Gaussian Processes

They check all the boxes

Introduction to Gaussian Processes

Gaussian Processes are a type of ML model

...Capable of doing inference based on set of observations

- For input values close to those of known observations
- ...Their output can be close to those of the observations themselves

Finally, their output is a full probability distribution (not a point estimate)

Intuitively, they model a conditional probability

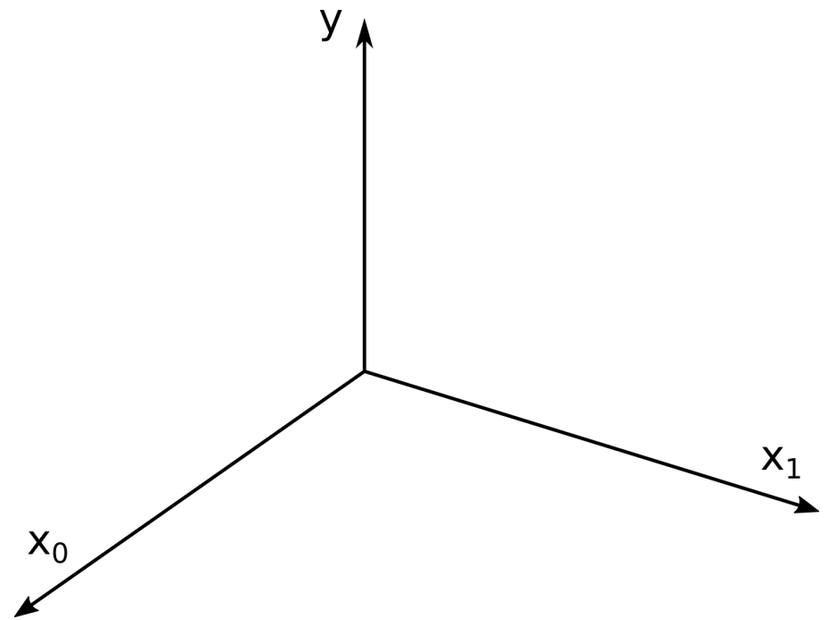
$$P(y \mid x, \hat{x}, \hat{y}) \simeq f(y, x, \hat{x}, \hat{y}, \omega)$$

- The model is parameterized with a numeric vector, i.e. ω
- ...But also with a set of examples with input $\hat{x}$ and output $\hat{y}$

They achieve this by relying on properties of the Normal (Gaussian) distribution

Introduction to Gaussian Processes

We will introduce the key concepts in GPs via an example:



- Say we want to model how rainfall changes over a stretch of land
- $y =$ rainfall, $(x_0, x_1) =$ position on the surface of land

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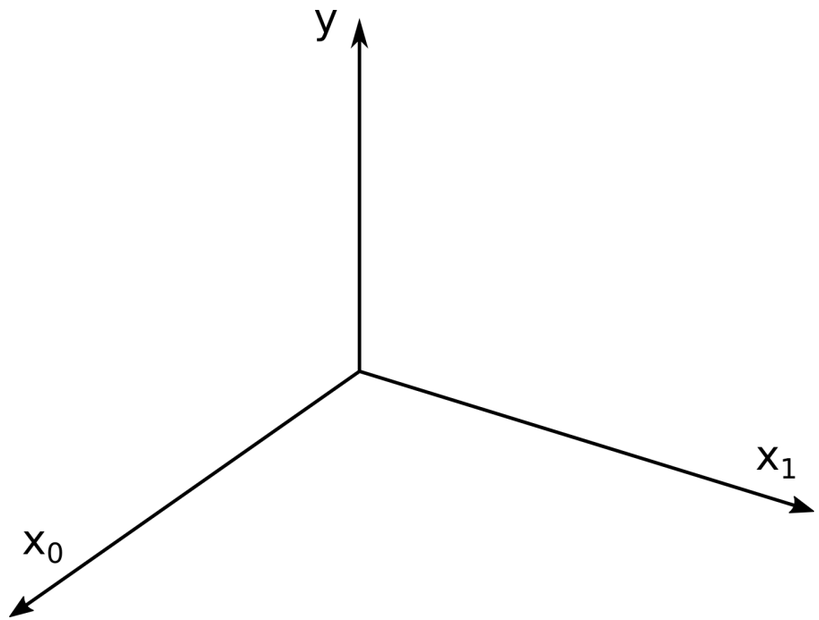

Since this is a physical phenomenon...

- ...We can reasonably assume that $\boldsymbol{y}$ is Normally distributed
- But unless we know more, we can say nothing else

Introduction to Gaussian Processes

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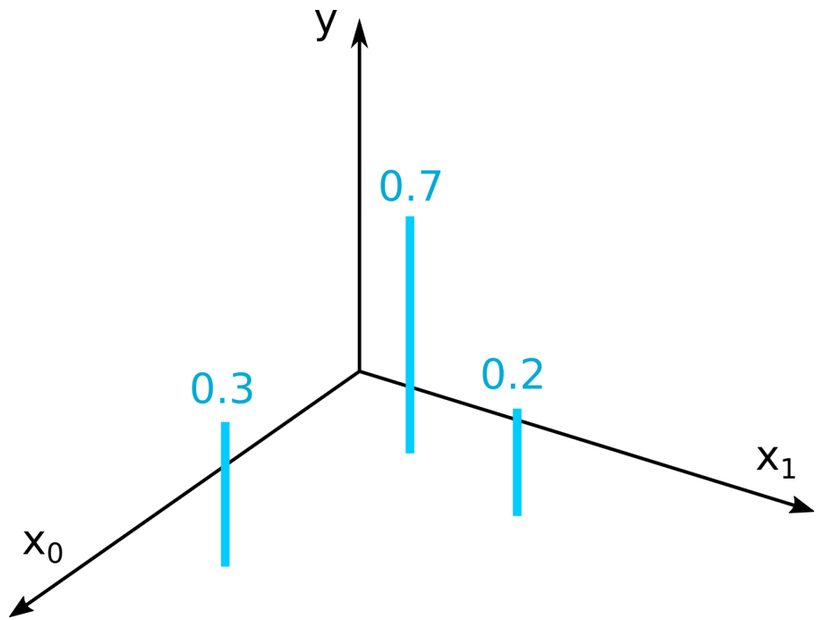

However, if we have a few measurements...

- ...Then we can assume that rainfall in nearby locations is similar
- ...So we can infer rainfall for positions for which we lack measurements

Introduction to Gaussian Processes

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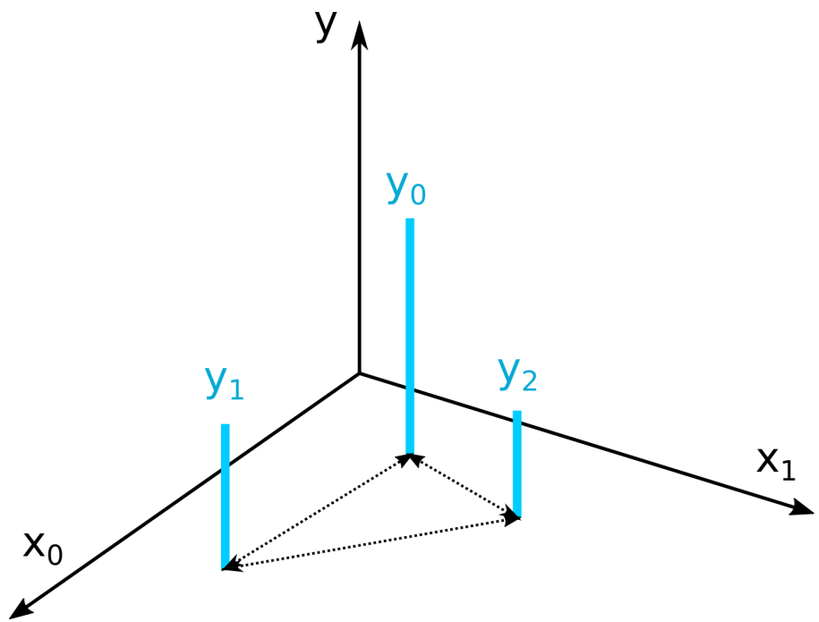


E.g. we can view the measurements as components of a variable

$y_X = (y_0, y_1, y_2)$

- y_X will follow a multivariate Normal distribution
- ...And we can assume the covariance will depend on the distances

Gaussian Processes, Formally

Formally:

A GP is a stochastic process, i.e. a collection of indexed random variables

- Each variable y_x is indexed via a tuple x (e.g. location, time...)
- The index is continuous and the collection infinite
- Every finite subset of y_x variables follows a Multivariate Normal Distribution

Translating back to our original conditional probability:

$$P(y \mid x, \hat{x}, \hat{y}) \equiv P(y_x \mid \hat{y}_{\hat{x}})$$

- x is the GP input
- y_x is the (stochastic) variable we want to estimate
- $\hat{x}$ is the input for all available observations
- ...And $\hat{y}_{\hat{x}}$ is the (stochastic) output

Gaussian Processes, Formally

A GP has access to:

- The input vector $\boldsymbol{x}$ for an unobserved point
- The input $\hat{x}_1, \hat{x}_2, \ldots$ for a number of observed points

Overall, let $\tilde{x} = (x, \hat{x}_1, \hat{x}_2, \ldots$

We view the output $\tilde{y} = (y_x, \hat{y}_1, \hat{y}_2, \ldots)$ as a Multivariate Normal Variable

$$\tilde{y} \sim \mathcal{N}(\mu, \Sigma)$$

With the aim to define the distribution, we make two assumptions:

- $\mu = 0$ (we can satisfy this by centering the data)
- The covariance matrix depends on the set of inputs...
- ...And on the the ω parameter vector, i.e. $\Sigma(\tilde{x}, \omega)$

Gaussian Processes, Formally

This is enough to estimate the distribution we need

The PDF for multivariate normal distribution is available in closed form

$$\phi(x, \mu, \Sigma) = \det(2\pi\Sigma)^{-\frac{1}{2}} e^{(x-\mu)^T \Sigma^{-1}(x-\mu)}$$

- Therefore, for our y variable we have:

$$P(y|\hat{y}) = \frac{\phi(\tilde{y}, 0, \Sigma(\tilde{x}, \omega))}{\phi(\hat{y}, 0, \Sigma(\hat{x}, \omega))}$$

- Which implies we can also easily get the PDF for $\hat{y}_{\hat{x}}$
- In fact, we can do it for every finite subset of observations

The catch is that we need to define how to compute $\Sigma(x, \omega)$

Gaussian Processes, Formally

We build Σ by means of a user-defined kernel function K

Given a set of (random) variables $y = (y_{x_1}, y_{x_2}, \ldots)$, we have:

$$\Sigma_{ij}(x, \omega) = K(x_i, x_j, \omega)$$

- Where the x_i, x_j are the input for the considered pair
- ...And ω is a (kernel-dependent) parameter vector

The overall covariance matrix will be structured as:

$$\Sigma(x, \omega) = \begin{pmatrix} K(x_1, x_1, \omega) & K(x_1, x_2, \omega) & \cdots & K(x_1, x_n, \omega) \\ K(x_2, x_1, \omega) & K(x_2, x_2, \omega) & \cdots & K(x_2, x_n, \omega) \\ \vdots & \vdots & \vdots & \vdots \\ K(x_n, x_1, \omega) & K(x_n, x_2, \omega) & \cdots & K(x_n, x_n, \omega) \end{pmatrix}$$

Training a Gaussian Process

In practice, to setup a GP model we

- Collect training observations $\hat{y}_{\hat{x}}$
- Pick a parameterized kernel function $K(x_i, x_j, \omega)$

Then we choose ω by maximizing the likelihood of the training data:

$$\text{argmax}_{\omega} \phi(\hat{y}, 0, \Sigma(\hat{x}, \omega))$$

- After this is done, we can store the training observations
- ...And use the to condition our predictions

The training problem

- Is a (possibly challenging) numerical optimization problem
- ...Which is typically solved to local optimality (e.g. via gradient descent)

Gaussian Processes in Practice

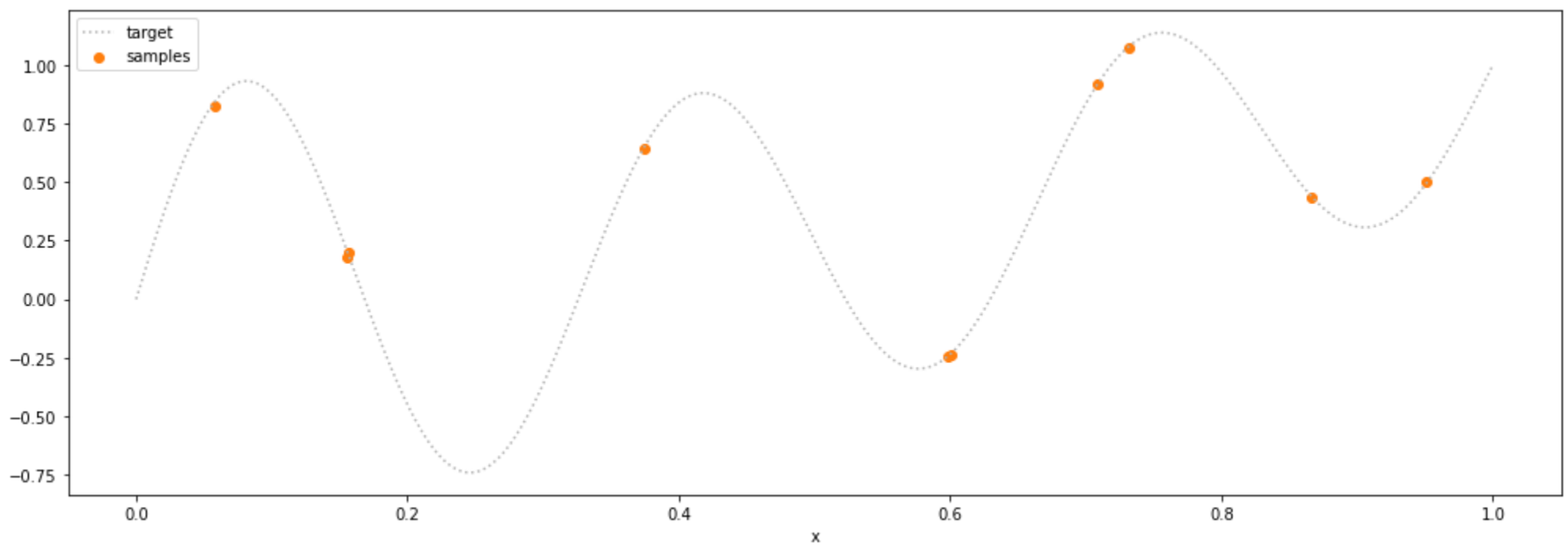
This is When It will all make sense... Hopefully

Target and Training Set

Let's see how to use GPs in scikit-learn

First, we need to collect a training setusing our example function and some noise

In [2]:
```
np.random.seed(42)
x_tr = np.random.rand(10)
y_tr = pd.Series(index=x_tr, data=f(x_tr) + 0.01*np.random.randn(10))
util.plot_series(samples=y_tr, target=target, figsize=figsize, xlabel='x')
```



Radial Basis Functions

Next we need to pick a kernel function

- There are many available options
- ...But we will focus on those typically used in Bayesian Optimization

We will start with a Radial Basis Function kernel

This is in the form:

$$K(x_i, x_j, \omega) = e^{-\frac{d(x_i,x_j)^2}{2l}}$$

The correlation decreases with the (Euclidean) distance $d(x_i, x_j)$:

- Intuitively, the closer the points, the higher the correlation
- The l parameter (scale) control the rate of the reduction

The ω vector will just be the collection of all kernel parameters

Untrained Guassian Processes

Let's start by building an RBF kernel with default parameters

In [3]:
```
kernel = RBF()
kernel
```

Out[3]:
```
RBF(length_scale=1)
```

Then we build a GP regressor and obtain our predictions

In [4]:
```
gp = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9, normalize_y=True)
y_mu, y_std = gp.predict(x.reshape(-1,1), return_std=True)
```

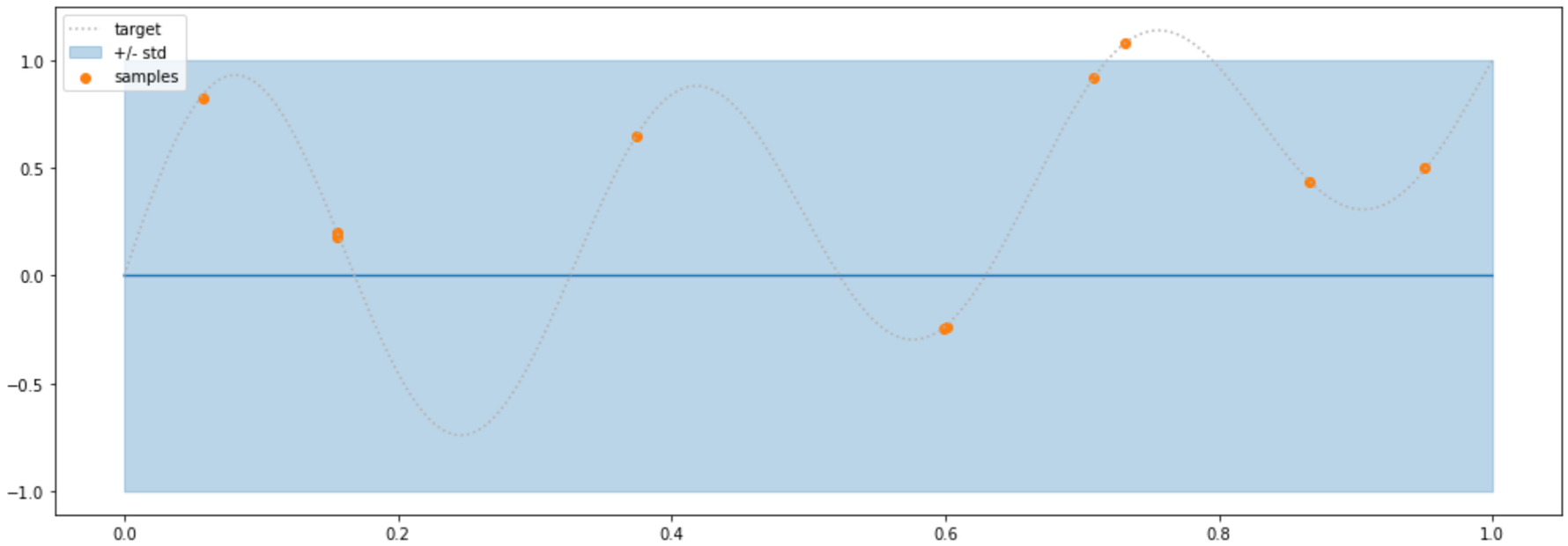
The "predictions" in this case are full probability distribution

- Since we know they are Normal
- ...They are characterized via a mean and standard deviation

Untrained Guassian Processes

Here's how the prediction look before training

In [5]:
```
y_mu, y_std = pd.Series(index=x, data=y_mu), pd.Series(index=x, data=y_std)
util.plot_series(series=y_mu, std=y_std, samples=y_tr, target=target, figsize=figsize)
```



- The mean is 0 everywhere
- ...And we are not exploiting Σ, since there is no stored observarion

Training a Gaussian Process

Now, let's train our model:

In [6]:
```
gp.fit(y_tr.index.values.reshape(-1,1), y_tr.values)
```

Out[6]:
```
GaussianProcessRegressor(kernel=RBF(length_scale=1), n_restarts_optimizer=9,
                         normalize_y=True)
```

During this process, two things happen:

- First, the kernel parameters are optimized
- Second, the training observations are stored in the model

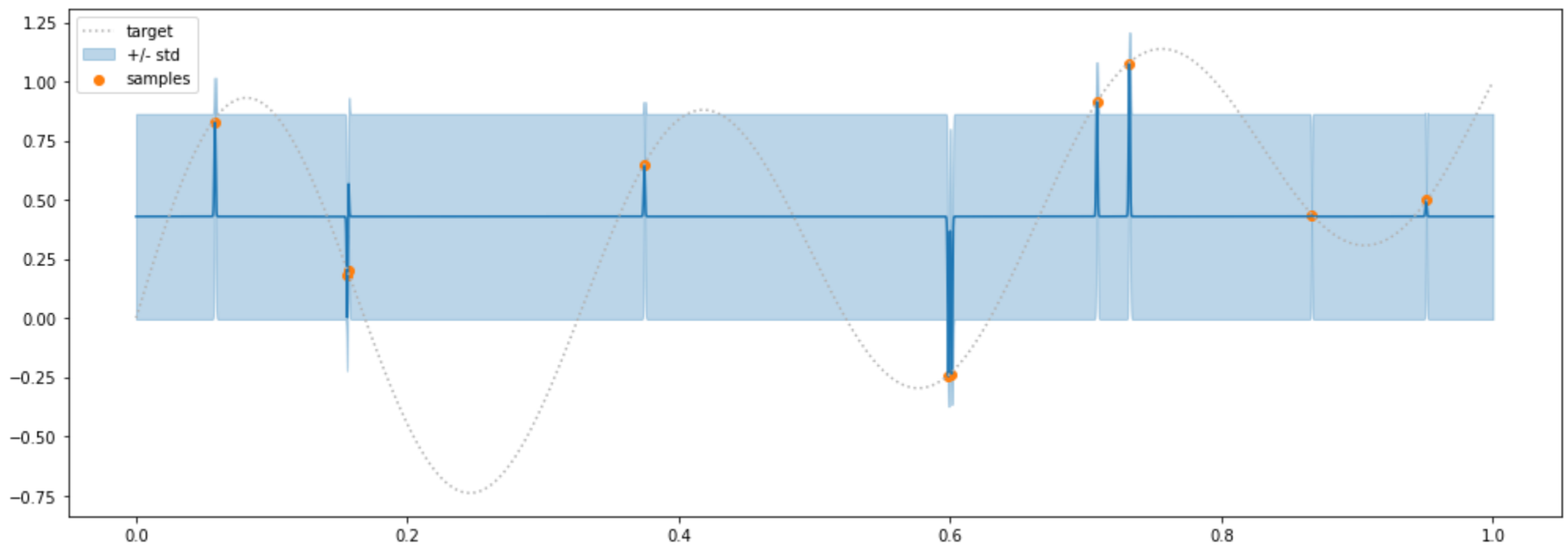
In [7]:
```
print(gp.kernel_)
print('X_train_:', str(gp.X_train_).replace('\n', ','))
print('y_train_:', str(gp.y_train_).replace('\n', ','))
```

```
RBF(length_scale=0.000494)
X_train_: [[0.37454012], [0.95071431], [0.73199394], [0.59865848], [0.15601864], [0.15599452],
[0.05808361], [0.86617615], [0.60111501], [0.70807258]]
y_train_: [ 0.49936961  0.16078846  1.49069525 -1.55533978 -0.52939824 -0.57819753,  0.9157736
6  0.01106198 -1.5385743   1.12382089]
```

Not Yet There

Let's check the updated predictions

In [8]:
```
y_mu, y_std = gp.predict(x.reshape(-1,1), return_std=True)
y_mu, y_std = pd.Series(index=x, data=y_mu), pd.Series(index=x, data=y_std)
util.plot_series(series=y_mu, std=y_std, samples=y_tr, target=target, figsize=figsize)
```



- The predicted means are close to all the observations (good news)
- ...But they get far from them very quickly (bad news)

White Noise

The issue is that we never told our model there is noise in the data

This can be done by adding a while noise kernel:

$$K(x_i, x_j, \omega) = e^{-\frac{d(x_i,x_j)^2}{2l}} + \nu(i, j)$$

Where:

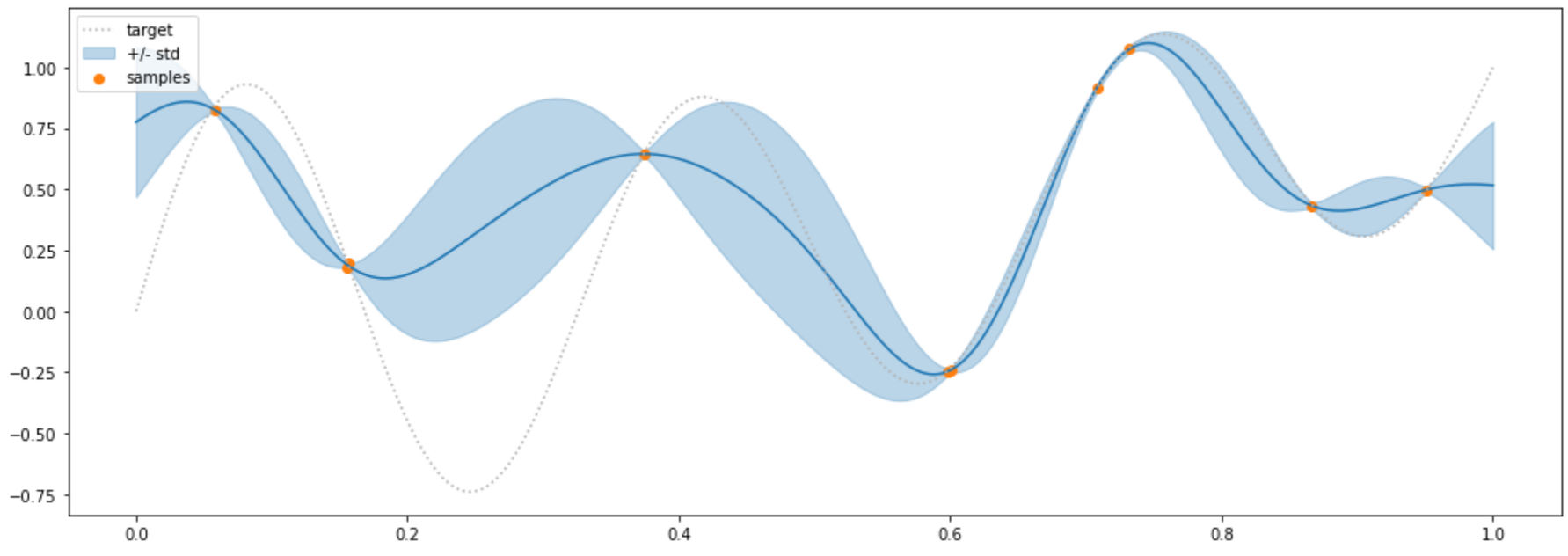
$$\nu(i, j) = \begin{cases} \sigma^2 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

- σ is the only kernel parameter
- We are telling the GP that observations have some intrinsic variance
- ...Freeing it from the need to interpolate exactly all observations

A Decent, Trained, Gaussian Process

Let's repeat training and display the results

In [9]:
```
y_mu, y_std = util.univariate_gp_tt(RBF()+WhiteKernel(), x_tr, y_tr, x)
util.plot_series(series=y_mu, std=y_std, samples=y_tr, target=target, figsize=figsize)
```



- All the predicted means are close to the observed ones
- ...And we get meaningful confidence intervals elsewhere