Gaussian Processes

Filling Values Using a Model

If we want to fill missing values better, we need to predict them

We need a model, which can infer their value

- All the approaches seen so far can be considered (extremely simple) models
- ...We just need a more advanced one!

What are the desired properties of the model we seek?

Given a gap (i.e. one or more contiguous missing values), the model:

- Must be able to make a prediction about the missing values
- ...Which is consistent with all the available observations
- I.e. it should be able to interpolate the data (in generalized sense)

Most ML models cannot be used for filling (in a straightforward fashion)

Filling Values Using a Model

Density estimation does not (natively) provide predictions

To be fair, predictions can be extracted from a density estimator:

- Given an estimator $f(\mathbf{x}, \theta)$ for $P(\mathbf{x})$ we can find the most likely value for $\mathbf{x}$ by solving:

$$\text{argmax}_{\mathbf{x}} f(\mathbf{x}, \theta)$$

- This is a Maximum A Posteriori (MAP)
- ...And its what most regressors/classifiers natively compute

However, with a density estimator, computing the MAP can be very expensive

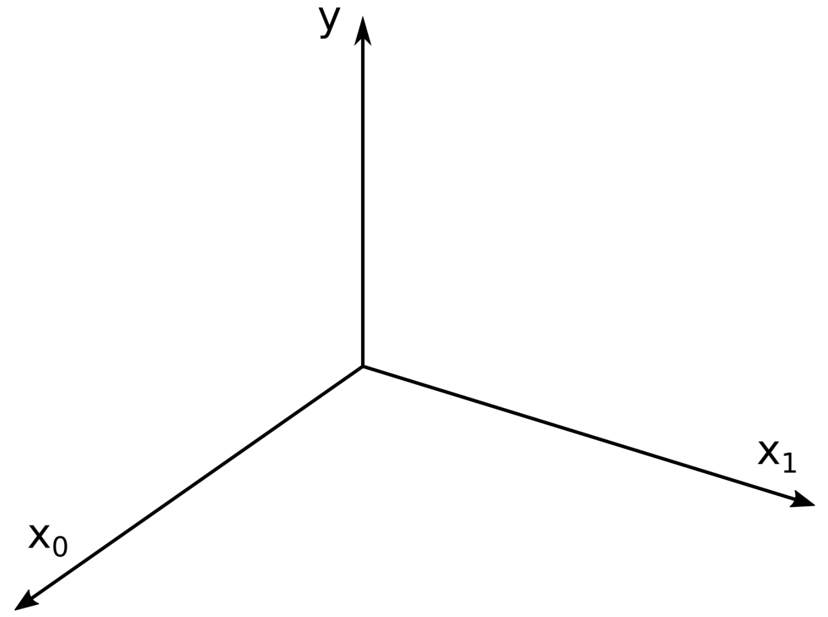
Auto-regressors makes use of past observations, but not the future ones

- They are designed for extrapolation (predict beyond the boundaries)
- ...And not for interpolation

Gaussian Processes

One of the few viable ML models is given by Gaussian Processes (GP)

We will introduce their key concepts via an example:

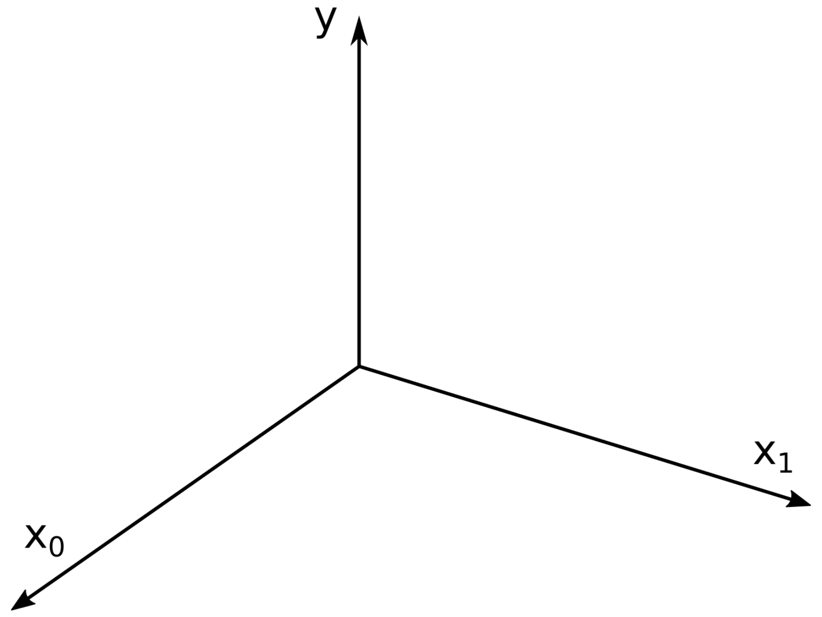


- Say we want to model how rainfall changes over a stretch of land
- $y =$ rainfall, $(x_0, x_1) =$ position on the surface of land

Gaussian Processes

One of the few viable ML models is given by Gaussian Processes (GP)

Since this is a physical phenomenon...

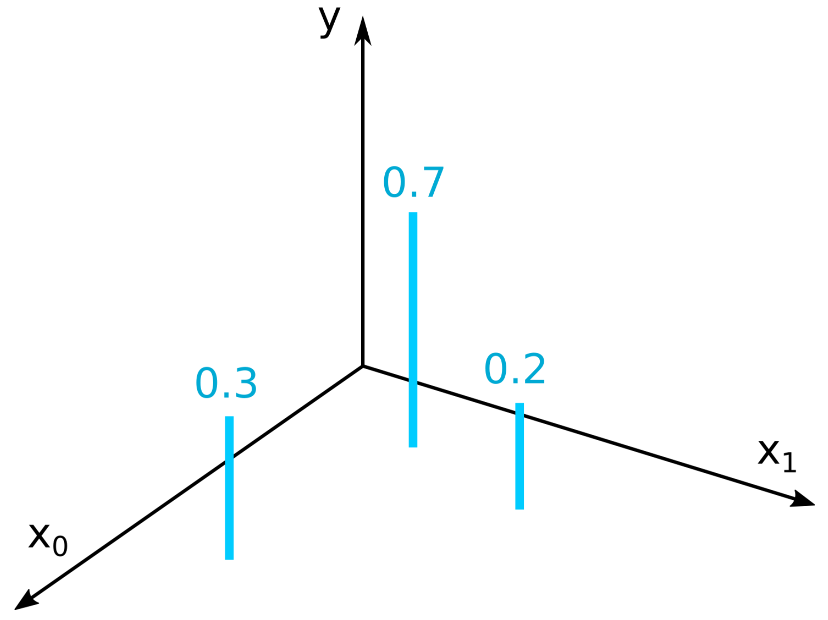


- ...We can reasonably assume that y is Normally distributed
- But unless we know more, we can say nothing else

Gaussian Processes

One of the few viable ML models is given by Gaussian Processes (GP)

However, if we have a few measurements...



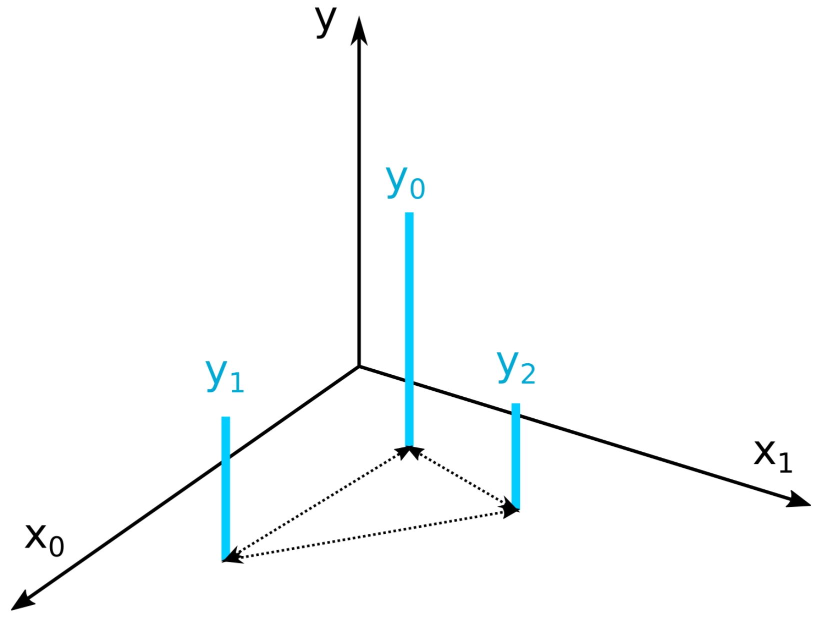
We can assume that rainfall in nearby locations is similar

- We can rely on this to estimate the chance of the measurements themselves
- ...And of rainfall at positions for which we lack measurements

Gaussian Processes

One of the few viable ML models is given by Gaussian Processes (GP)

We 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 the covariance will depend on the distance between measurements

Gaussian Processes

Formally:

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

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

Some examples:

- $\boldsymbol{y_x}$ could be the rainfall rate at location $\boldsymbol{x}$
- $\boldsymbol{y_x}$ could be the twitter volume at time $\boldsymbol{x}$
- $\boldsymbol{y_x}$ could be the traffic volume at time $\boldsymbol{x}$

In general y_x is the value of a (stochastic) function for input x

Multivariate Normal Distritbuion

The multivariate normal distribution?

- It works for many real world phenomena
- It has a closed-form density function that is (relatively) easy to compute
- The PDF is defined via a (vector) mean $\boldsymbol{\mu}$ and a covariance matrix Σ
- ...And often we can assume $\boldsymbol{\mu} = \mathbf{0}$, so knowing Σ is enough

So, given a set of indexes/input values of interest X

Then, if we manage to know Σ, we can compute:

- The probability density $f(\hat{\mathbf{y}}_{\mathbf{X}})$ of some given observations
  - I.e. the probability of a dataset
- The conditional density $f(\hat{y}_x \mid \hat{\mathbf{y}}_{\mathbf{X}})$ of a new observation
  - I.e. a prediction w.r.t. a set of know observations $\hat{y}_X$

Defining the Covariance Matrix

How do we define Σ?

We assume that the covariance depends on $\boldsymbol{x}$ (and not on the $\boldsymbol{y}$)

- Given two variables $\boldsymbol{y}_{x_i}$ and $\boldsymbol{y}_{x_j}$, their covariance is given by $K(x_i, x_j)$
- Where K is called a kernel function (and is user chosen)

Given any finite set of variables $\{y_{x_1}, \dots y_{x_n}\}$, the covariance matrix is:

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

- I.e. it's entirely specified via the kernel

Unfortunately, choosing the kernel completely by hand would still be too difficult

Fitting a Gaussian Process

In practice, to define the kernel we:

- Pick a parameterized kernel function $K_\theta(x_i, x_j)$, where $\boldsymbol{\theta}$ = parameter vector
- Collect training observations $\hat{\mathbf{y}}_{\mathbf{X}}$

Then we choose θ so as to maximize the likelihood of the training data, i.e.:

$$\text{argmax}_\theta f(\hat{\mathbf{y}}_{\mathbf{X}}, \theta)$$

- Where $f(\hat{\mathbf{y}}_{\mathbf{X}}, \theta)$ is the estimated probability density of the observations

The training problem

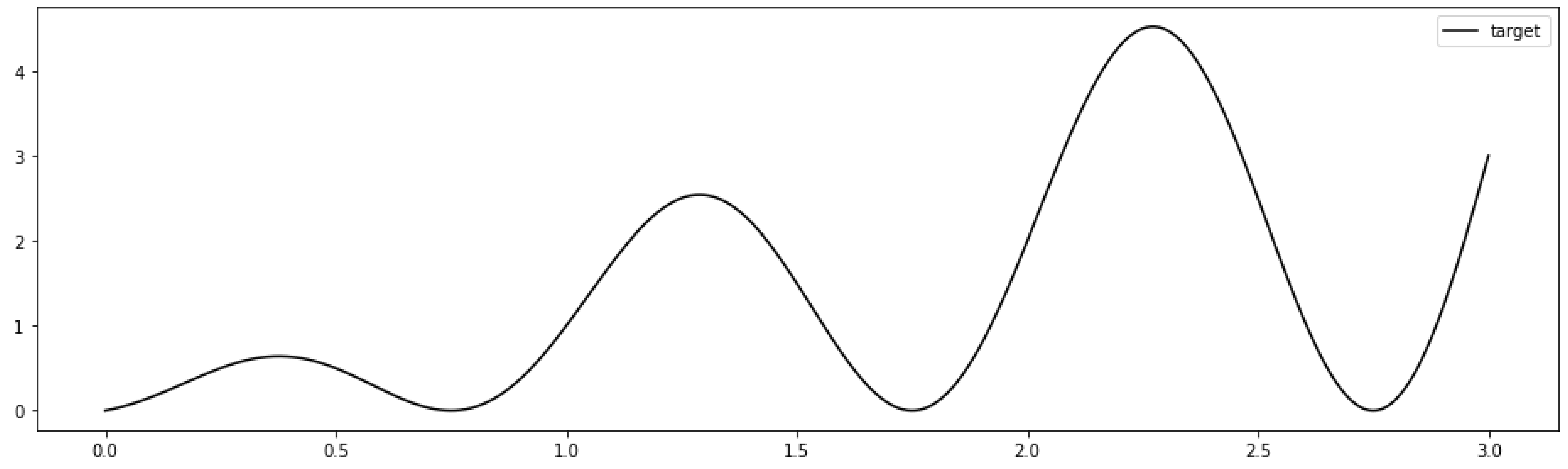
- Is a (possibly challenging) numerical optimization problem
- ...Which is typically solved to local optimality (e.g. via gradient descent)

Gaussian Processes in scikit-learn

Let's see how to use Gaussian Processes in scikit-learn

First, let us choose a target function:

```
In [2]: f = lambda x: x * np.sin(2*np.pi*x) + x # target function
        x = np.linspace(0, 3, 1000)
        y = pd.Series(index=x, data=f(x))
        nab.plot_gp(target=y, figsize=figsize)
```

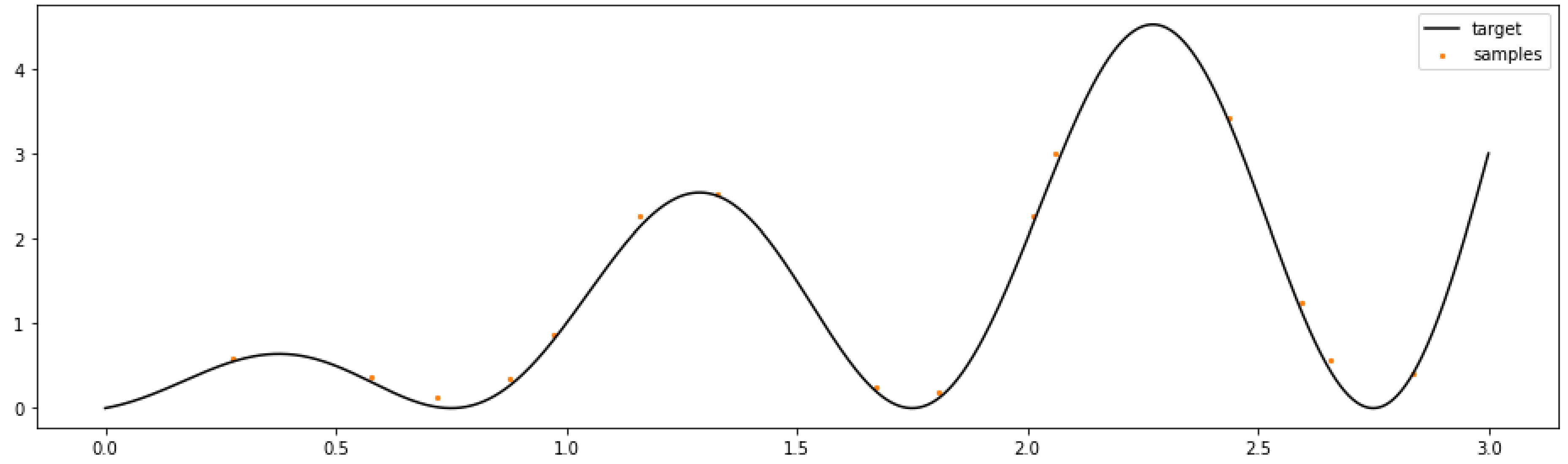


Gaussian Processes in scikit-learn

Let's see how to use Gaussian Processes in scikit-learn

Then we build a small training set:

In [3]:
```
np.random.seed(42)
n_tr = 15
x_tr = np.linspace(0.2, 2.8, n_tr) + 0.2*np.random.rand(n_tr)
x_tr.sort()
y_tr = pd.Series(index=x_tr, data=f(x_tr) + 0.2*np.random.rand(n_tr))
nab.plot_gp(target=y, samples=y_tr, figsize=figsize)
```



Gaussian Processes in scikit-learn

Let's see how to use Gaussian Processes in scikit-learn

Then we need to choose a kernel

- There are many available options
- We will start with a simple Radial Basis Function (i.e. Gaussian) kernel

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

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

We have 15 indexes, so the kernel will define a 15×15 covariance matrix

Gaussian Processes in scikit-learn

Here's how to use an RBF kernel in scikit-learn

```
In [4]: from sklearn.gaussian_process.kernels import RBF

        kernel = RBF(1, (1e-3, 1e3))
```

The RBF kernel has a single parameter, representing its scale

The extra (tuple) parameter represents a pair of bounds

- During training only parameter values within the boundaries will be considered
- Bounds can be very useful for controlling the training process
- ...Based on the available domain information

Gaussian Processes in scikit-learn

Now we can train a Gaussian Process

```
In [5]: from sklearn.gaussian_process import GaussianProcessRegressor
        gp = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
        gp.fit(y_tr.index.values.reshape(-1,1), y_tr.values) # needs 2D input
        gp.kernel_

Out[5]: RBF(length_scale=0.229)
```

- Training uses Gradient Descent...
- ...To maximize the likelihood (density) of the training data
- Restarts are needed to mitigate issues due to local optima

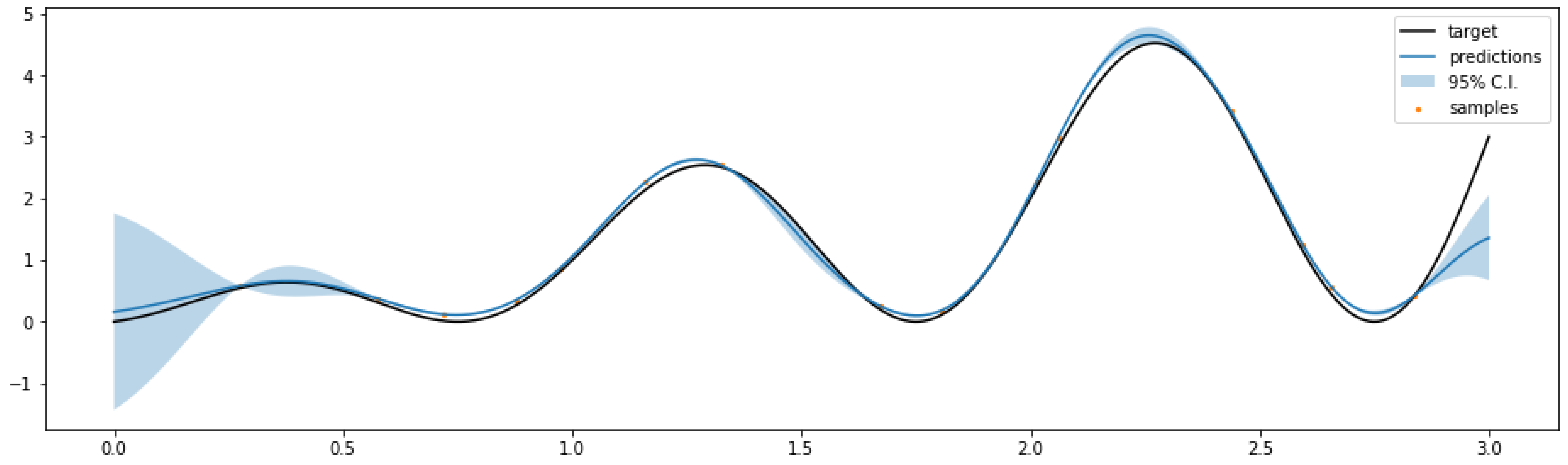
And then we can obtain the predictions:

```
In [6]: xp, std = gp.predict(x.reshape(-1,1), return_std=True)
        xp = pd.Series(index=y.index, data=xp)
        std = pd.Series(index=y.index, data=std)
```

Gaussian Processes in scikit-learn

We can now plot the predictions

```
In [7]: nab.plot_gp(target=y, samples=y_tr, pred=xp, std=std, figsize=figsize)
```



- We get both a point estimate (the blue line)
- ...And a confidence interval (the light blue areas)

But how did we manage that?

Behind the Scenes

There are two tricks at work here:

1) The training examples $\hat{\mathbf{y}}_{\mathbf{X}}$ are part of the GP parameters

- This is similar to what we have (e.g.) in KDE
- ...And quite different from other ML methods (e.g. NN, DTs, SVMs...)

Given an new input value $\boldsymbol{x}$, the GP output corresponds to:

$$f\left(y_x \mid \hat{\mathbf{y}}_{\mathbf{X}}\right)$$

- I.e. the probability of y_x conditioned on the known examples

2) For computing Σ, we only need to know the input values (i.e. X and x)

- This is by construction: all our kernels $K(x_i, x_j)$ are built this way
- Which means that we can compute $f\left(y_x \mid \hat{\mathbf{y}}_{\mathbf{X}}\right)$ via a closed-form expression

Behind the Scenes

Thanks to this, for $f\left(y_x \mid \hat{\mathbf{y}}_{\mathbf{X}}\right)$ we can get

The conditional mean (which is also the MAP):

$$\arg\max_{y_x} f\left(y_x \mid \hat{\mathbf{y}}_{\mathbf{X}}\right)$$

- This will be our "prediction"

The conditional standard deviation

$$\sqrt{\text{Var}\left[f\left(y_x \mid \hat{\mathbf{y}}_{\mathbf{X}}\right)\right]}$$

- This is used to define the confidence intervals

In practice, we GP output is a probability distribution

A Numeric Example

As an example, say we want a prediction for $x = 2.5$, i.e. $y_{2.5}$

...And let's assume that our training set contains only one example

- We will consider separately the tenth and first example in our dataset
- We have: $(\hat{x}_9, \hat{y}_{\hat{x}_9}) \simeq (2.01, 2.27)$ and $(\hat{x}_0, \hat{y}_{\hat{x}_0}) \simeq (0.27, 0.58)$

The covariance matrix in the two cases is therefore:

$$\Sigma_{y_x, \hat{y}_{\hat{x}_9}} = \begin{pmatrix} K(2.01, 2.01) & K(2.01, 2.5) \\ K(2.5, 2.01) & K(2.5, 2.5) \end{pmatrix}$$

$$\Sigma_{y_x, \hat{y}_{\hat{x}_0}} = \begin{pmatrix} K(0.27, 0.27) & K(0.27, 2.5) \\ K(2.5, 0.27) & K(2.5, 2.5) \end{pmatrix}$$

- Each matrix defines a multivariate Normal distribution

Behind the Scenes

Let's actually build the matrices in Python

- Note: scikit-learn kernels are not designed to be used on individual points
- So, for this we will rely on basic numpy methods

We start with $\hat{x}_9$ and x, which are close to each other

In [8]:
```
from scipy.stats import multivariate_normal
X9, X0, X = [[x_tr[9]]], [[x_tr[0]]], [[2.5]] # Must be 2D
sigma_9x = np.array([[kernel(X9, X9)[0,0], kernel(X9, X)[0,0]],
                     [kernel(X, X9)[0,0], kernel(X, X)[0,0]]])
f_9x = multivariate_normal([0, 0], cov=sigma_9x)
```

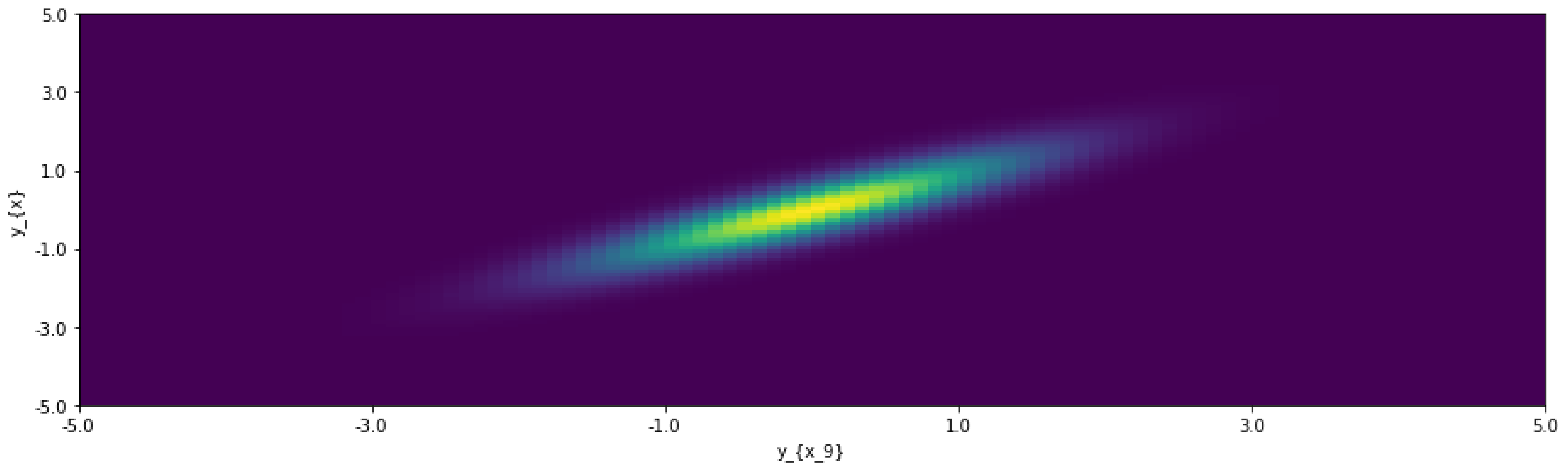
Then we do the same for $\hat{x}_0$ and x, which are far apart

In [9]:
```
sigma_0x = np.array([[kernel(X0, X0)[0,0], kernel(X0, X)[0,0]],
                     [kernel(X, X0)[0,0], kernel(X, X)[0,0]]])
f_0x = multivariate_normal([0, 0], cov=sigma_0x)
```

Behind the Scenes

$\hat{x}_9$ and x are close to each other, so $\hat{y}_{\hat{x}_9}$ and y_x are strongly correlated

```
In [10]: yr = np.linspace(-5, 5, 100)
         nab.plot_distribution_2D(f_9x, yr, yr, figsize=figsize)
         plt.xlabel('y_{x_9}'); plt.ylabel('y_{x}'); plt.tight_layout()
```

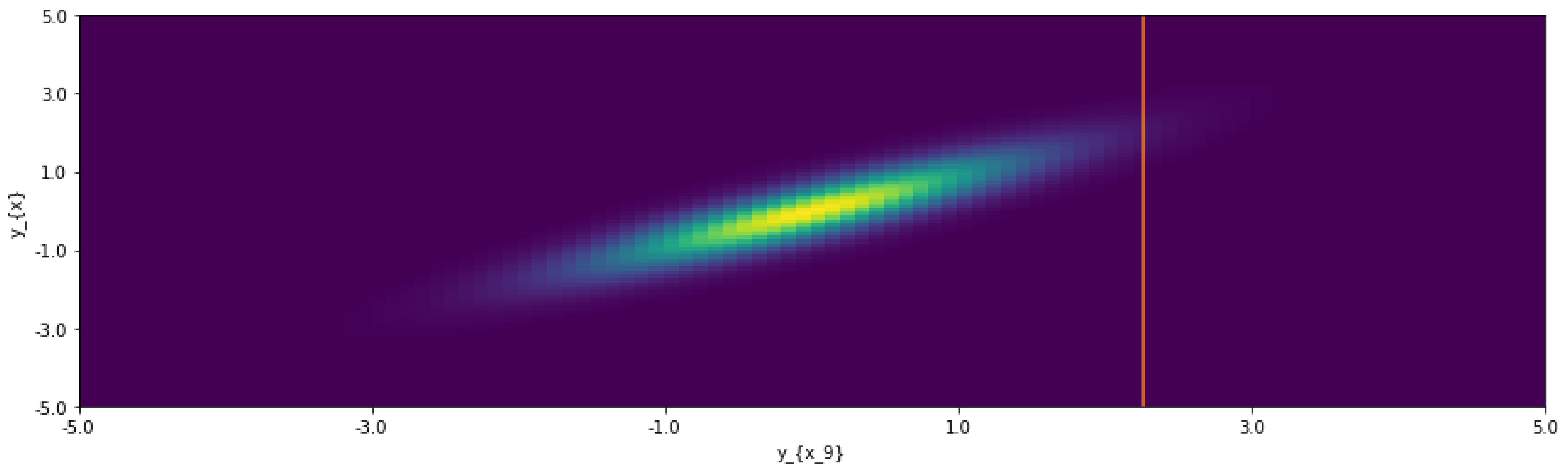


- Still, if we know neither $\hat{y}_{\hat{x}_9}$ nor y_x, we can only say that they are likely both zero

Behind the Scenes

But we do know $\hat{y}_{\hat{y}_9}$! So, we can use this information_

```
In [11]: nab.plot_distribution_2D(f_9x, yr, yr, figsize=figsize)
         plt.axvline(10*(y_tr[x_tr[9]] + 5), color='tab:orange');
         plt.xlabel('y_{x_9}'); plt.ylabel('y_{x}'); plt.tight_layout()
```

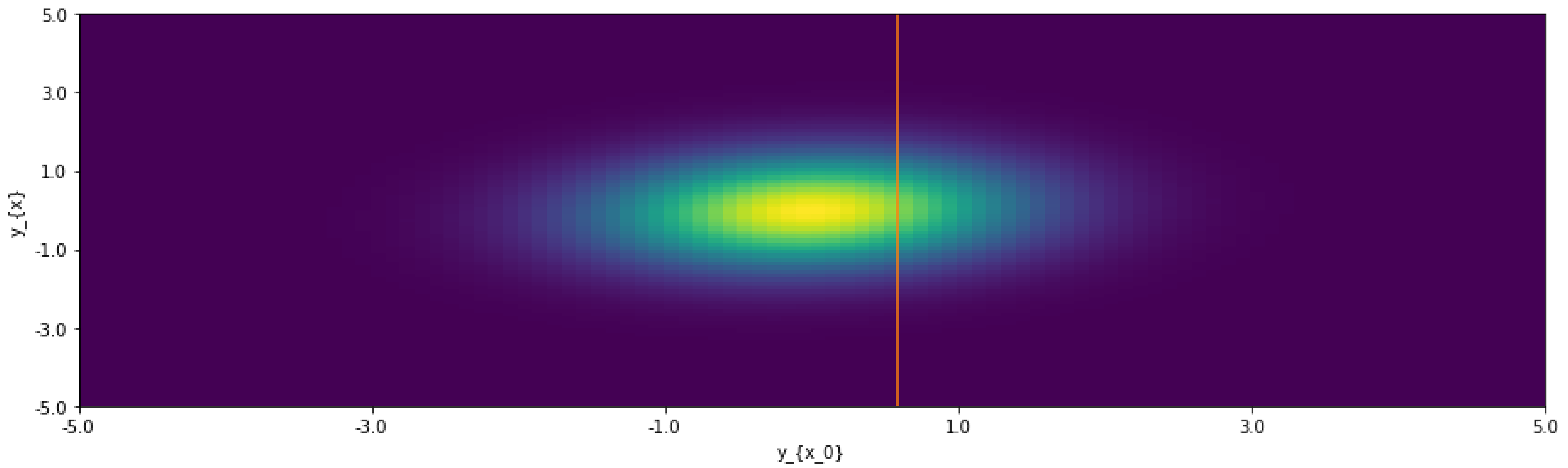


- Given the observation, the most likely value for y_x changes considerably

Behind the Scenes

$\hat{x}_0$ and x are far apart, so $\hat{y}_{\hat{x}_0}$ and y_x are loosely correlated

In [12]:
```
nab.plot_distribution_2D(f_0x, yr, yr, figsize=figsize)
plt.axvline(10*(y_tr[x_tr[0]] + 5), color='tab:orange');
plt.xlabel('y_{x_0}'); plt.ylabel('y_{x}'); plt.tight_layout()
```



- Knowing $\hat{y}_{\hat{x}_0}$ is not going to be of much help here

Behind the Scenes

So, a few key insight to keep in mind:

- Superficially, GPs behave like functions that output probability distribution
- Internally, this is enabled by two components:
  - The kernel, defining how all the points are correlated
  - A set of observations, use to obtain conditional distributions

In scikit-learn:

When we call the `fit` method:

- The optimizer adjusts the kernel parameters
- ...And the observations $\hat{y}_{\hat{x}}$ are stored

When we call the `predict` method:

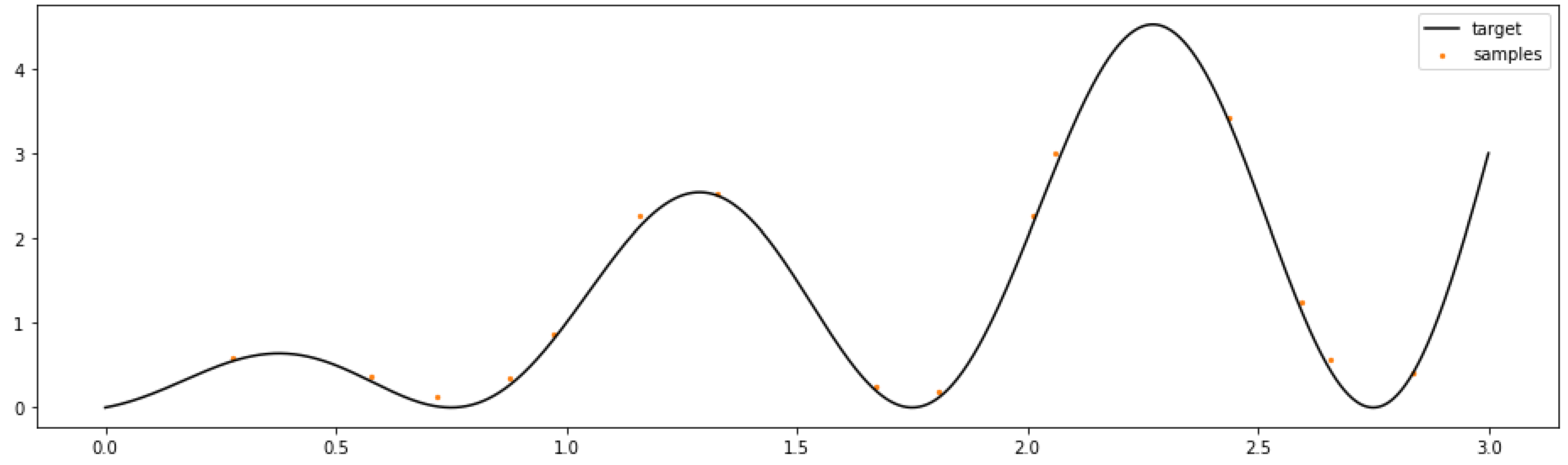
- The covariance matrix is built
- The model computes the conditional distributions

How to Improve the Model

Now, let's try to improve our model

We need to choose a kernel appropriate to our dataset

```
In [13]: nab.plot_gp(target=y, samples=y_tr, figsize=figsize)
```



- We a bit of noise, a period, and a trend

How to Improve the Model

So, let us deal with the noise first

```
In [14]: from sklearn.gaussian_process.kernels import WhiteKernel

         kernel = WhiteKernel(0.1, (1e-3, 1e3))
         kernel += RBF(1, (1e-2, 1e2))
```

`WhiteKernel` captures the presence of noise in the data

$$K(x_i, x_j) = \sigma^2 \text{ iff } x_i = x_j, 0 \text{ otherwise}$$

- The only parameter of `WhiteKernel` represents the noise level σ^2
- A small noise level prevent overfitting the data
- ...But too much noise leads to useless predictions!

How to Improve the Model

It's often a good idea to have magnitude parameters in the kernel

In [15]:
```
from sklearn.gaussian_process.kernels import ConstantKernel

kernel = WhiteKernel(0.1, (1e-2, 1e2))
kernel += ConstantKernel(1, (1e-2, 1e2)) * RBF(1, (1e-2, 1e2))
```

`ConstantKernel` is a constant factor (in this case a relative weight)

- ...And allows the optimizer to tune the magnitude of the RBF kernel

Let's repeat training again:

In [16]:
```
gp = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
gp.fit(y_tr.index.values.reshape(-1,1), y_tr.values) # needs 2D input
print(gp.kernel_)
```

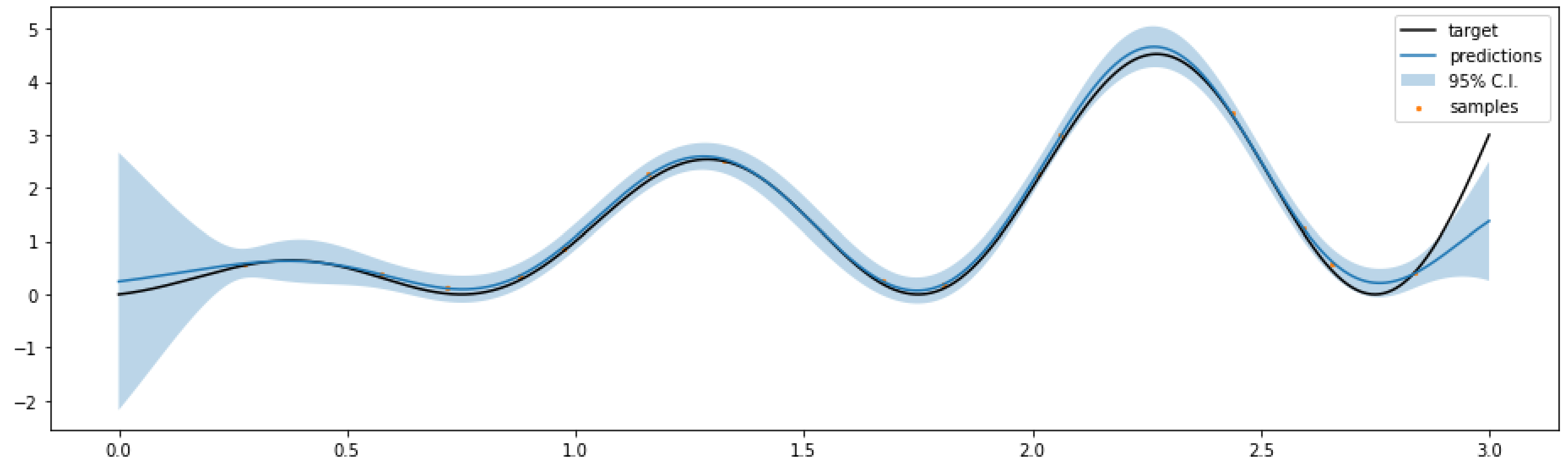
```
WhiteKernel(noise_level=0.01) + 2.21**2 * RBF(length_scale=0.321)
```

```
/usr/local/lib/python3.9/site-packages/sklearn/gaussian_process/kernels.py:402: ConvergenceWar
ning: The optimal value found for dimension 0 of parameter k1__noise_level is close to the spe
cified lower bound 0.01. Decreasing the bound and calling fit again may find a better value.
  warnings.warn("The optimal value found for "
```

How to Improve the Model

Let us see the new predictions

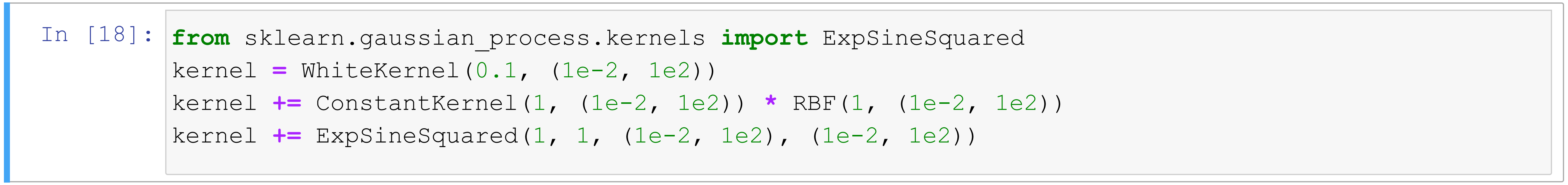
In [17]:
```
xp, std = gp.predict(x.reshape(-1,1), return_std=True)
xp = pd.Series(index=y.index, data=xp)
std = pd.Series(index=y.index, data=std)
nab.plot_gp(target=y, samples=y_tr, pred=xp, std=std, figsize=figsize)
```



- Better, but we are still not exploiting the period and the trend

How to Improve the Model

So, let us take them into account, starting with the period



```
In [18]: from sklearn.gaussian_process.kernels import ExpSineSquared
         kernel = WhiteKernel(0.1, (1e-2, 1e2))
         kernel += ConstantKernel(1, (1e-2, 1e2)) * RBF(1, (1e-2, 1e2))
         kernel += ExpSineSquared(1, 1, (1e-2, 1e2), (1e-2, 1e2))
```

`ExpSineSquared` captures the period:

$$K(x_i, x_j) = e^{-2\frac{\sin^2\left(\pi \frac{d(x_i,x_j)}{p}\right)}{l^2}}$$

- The correlation grows is the distance is close to a multiple of the period p
- The scale parameter l control the rate of decrease/increase
- In the implementation, the first parameter is l and the second p

How to Improve the Model

Now, let's try to capture the trend

```
In [19]: from sklearn.gaussian_process.kernels import DotProduct
         kernel = WhiteKernel(0.1, (1e-2, 1e2))
         kernel += ConstantKernel(1, (1e-2, 1e2)) * RBF(1, (1e-2, 1e2))
         kernel += ExpSineSquared(1, 1, (1e-2, 1e2), (1e-2, 1e2))
         kernel += DotProduct(1, (1e-2, 1e2))
```

`DotProduct` (somewhat) captures the trend:

$$K(x_i, x_j) = \sigma^2 + x_i x_j$$

- The larger the x values, the larger the correlation
- This allows the distance from the mean (which is zero) to grow
- The σ parameter controls the base level of correlation
- Unlike all kernels so far `DotProduct` is not translation-invariant (we sa!

How to Improve the Model

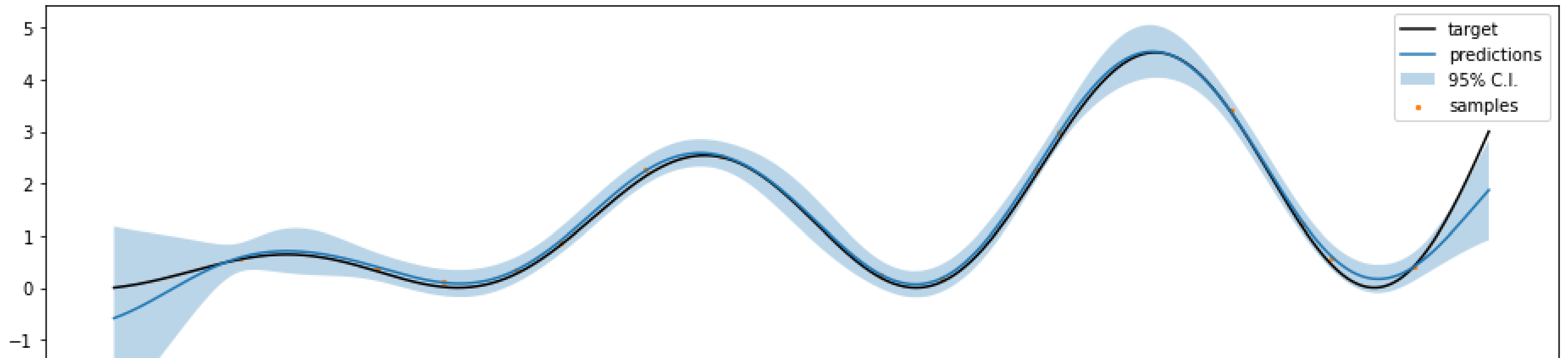
The new predictions are a bit better at the edges of the plot

In [20]:

```
gp = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
gp.fit(y_tr.index.values.reshape(-1,1), y_tr.values) # needs 2D input
print(gp.kernel_)
xp, std = gp.predict(x.reshape(-1,1), return_std=True)
xp = pd.Series(index=y.index, data=xp)
std = pd.Series(index=y.index, data=std)
nab.plot_gp(target=y, samples=y_tr, pred=xp, std=std, figsize=figsize)
```

```
/usr/local/lib/python3.9/site-packages/sklearn/gaussian_process/kernels.py:402: ConvergenceWar
ning: The optimal value found for dimension 0 of parameter k1__k1__k1__noise_level is close to
the specified lower bound 0.01. Decreasing the bound and calling fit again may find a better v
alue.
  warnings.warn("The optimal value found for "
```

```
WhiteKernel(noise_level=0.01) + 1.17**2 * RBF(length_scale=0.305) + ExpSineSquared(length_scal
e=2.17, periodicity=0.939) + DotProduct(sigma_0=0.0197)
```



Considerations

Gaussian Processes are a very flexible ML technique

- They can be used to making predictions
- ...Together with their confidence intervals
- ...But also for (conditional) density estimation
- ...And for generating data

They are non-trivial to use:

- In particular, choosing a kernel requires some practice and some understanding
- Automating the process is possible, but complex (grid search is likely not enough)

Gaussian processes tend to perform better: