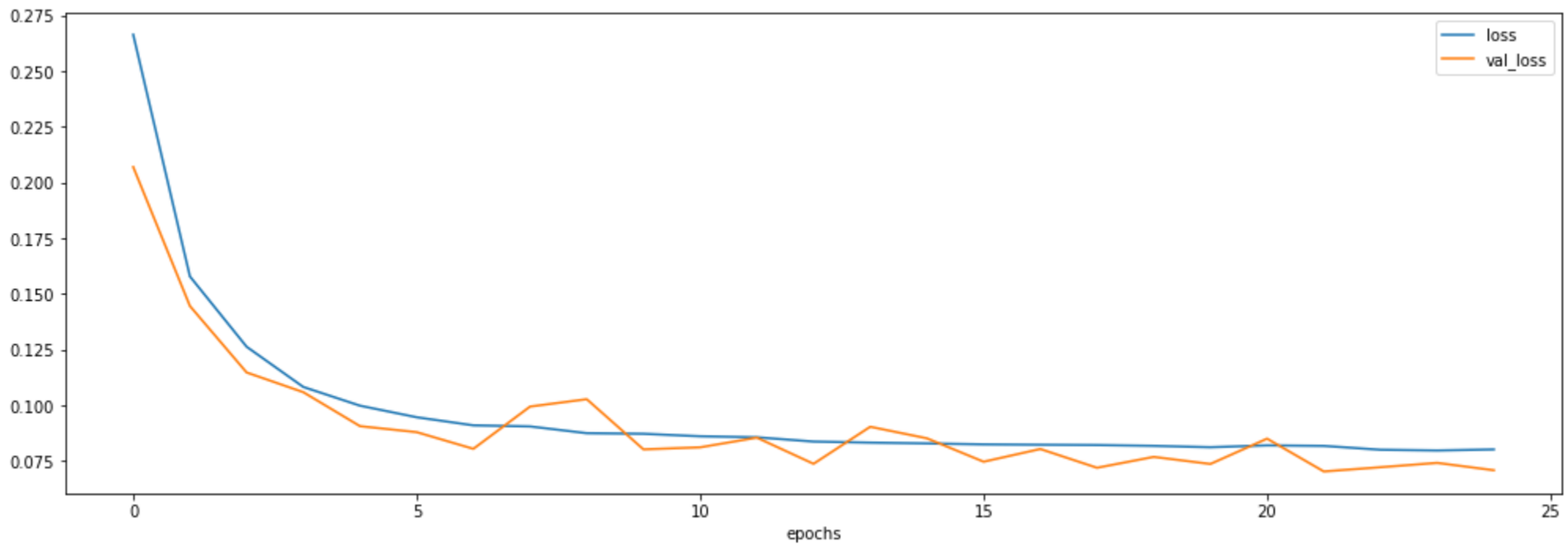
- Classes are rather imbalanced, but we'll think about that later

Training the Classifier

We can now train our classifier

In [4]:
```
%time history = util.train_ml_model(nn, tr_s[dt_in], tr_lbl, epochs=25, validation_split=0.2, lo
nn.save('rul_classifier')
util.plot_training_history(history, figsize=figsize)
```

```
CPU times: user 23.7 s, sys: 1.96 s, total: 25.6 s
Wall time: 16 s
INFO:tensorflow:Assets written to: rul_classifier/assets
```

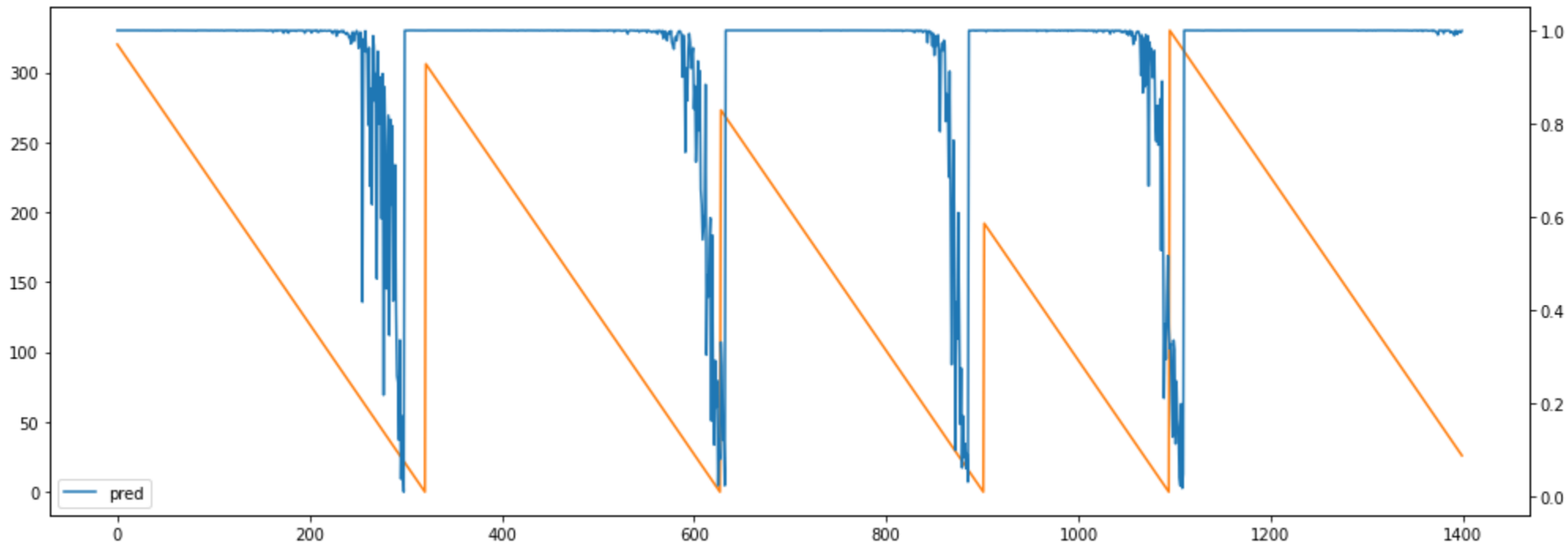


Model loss: 0.0817 (training) 0.0703 (validation)

Training the Classifier

The estimated probabilities follow the correct pattern:

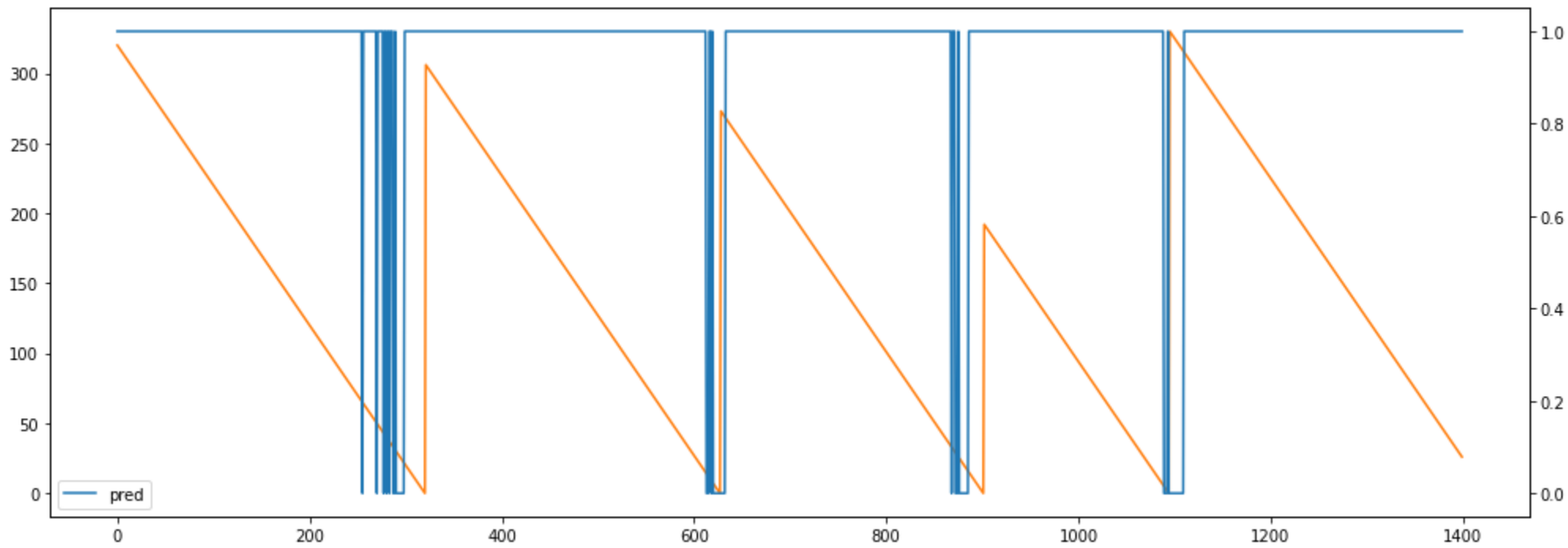
In [5]:
```
ts_prob = nn.predict(ts_s[dt_in]).ravel()
util.plot_rul(ts_prob[:stop], tr['rul'][:stop], same_scale=False, figsize=figsize)
```



Inspecting the Predictions

After rounding is applied, this is what we get

In [6]:
```
ts_pred = np.round(nn.predict(ts_s[dt_in]).ravel())
util.plot_rul(ts_pred[:stop], tr['rul'][:stop], same_scale=False, figsize=figsize)
```



Evaluation

We can evaluate the classifier directly

...Because it defines the whole policy

In [7]:
```
tr_pred = np.round(nn.predict(tr_s[dt_in]).ravel())
tr_c, tr_f, tr_sl = cmodel.cost(tr['machine'].values, tr_pred, 0.5, return_margin=True)
ts_c, ts_f, ts_sl = cmodel.cost(ts['machine'].values, ts_pred, 0.5, return_margin=True)
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)
```

It's already working reasonably, but is this the best we can do?

- If we want to know that, we need to search over θ
- ...Except that every evaluation will required up to 20 seconds


Surrogate Based Black-Box Optimization

Of which Bayesian Optimization is a prime example

Motivation

Let's recap our situation. Our problem is in the form:

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

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

We need to optimize only over θ, but every evaluation is rather slow

How can we efficiently solve it?

Motivation

Let's recap our situation. Our problem is in the form:

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

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

We need to optimize only over θ, but every evaluation is rather slow

How can we efficiently solve it?

- We need make the best possible use of the available information
- E.g. by learning as much as possible from every evaluated solution

Surrogate-Based Black Box Optimization

Classical Black-box optimization approaches

...Are concerned with problems in the form:

$$\text{argmin}_x \{ f(x) \mid l \leq x \leq u \}$$

- Where x is a variable in $\mathbb{R}^n$
- ...And f is a function that we can only evaluate (black-box)
- l and u are bounds for the input variables

Most black-box optimization solvers rely on a surrogate model

- They approximate f via an internal model $\tilde{f}$
- They choose solutions based on $\tilde{f}$
- They use evaluated solutions to refine $\tilde{f}$

Surrogate-Based Black Box Optimization

The basic loop of the algorithm is as follows:

- 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 # No more improvements possible
    - return x^*
  - If $f(x') < f(x^*)$, then $x^* = x'$ # Evaluate and possibly update the solution
  - update $\tilde{f}$ # Refine the surrogate model

Where:

- g is called an acquisition function and is related to $\tilde{f}$
- n_i is the maximum number of iterations

Surrogate-Based Black Box Optimization

The surrogate model is key to the method operation

...And it represents a posterior probability distribution

- It represents all we know about the true cost function
- We keep it up to date by retraining after each evaluation

For this reason, the approach is also known as Bayesian Optimization

The surrogate exists to support the the g (acquisition) function

...Which seeks an $\boldsymbol{x}$ with a large-enough improvement chance

- This chance is evaluated on the surrogate/posterior $\tilde{f}$
- If f is well behaved, we can give probabilistic optimality guarantees

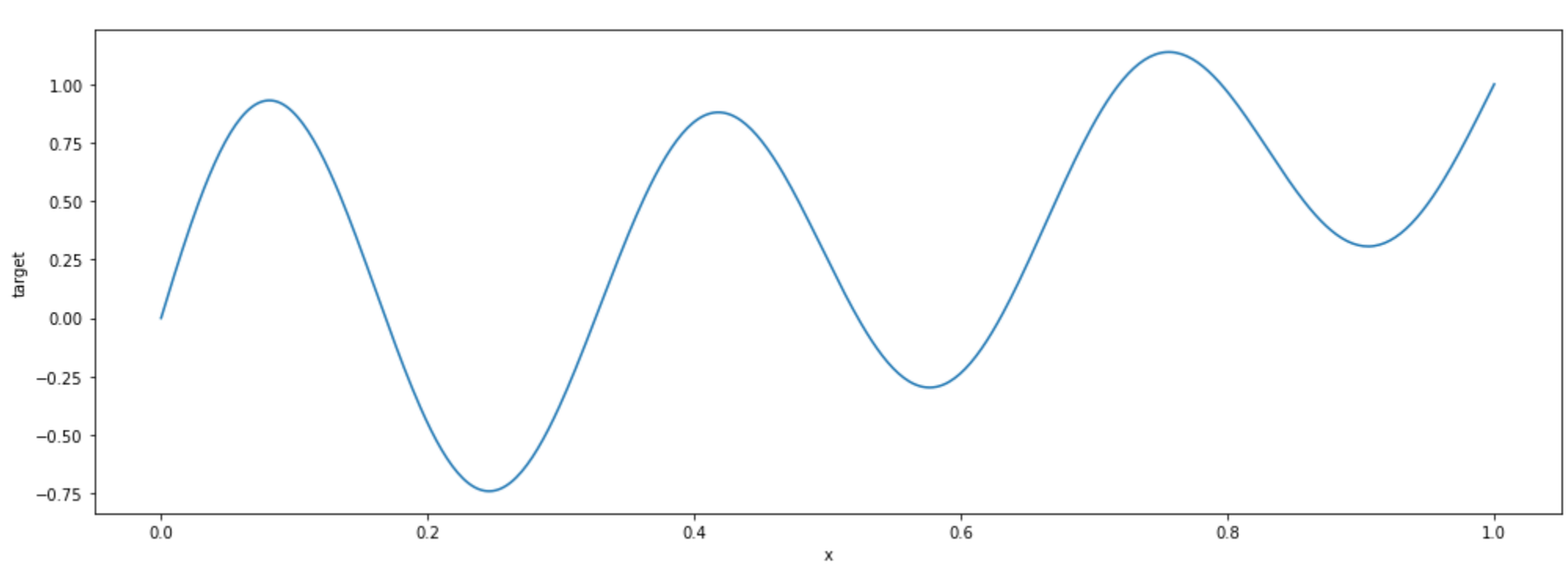
Different surrogate-based methods differ by:

- The type of acquisition function
- How they balance exploration and exploitation

A Numeric Example

Say we want to obtain a minimizer for $f(x) = \frac{1}{1+x} sin(6\pi x) + x^2$

In [8]:
```
f = lambda x: 1/(1+x) * np.sin(6 * np.pi * x) + x**2
x = np.linspace(0, 1, 500)
target = pd.Series(index=x, data=f(x))
util.plot_series(target, figsize=figsize, ylabel='target', xlabel='x')
```

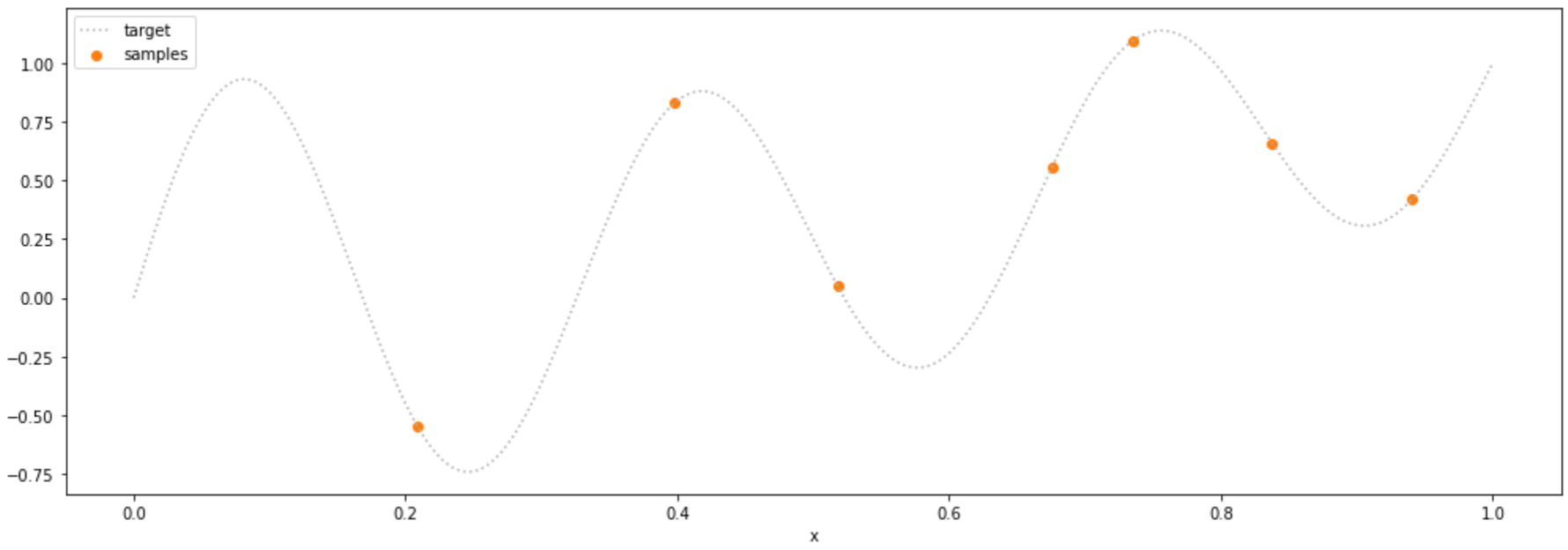


This is easy to plot and compute, but challenging due to multiple local optima

A Numeric Example

Before updating the surrogate, we would be in this kind of situation:

In [9]:
```
x_sample = np.random.rand(7)
y_sample = pd.Series(index=x_sample, data=f(x_sample))
util.plot_series(samples=y_sample, target=target, figsize=figsize, xlabel='x')
```



- We would have access to a number of samples (evaluated solutions)
- ...And we wished to obtain an approximation of the true function

Which Surrogate Model?

Some desiderata for our surrogate model

...Keeping in mind its goal is to support the acquisition function:

- The surrogate $\tilde{f}$ should output a probability distribution
  - ...Or we wouldn't be able to estimate optimality chances
- When we are near a sampled solution, i.e. $x \simeq x'$
  - It should be very close to its value, i.e $f(x) \simeq f(x')$
  - ...Or it would be hard to provide guarantees
- It should change considerably when a single new solution is evaluated
  - ...Or we would need to sample points too close to each other
  - ...Before we finally explore another area

There aren't many ML method that fit this description