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):

- 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. time, space, temperature...)
- The index is continuous and the collection infinite
- Every finite subset of y_x variables follows a Multivariate Normal Distribution

Intuitively: it's a bunch of correlated, named, Normally-distributed variables

For example:

- y_x could be the occupancy/twitter volume at time x
- y_x could be the rainfall rate at location x

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

Multivariate Normal Distritbuion

The multivariate normal distribution:

- Has a closed-form density function that is (relatively) easy to compute
- Is uniquely defined by its (vector) mean $\boldsymbol{\mu}$
- ...And its covariance matrix $\boldsymbol{\Sigma}$

If we assume centered data ($\boldsymbol{\mu} = \mathbf{0}$), then knowing $\boldsymbol{\Sigma}$ is enough

Say we have a vector of observations $\hat{\mathbf{y}}_{\mathbf{X}}$, for a set of indexes/input values X

Then, if we manage to know $\boldsymbol{\Sigma}$, we can compute:

- The probability density $f(\hat{\mathbf{y}}_{\mathbf{X}})$
- The conditional density $f(\hat{y}_x \mid \hat{\mathbf{y}}_{\mathbf{X}\setminus\mathbf{x}})$ of one observation w.r.t. the others

There are closed-form expressions for doing that

Defining the Covariance Matrix

We define Σ by assuming that the covariance depends on the indexes

Intuitively, it depends on the input values

- Given two variables y_{x_i} and 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 $\{ y_{x_1}, \ldots y_{x_n} \}$, 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
- But 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 θ = 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

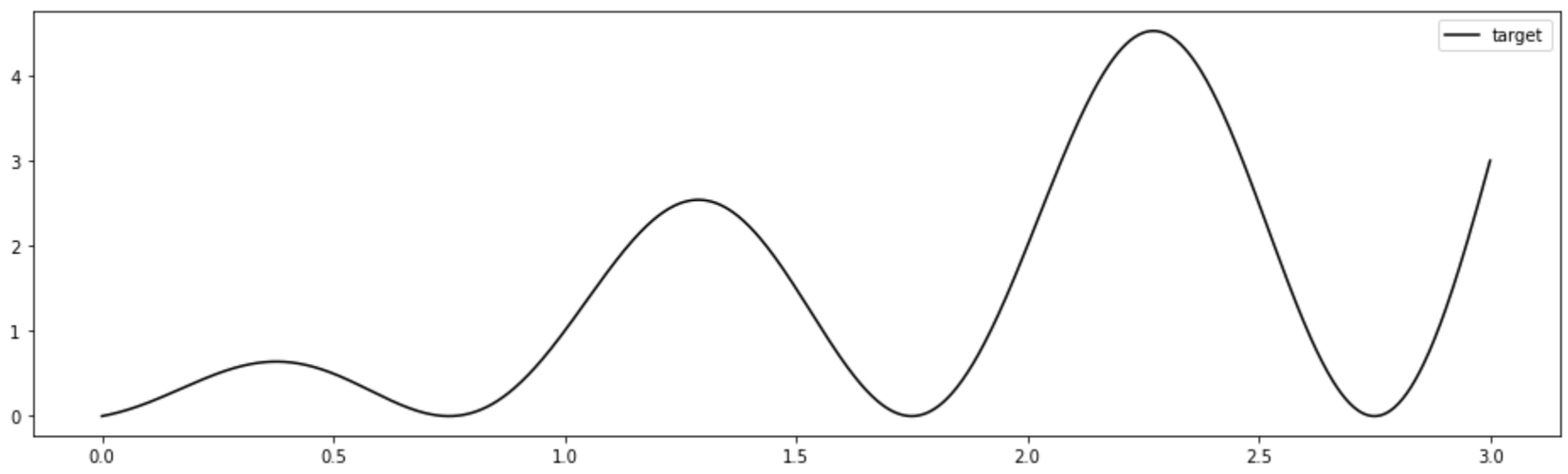
- Is a (possibly challenging) numerical optimization problem
- ...Which is typically solved to local optimality (e.g. via gradient descent)

Gaussian Processes in scikit-learn

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

First, let us choose a target function:

In [3]:
```
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)
```

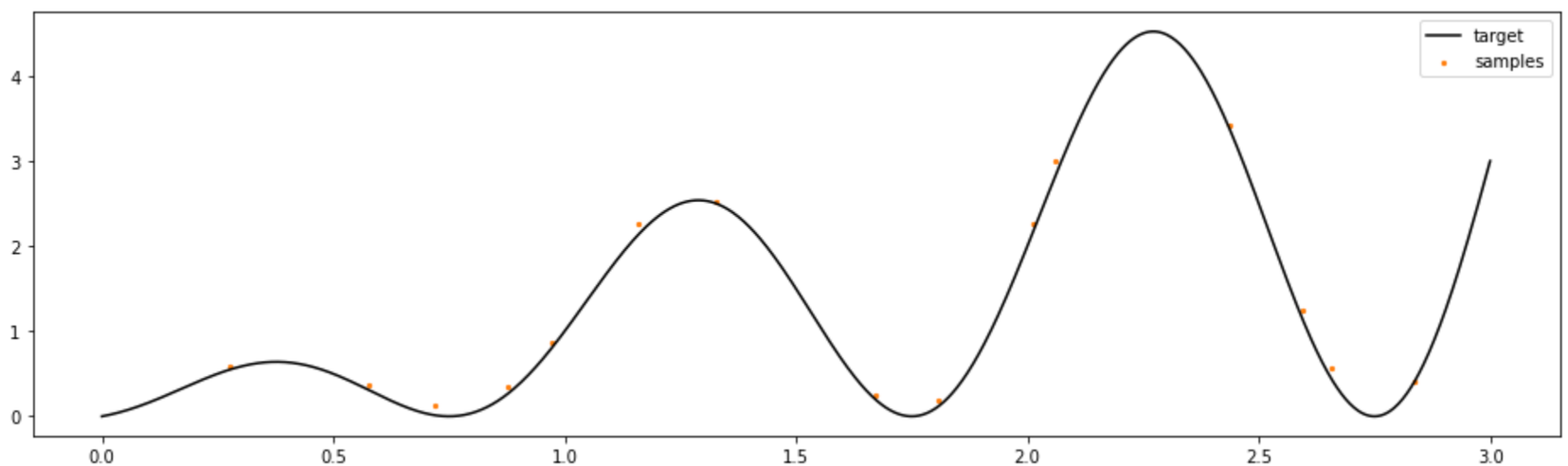


Gaussian Processes in scikit-learn

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

Then we build a small training set:

In [4]:
```
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 exponentially 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

Gaussian Processes in scikit-learn

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

In [5]:
```
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 [6]:
```
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[6]:
```
RBF(length_scale=0.229)
```

- Restarts are needed to mitigate issues due to local optima

And then we can obtain the predictions:

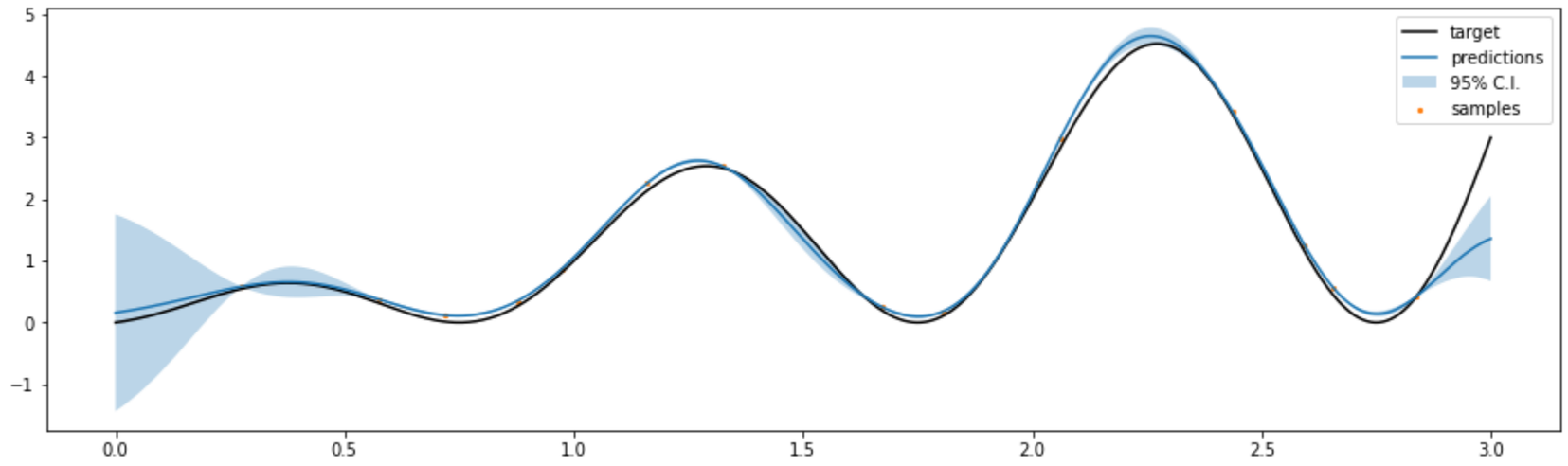
In [7]:
```
xp, std = gp.predict(x.reshape(-1,1), return_std=True)
xp = pd.Series(index=y.index, data=xp)
std = pd.Series(index=y.index, data=std)
```

- The model returns predictions (i.e. the estimated mean of the distribution)
- ...But can also return their standard deviation!

Gaussian Processes in scikit-learn

We can now plot the predictions

In [8]:
```
nab.plot_gp(target=y, samples=y_tr, pred=xp, std=std, figsize=figsize)
```



- The prediction (point estimates) correspond to the blue line
- The confidence interval to 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 $\boldsymbol{K}(\boldsymbol{x}_i, \boldsymbol{x}_j)$ 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

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

- 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 [9]:
```
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)
```

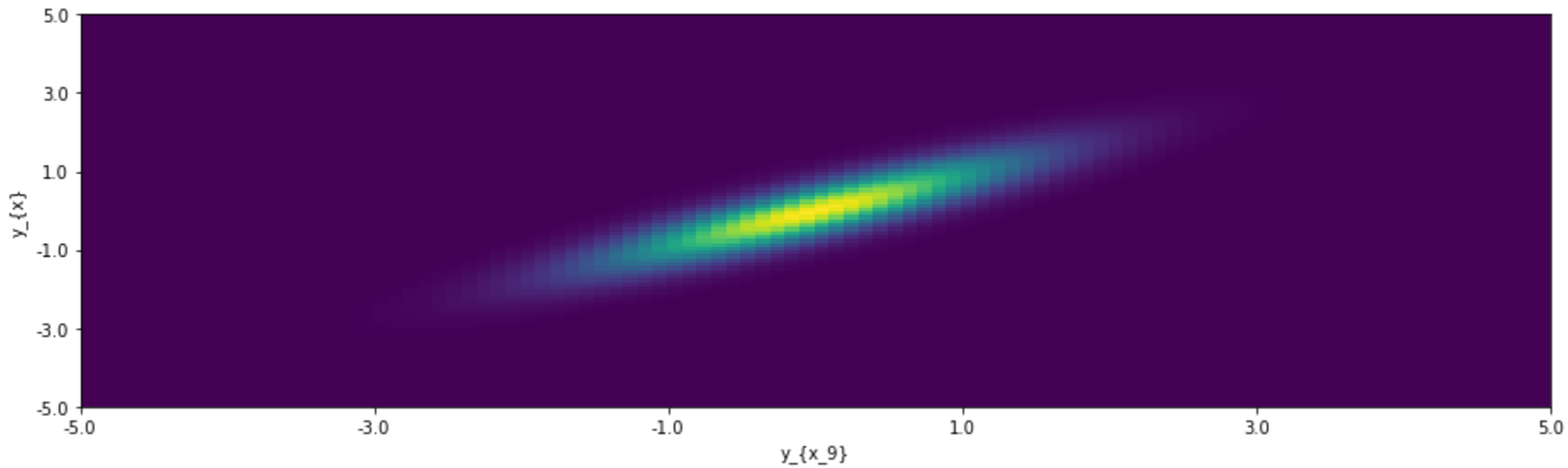
Then we do the same for $\hat{x}_0$ and x, which are far apart

In [10]:
```
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 [12]:
```
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()
```

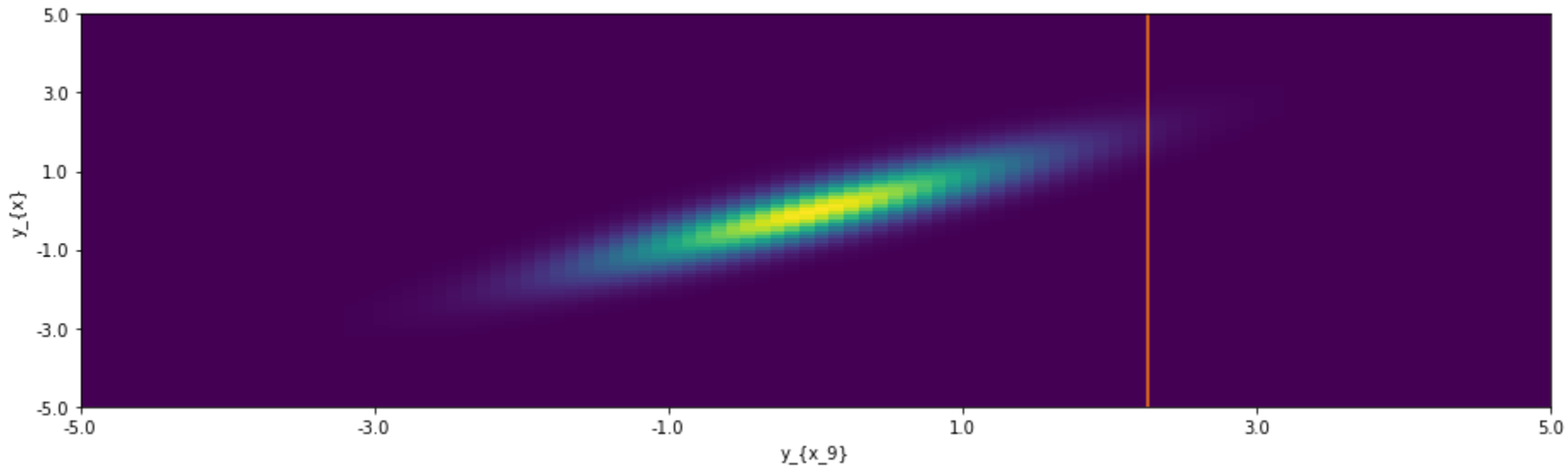


- Still, if we know neither $\hat{y}_{\hat{x}_9}$ nor y_x, we can only say that they are likely both zero

Behind the Scenes

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

In [13]:
```
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()
```

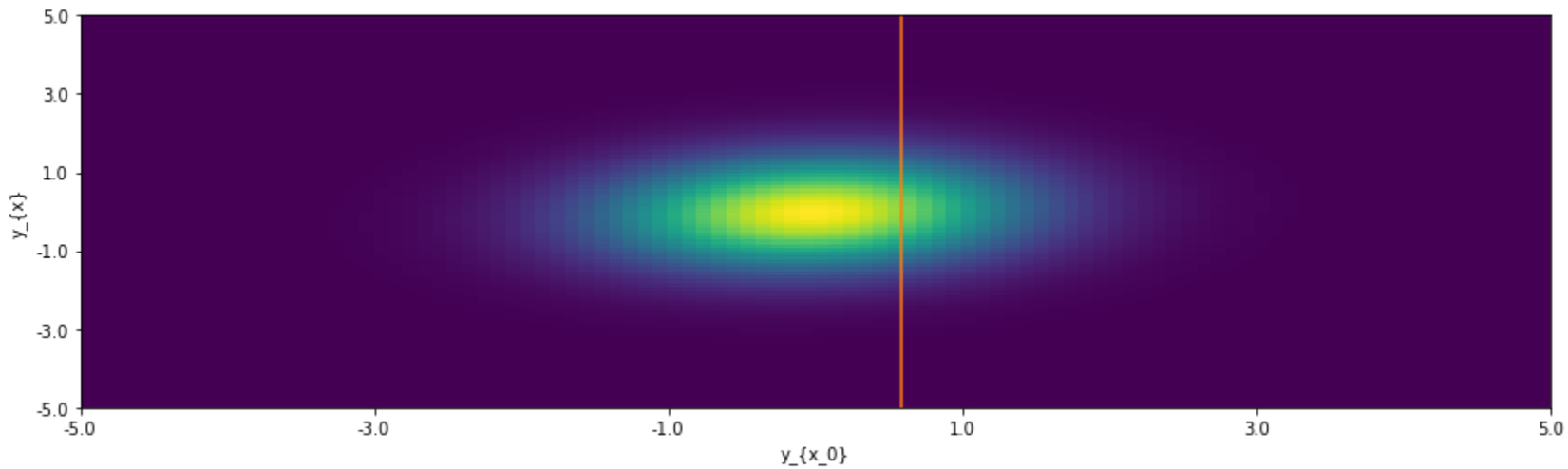


- Given the observation, the most likely value for y_x changes considerably

Behind the Scenes

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

In [14]:
```
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:

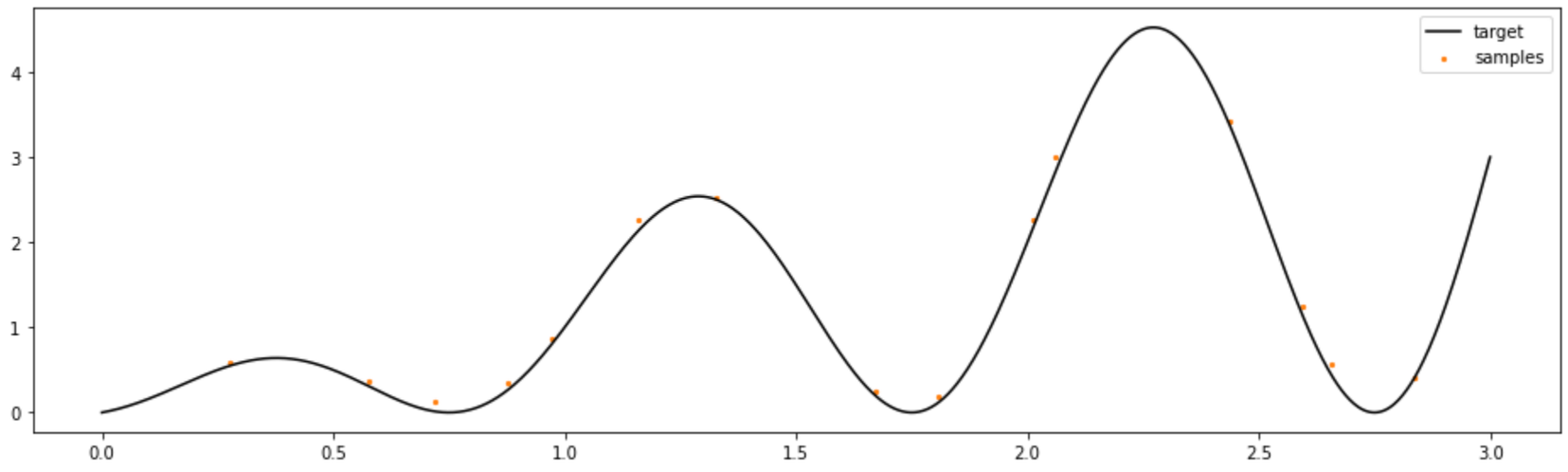
- The covariance matrix is built
- The model computes the conditional distributions

How to Improve the Model

Now, let's try to improve our model

We need to choose a kernel appropriate to our dataset

In [15]:
```
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 [16]:
```
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 [17]:
```
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 [18]:
```
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_)
```

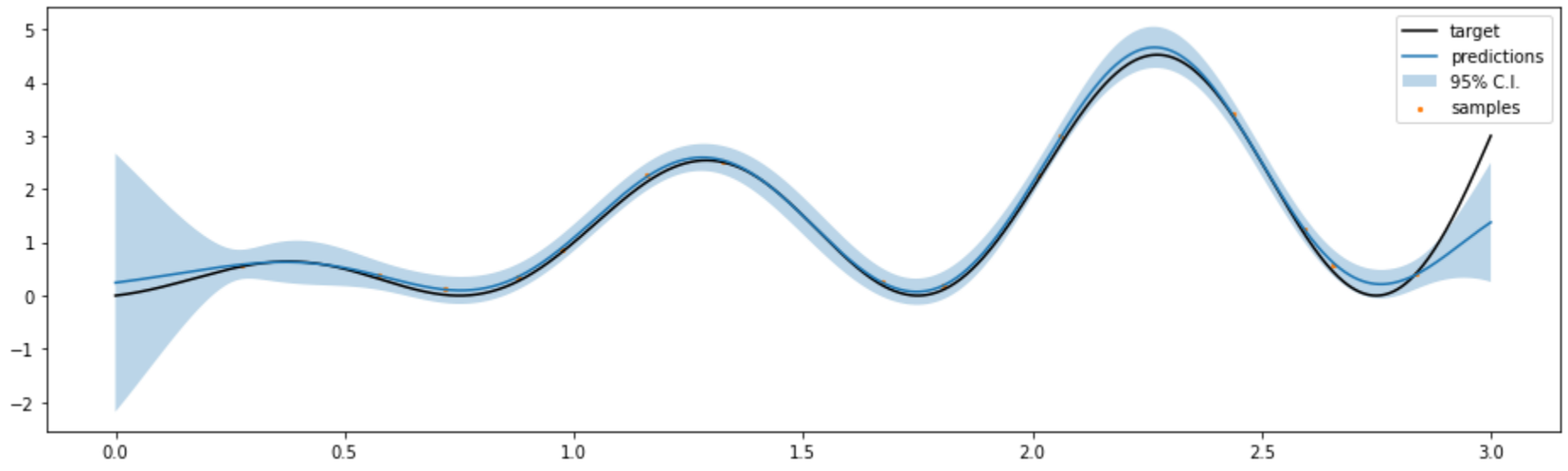
```
WhiteKernel(noise_level=0.01) + 2.21**2 * RBF(length_scale=0.321)
```

```
/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 [20]:
```
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 [21]:
```
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 [22]:
```
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!

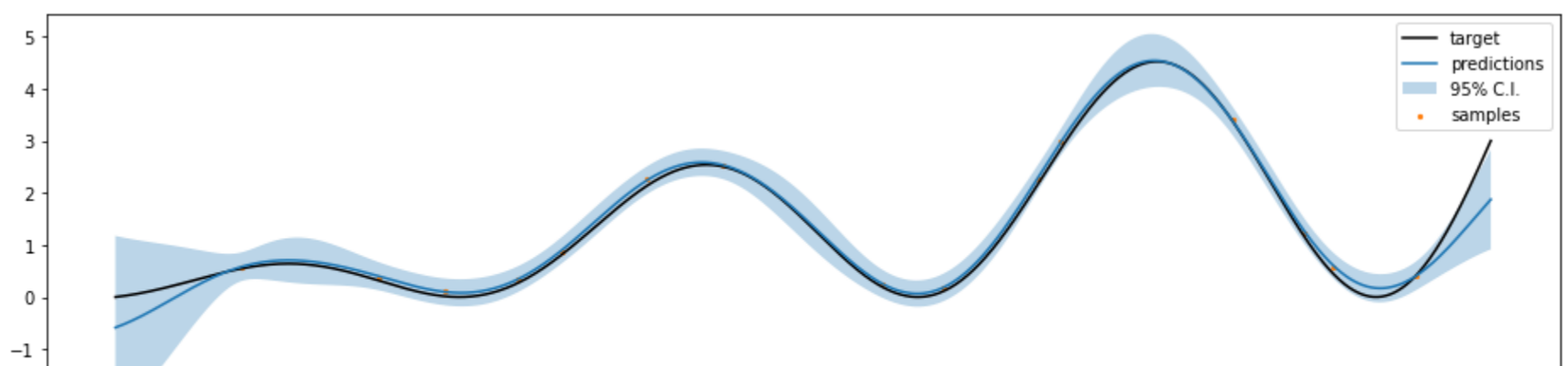
How to Improve the Model

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

In [23]:
```
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: