Gaussian Processes

If we want to do better, we need a better predictor

What would be some desired properties?

Filling Values Using a Model

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

- Should be able to make a prediction about the missing values
- It should take into account the values that are before the hole
- ...But also those that are after the hole

I.e. it should be able to interpolate all the available data

Can you think of an ML model that can to that?

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Can you think of an ML model that can to that?

If you have trouble, that's normal: there aren't many!

- Most ML models cannot be used for filling (at least not easily)
- We will see a couple of examples now

Filling Values Using a Density Estimator

Density estimation does take into account all data

...But it cannot easily provide predictions

To be fair, predictions can be obtained from a density estimator

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

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

- This is called a Maximum A Posteriori (MAP)

In fact, it's what we naturally get out of most regressors/classifiers

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...But with density estimators, computing the MAP can be very expensive

Filling Values Using a Regressor

We can train a (auto)-regressor to predict the next value in a series

...Then we can fill holes by making a "rolling forecast"

- We make one prediction
- We incorporate the prediction in the input
- Then we make another prediction and so on

...But by doing so we only rely on past values

In fact, the last prediction can be far from the next true value

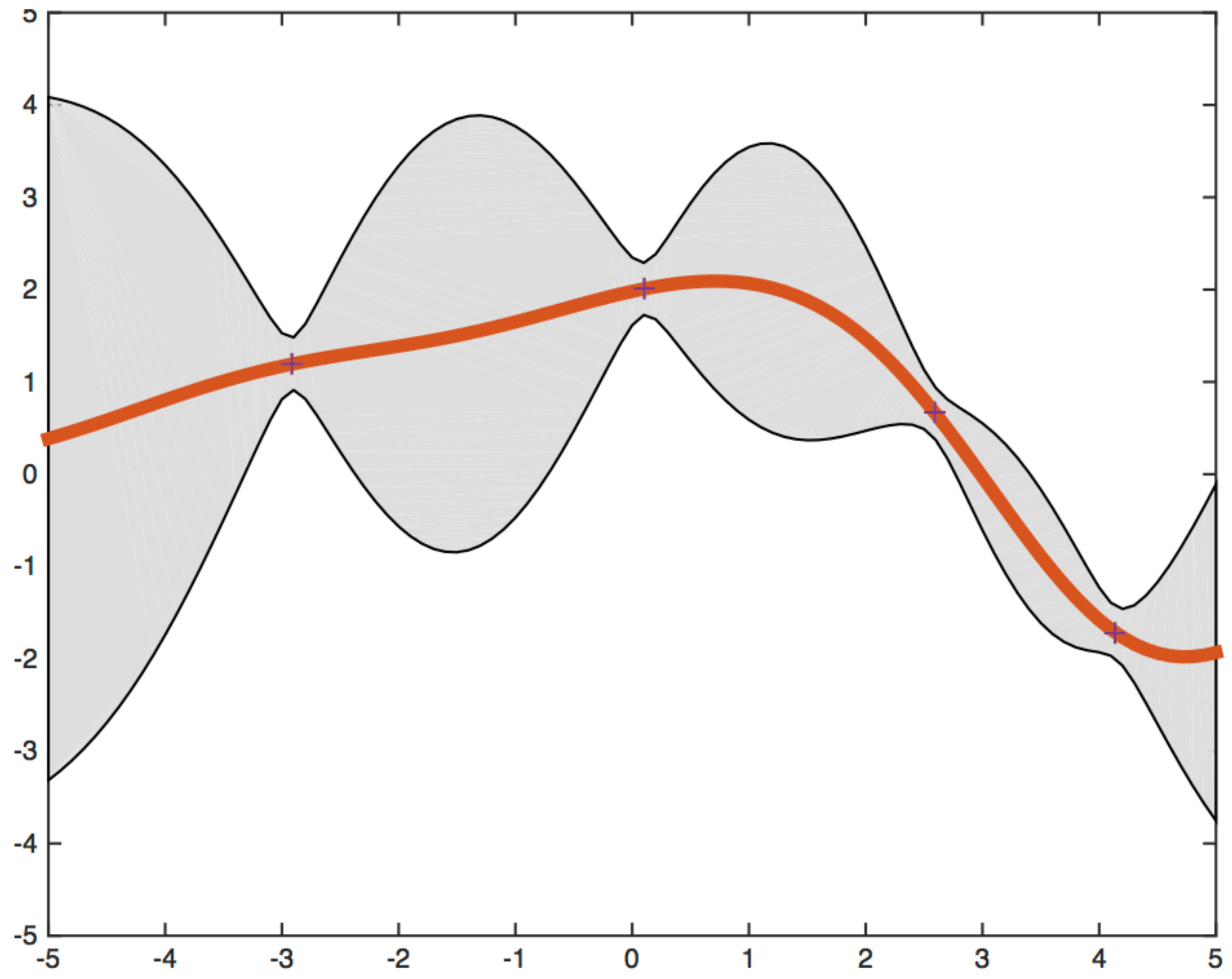
- In addition, every iteration of the process introduces approximation
- Formally, we get compound errors

This is partly unavoidable: predicting the far future is often difficult

Gaussian Processes

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

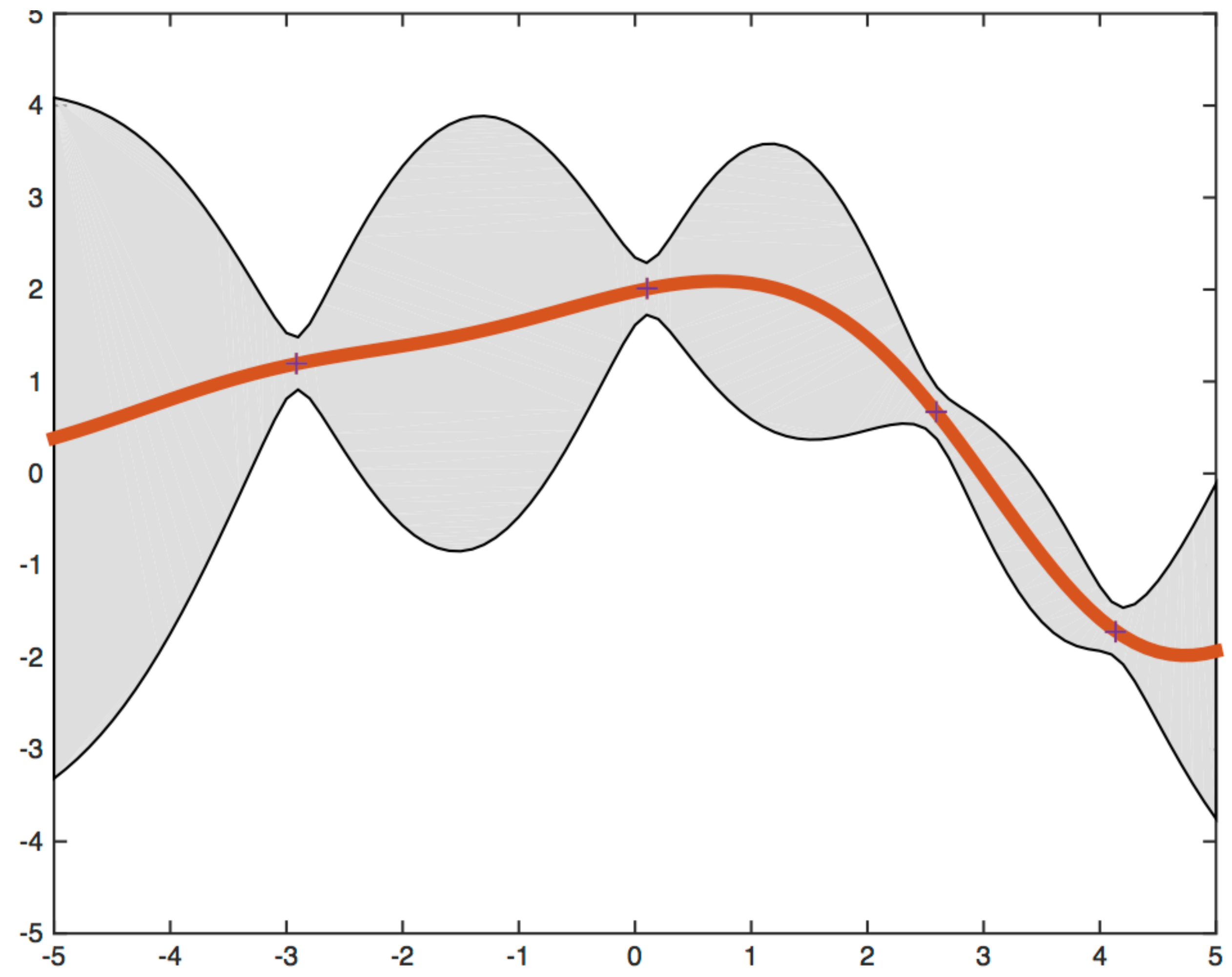
They are not easy to use, but can work well in the correct setting



- GPs define a probability distribution over an index (i.e. input) variable
- The distribution is based on the available observation and a few assumptions

Gaussian Processes

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



Assumption 1 (intuitively)

- For every value of the index variable the distribution is Gaussian
- Therefore it can be described by a mean and a standard deviation

Gaussian Processes

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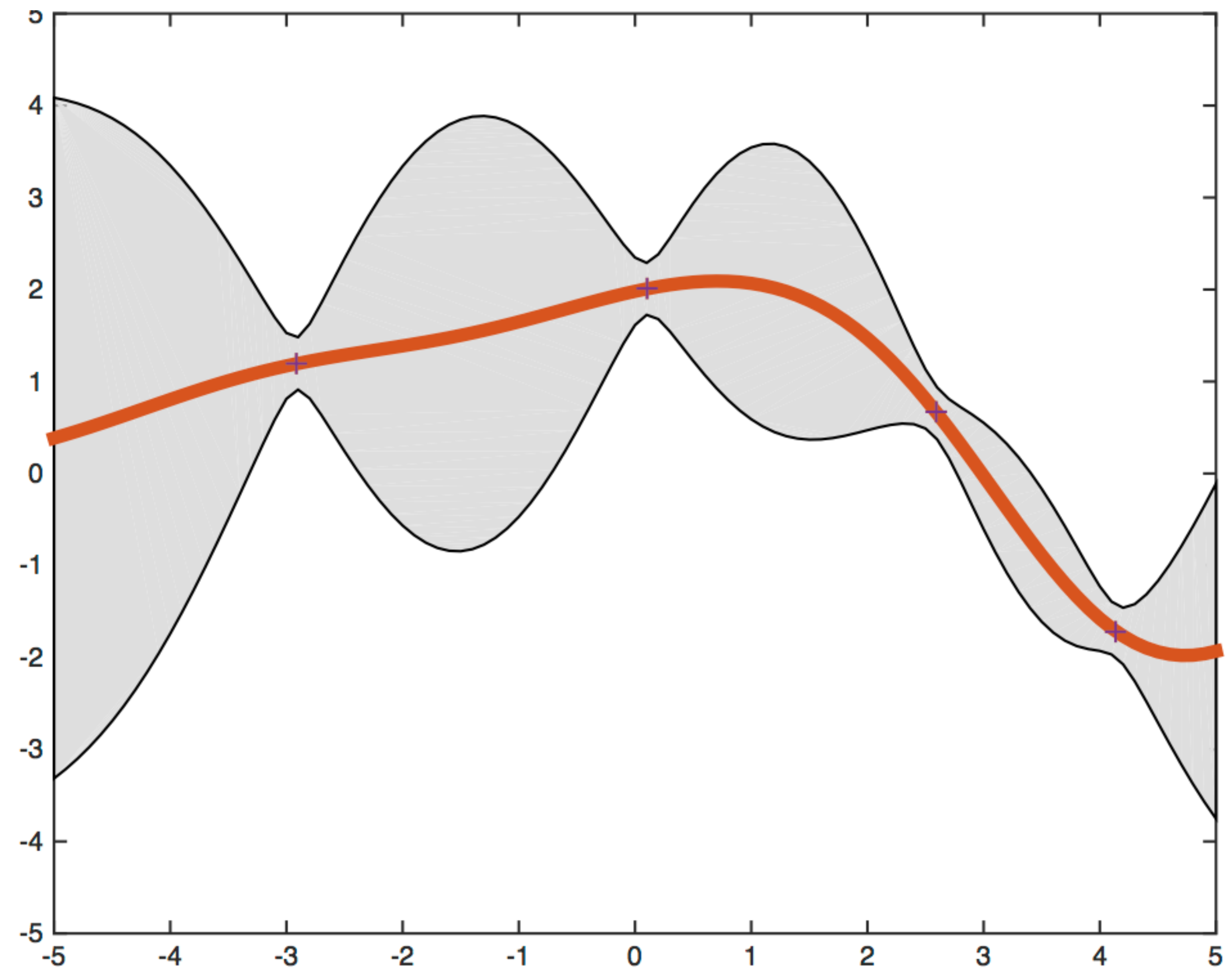

Assumption 2 (intuitively)

- The stdev depends on the distance between a point and the observations
- So it will be low when we are close to the observations, high when we are far

Gaussian Processes

Formally, things are a bit more complicated

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

- The index variable x represents an input (and can be a vector/tuple)
- Each variable y_x represents the output for input x
- The index is continuous and the collection is therefore infinite

You can think of y_x as the value of a (stochastic) function for input x

Some examples:

- y_x could be the rainfall rate at location $x = (\text{latitude}, \text{longitude})$
- y_x could be the traffic volume at time x

Each y_x follows a Normal Distribution, but the variables are correlated

- Therefore every finite subset of y_x variables
- ...Follows a Multivariate Normal Distribution

Multivariate Normal Distritbuion

Why the multivariate normal distribution?

- It works for many real world phenomena
- It has a (relatively) simple closed-form density function

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In particular, the PDF for a MND is defined via:

- A (vector) mean μ
- A covariance matrix Σ

By recentering we can assume $\mu = 0$, meaning that knowing Σ is enough

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In particular, the PDF for a MND is defined via:

- A (vector) mean $\boldsymbol{\mu}$
- A covariance matrix Σ

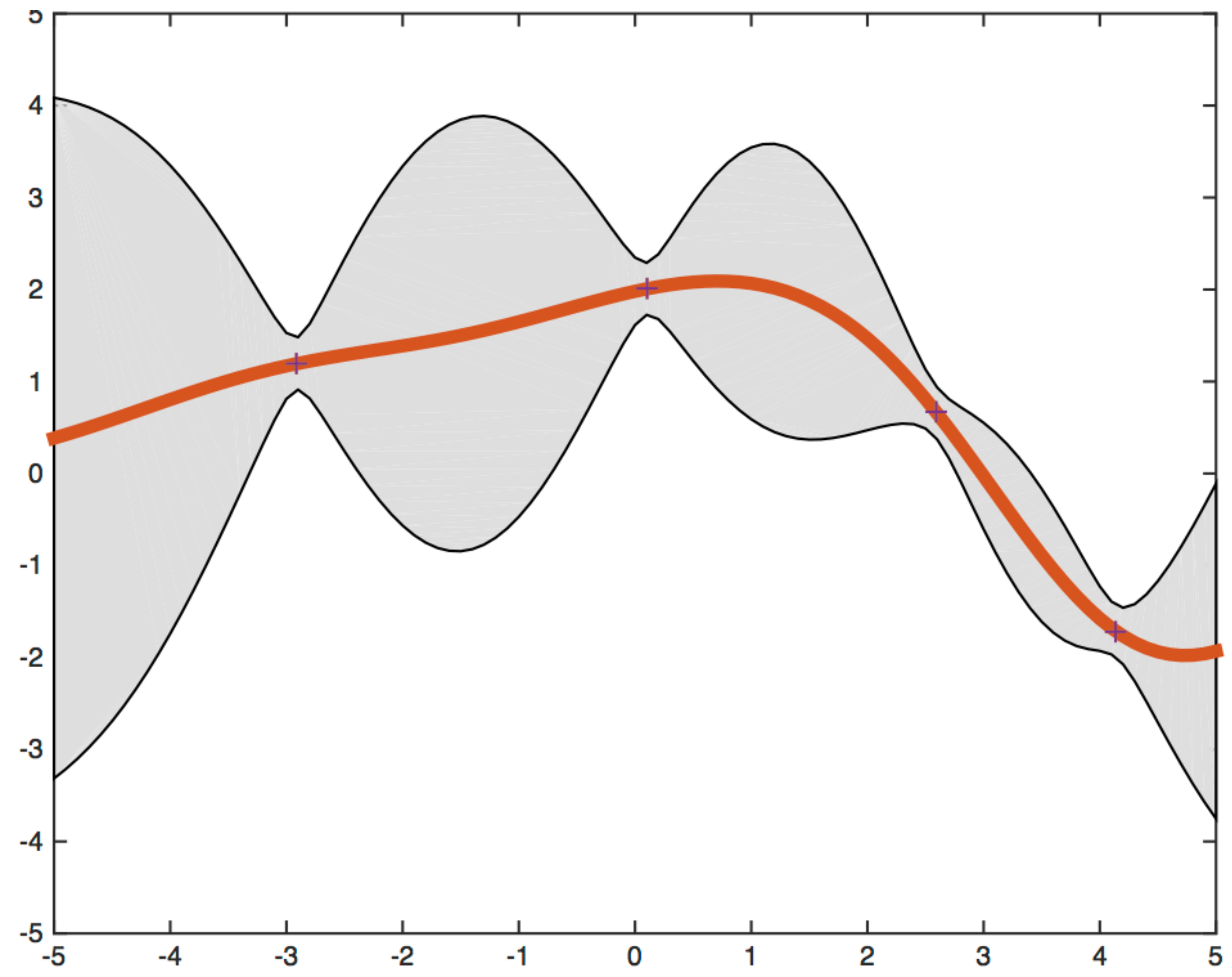
By recentering we can assume $\boldsymbol{\mu} = \mathbf{0}$, meaning that knowing Σ is enough

Therefore, if we know Σ we can easily compute

- The joint density $f(\bar{y}_{\bar{x}})$ for a set of observations
- The conditional density $f(y_x \mid \bar{y}_{\bar{x}})$ of an observation y_x, given $\bar{y}_{\bar{x}}$

Why do We Care?

We need the conditional density to perform inference!



- The line and grey areas represent the conditional density $f(y_x \mid \bar{y}_{\bar{x}})$ of y_x
- ...Based on the available observations, i.e. $\bar{y}_{\bar{x}}$

Why do We Care

We need the joint density to perform training!

...Because in practice we don't know Σ

- Therefore we'll assume that Σ is a parameterized function $\Sigma(\theta)$
- ...And we can optimize the parameters θ for maximum likelihood

Why do We Care

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- ...And we can optimize the parameters θ for maximum likelihood

Formally, given a set of training observations $\bar{y}_{\bar{x}}$

...We can calibrate the parameters by solving a problem in the form:

$$\arg\max_{\theta} f(\bar{y}_{\bar{x}})$$

- Here we are not using a product of probabilities over the training set
- ...Because the y_x variables are correlated
- No worries: since we have the joint PDF, we use it directly

Which Covariance Matrix?

We still have one big problem

Say that we a covariance matrix Σ for a set of observations $\bar{y}_{\bar{x}}$

- Now we want to perform inference for an input value x
- Formally: we want to compute $f(y_x \mid \bar{y}_{\bar{x}})$

In principle, we can use the formula:

$$f(y_x \mid \bar{y}_{\bar{x}}) = \frac{f(y_x, \bar{y}_{\bar{x}})}{f(\bar{y}_{\bar{x}})}$$

- By using our Σ, we can easily compute $f(\bar{y}_{\bar{x}})$
- ...But what about $f(y_x, \bar{y}_{\bar{x}})$?

Which Covariance Matrix?

Our Σ refers to our set of observed variables $\bar{y}_{\bar{x}}$

Therefore, if we have n variables, our matrix will be $n \times n$

$$\Sigma_{\bar{x}} = \begin{pmatrix} \sigma_{\bar{x}_1,\bar{x}_1} & \sigma_{\bar{x}_1,\bar{x}_2} & \cdots & \sigma_{\bar{x}_1,\bar{x}_n} \\ \sigma_{\bar{x}_2,\bar{x}_1} & \sigma_{\bar{x}_2,\bar{x}_2} & \cdots & \sigma_{\bar{x}_2,\bar{x}_n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{\bar{x}_n,\bar{x}_1} & \sigma_{\bar{x}_n,\bar{x}_2} & \cdots & \sigma_{\bar{x}_n,\bar{x}_2} \end{pmatrix}$$

- In every cell we have the covariance for variables $\bar{y}_{\bar{x}_i}$ and $\bar{y}_{\bar{x}_j}$
- With this matrix, we can compute $f(\bar{y}_{\bar{x}})$

bar## Which Covariance Matrix?

However, $f(y_x, \bar{y}_{\bar{x}})$ refers to one more variable

Meaning that it will be specified via an $(n+1) \times (n+1)$ matrix!

$$\Sigma_{x,\bar{x}} = \begin{pmatrix} \sigma_{x,x} & \sigma_{x,\bar{x}_1} & \sigma_{x,\bar{x}_2} & \cdots & \sigma_{x,\hat{x}_2} \\ \sigma_{\bar{x}_1,x} & \sigma_{\bar{x}_1,\bar{x}_1} & \sigma_{\bar{x}_1,\bar{x}_2} & \cdots & \sigma_{\hat{x}_1,\hat{x}_n} \\ \sigma_{\bar{x}_2,x} & \sigma_{\bar{x}_2,\bar{x}_1} & \sigma_{\bar{x}_2,\bar{x}_2} & \cdots & \sigma_{\bar{x}_2,\bar{x}_n} \\ \vdots & \vdots & \ddots & \vdots & \\ \sigma_{\bar{x}_n,x} & \sigma_{\bar{x}_n,\bar{x}_1} & \sigma_{\bar{x}_n,\bar{x}_2} & \cdots & \sigma_{\bar{x}_n,\bar{x}_2} \end{pmatrix}$$

- Assuming that $\bar{y}_{\bar{x}}$ are the training observations
- ...We could define $\boldsymbol{\sigma}_{\bar{x}_1,\bar{x}_2}$ at training time

But how do we define the new covariances, i.e. those related to y_x?

Defining the Covariance Matrix

We assume that covariance can be built from a set of inputs

Let x refer now to a vector of values for the index variable

- Given two variables y_{x_i} and y_{x_j}
- We specify their covariance via parameterized kernel function $K_\theta(x_i, x_j)$
- K typically depends on the distance between input values

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

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

...Which we can computed based on the input (and the parameters) alone!

The Whole Picture

In practice, at training time

- Pick a parameterized kernel function $K_\theta(x_i, x_j)$
- Collect training observations $\bar{y}_{\bar{x}}$
- Optimize the kernel for maximum likelihood (e.g. via gradient descent)

Both the parameters θ and the observations $\bar{y}_{\bar{x}}$ are stored in the model

- This is similar to what we have in Kernel Density Estimation

The Whole Picture

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- This is similar to what we have in Kernel Density Estimation

At inference time:

- Given a new input (i.e. index) value x
- We obtain the covariance matrix $\Sigma_{\bar{x}}$
- We obtain the covariance matrix $\Sigma_{x,\bar{x}}$

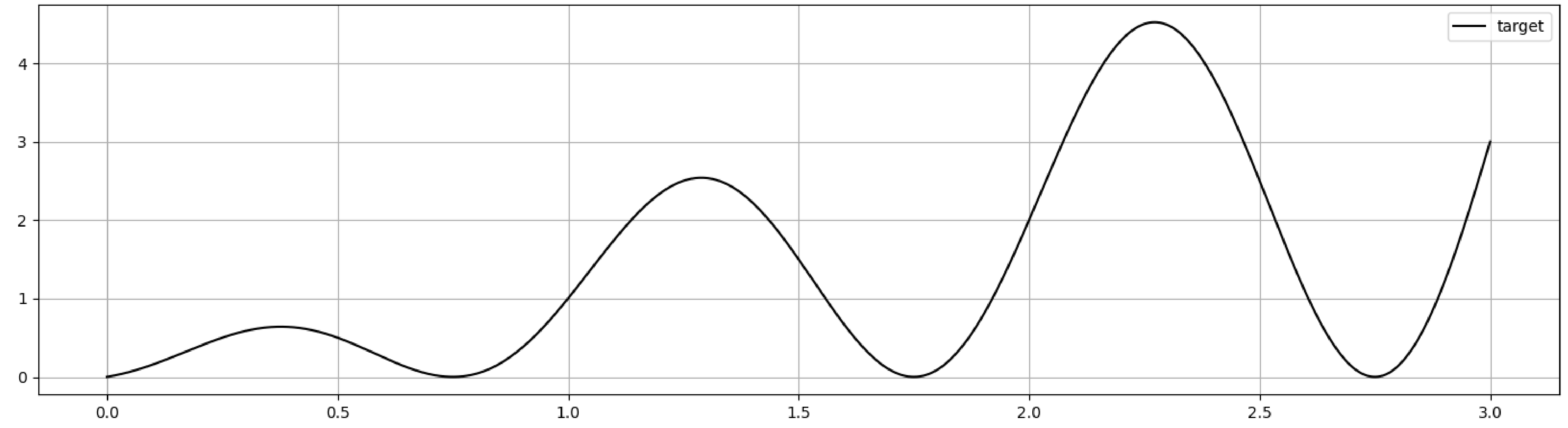
...And with this we can completely characterize $f(y_x, \mid \bar{y}_{\bar{x}})$

Gaussian Processes in scikit-learn

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

First, let us choose a function as our ground truth

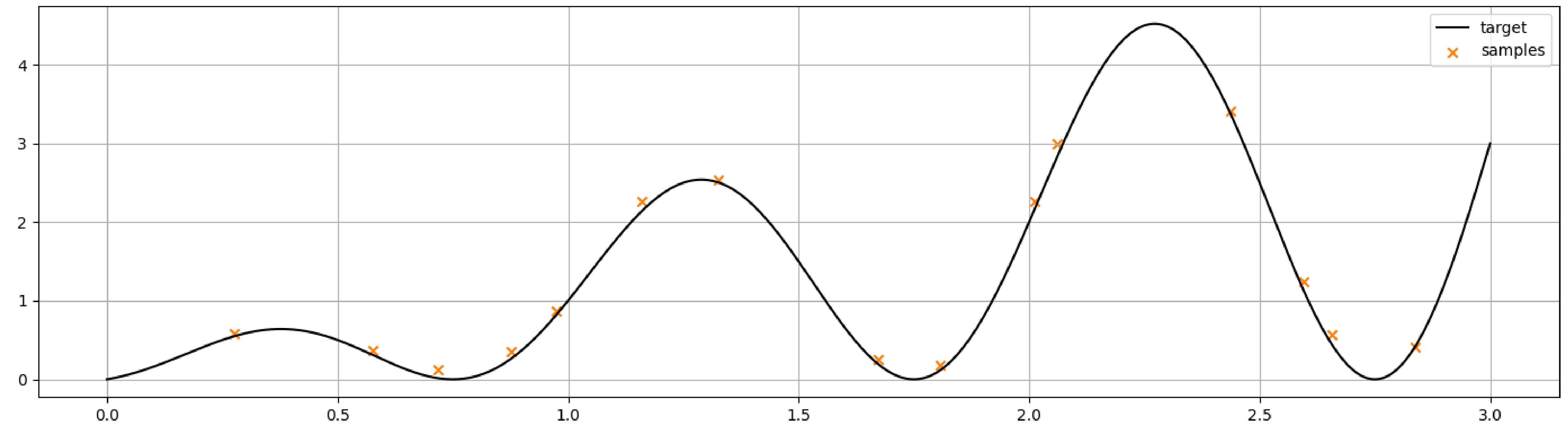
```
In [2]: f = lambda x: x * np.sin(2*np.pi*x) + x # target function
        x = np.linspace(0, 3, 1000)
        y = pd.Series(index=x, data=f(x))
        util.plot_gp(target=y, figsize=figsize)
```



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))
        util.plot_gp(target=y, samples=y_tr, figsize=figsize)
```



Gaussian Processes in scikit-learn

Now we are where we would normally start in a data analysis

...And we need to choose a kernel among are many available options

- Since we have 15 training points
- This will be used at training time to build a 15×15 covariance matrix

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 covariance 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

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-2, 1e2))
```

The RBF kernel has a single parameter, representing its scale

The extra (tuple) parameter represents a pair of bounds

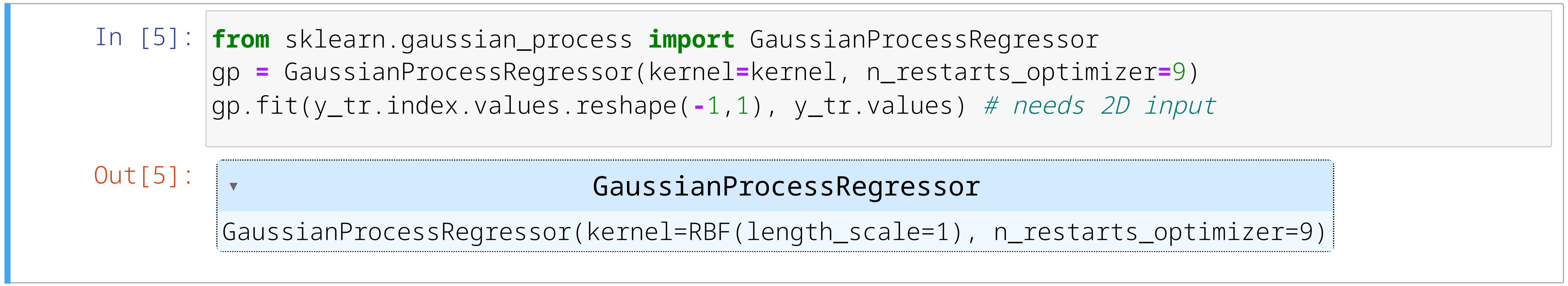
- During training, only values within the boundaries will be considere

Bounds can be very useful for controlling the training process

- They should be chosen based on the available domain information
- Multiples educated guesses are fine when little is known about the problem

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

Out[5]: ▾ GaussianProcessRegressor
        GaussianProcessRegressor(kernel=RBF(length_scale=1), n_restarts_optimizer=9)
```

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

Training can be an expensive process:

- Building the covariance matrix runs in $O(n^2)$ (where n is the training set size)
- ...And we need to that repeatedly during optimization!

Gaussian Processes in scikit-learn

Finally, 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)
```

The "predictions" are not point estimates!

- We actually get those (i.e. the means, called `xp` in the code)
- ...But we also obtain standard deviations

The model output is a fully characterized conditional distribution

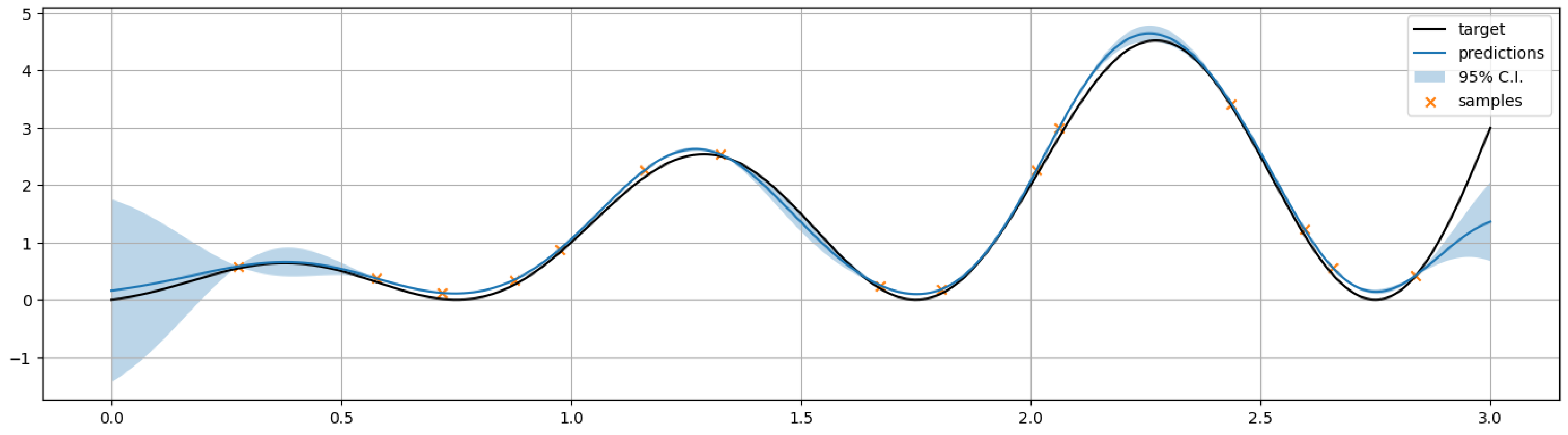
The distribution is conditional on:

- The input value x (passed at inference time)
- All the training observations (stored in the model)

Gaussian Processes in scikit-learn

We can now plot the predictions

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



Obtaining a full distribution as output is cool

- We obtain an estimated value (the mean)
- ...And we get to know how certain the model is about that

Behind the Scenes

Let's see how prediction works with a numeric example

We want a prediction for $x = 2.5$, i.e. $y_{2.5}$

- We consider two separate training set (and pre-optimized kernel parameters)
- The first set contains only $(\bar{x}_9, \bar{y}_{\bar{x}_9}) \simeq (2.01, 2.27)$
- The second set contains only $(\bar{x}_0, \bar{y}_{\bar{x}_0}) \simeq (0.27, 0.58)$

The covariance matrices in the two cases are therefore:

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

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

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 $\bar{x}_9$ 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)
```

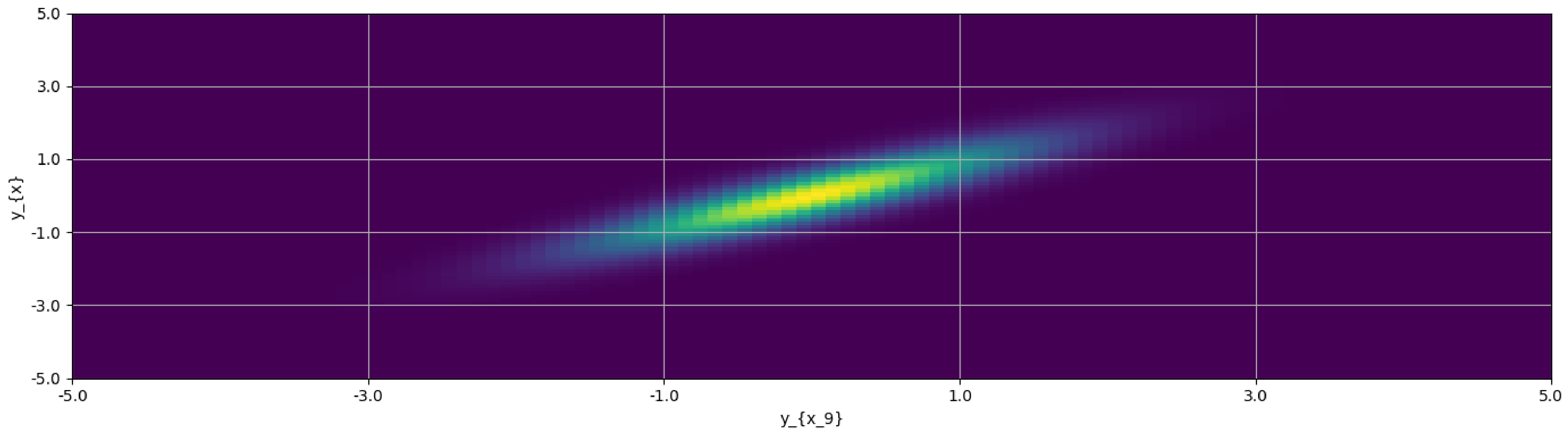
Then we do the same for $\bar{x}_0$ and x, which are far apart

```
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

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

```
In [11]: yr = np.linspace(-5, 5, 100)
         util.plot_distribution_2D(f_9x, yr, yr, figsize=figsize)
         plt.xlabel('y_{x_9}'); plt.ylabel('y_{x}'); plt.tight_layout()
```

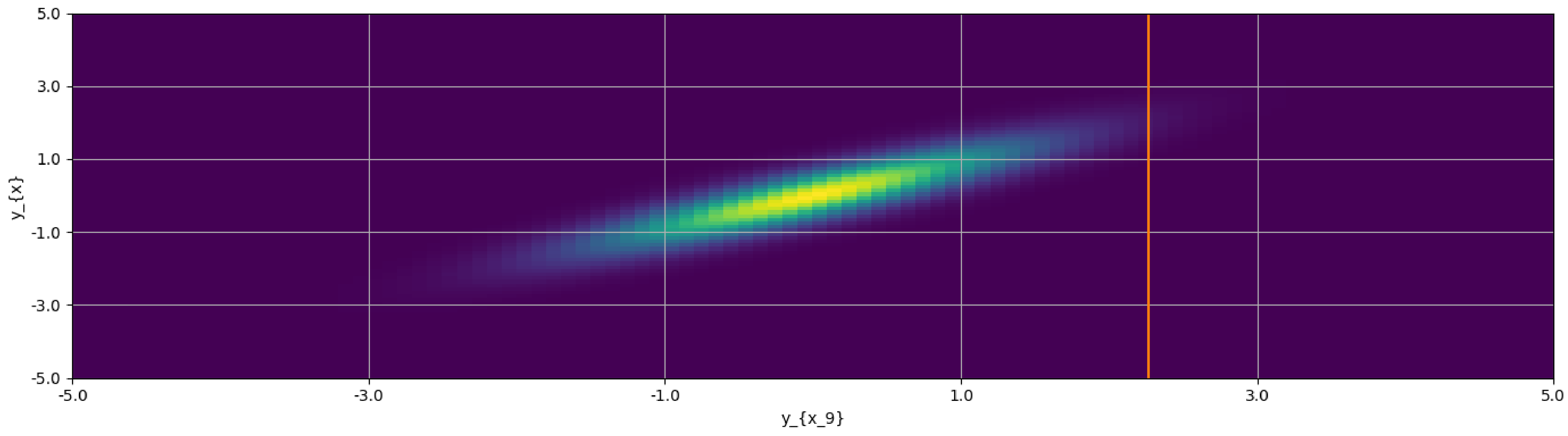


- If we know neither $\bar{y}_{\bar{x}_9}$ nor y_x, we can only say that they are likely both zero

Behind the Scenes

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

```
In [12]: util.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()
```

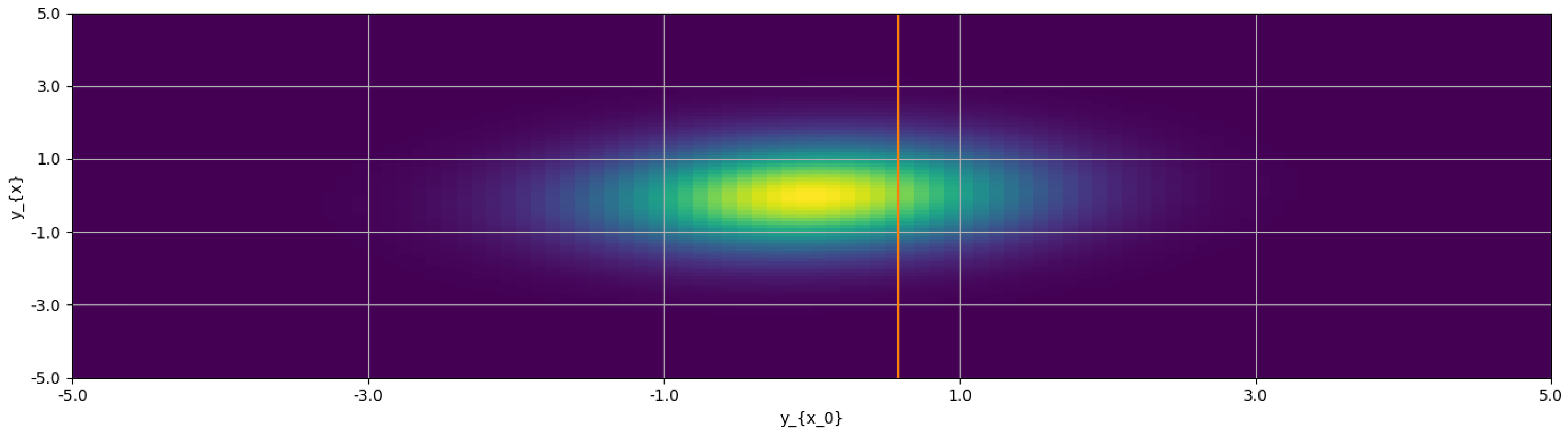


- Given the observation, the most likely value for y_x is $\simeq 2$

Behind the Scenes

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

In [13]:
```
util.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 $\bar{y}_{\bar{x}_0}$ is not going to be of much help here

Memento

So, a few key insight to keep in mind:

- Superficially, GPs behave like functions that output probability distribution
- Internally, they store the kernel, defining how all the points are correlated
- A set of observations, used 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:

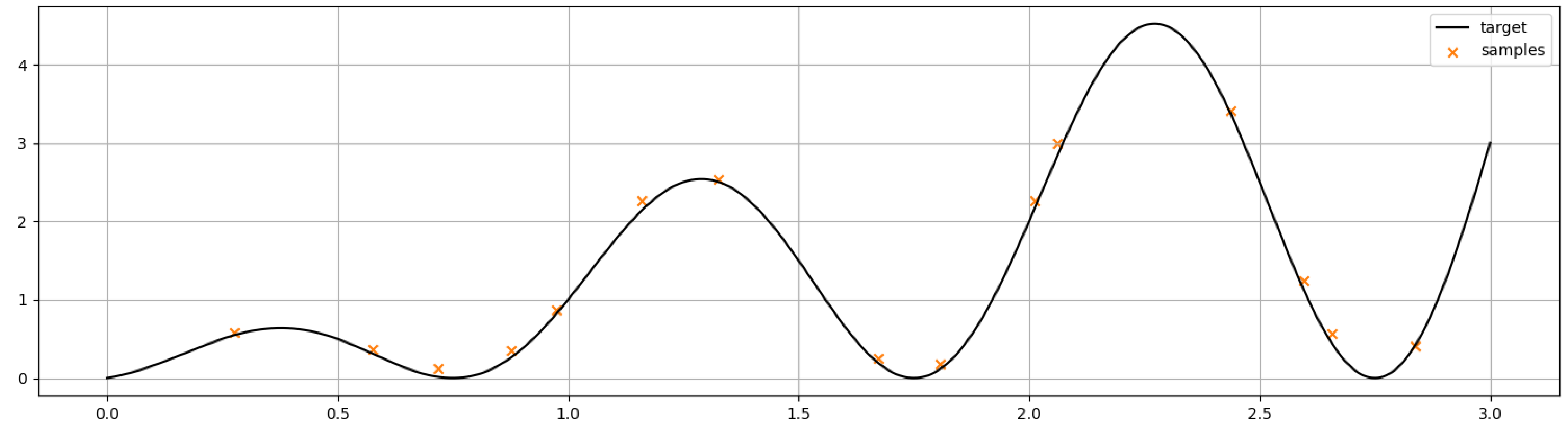
- The covariance matrix is built
- The model computes the conditional distributions

How to Improve the Model

We can improve the model by choosing a more appropriate kernel

- Let's (cheat and) look again at our ground truth and training data
- Which patterns and properties do you notice?

```
In [14]: util.plot_gp(target=y, samples=y_tr, figsize=figsize)
```



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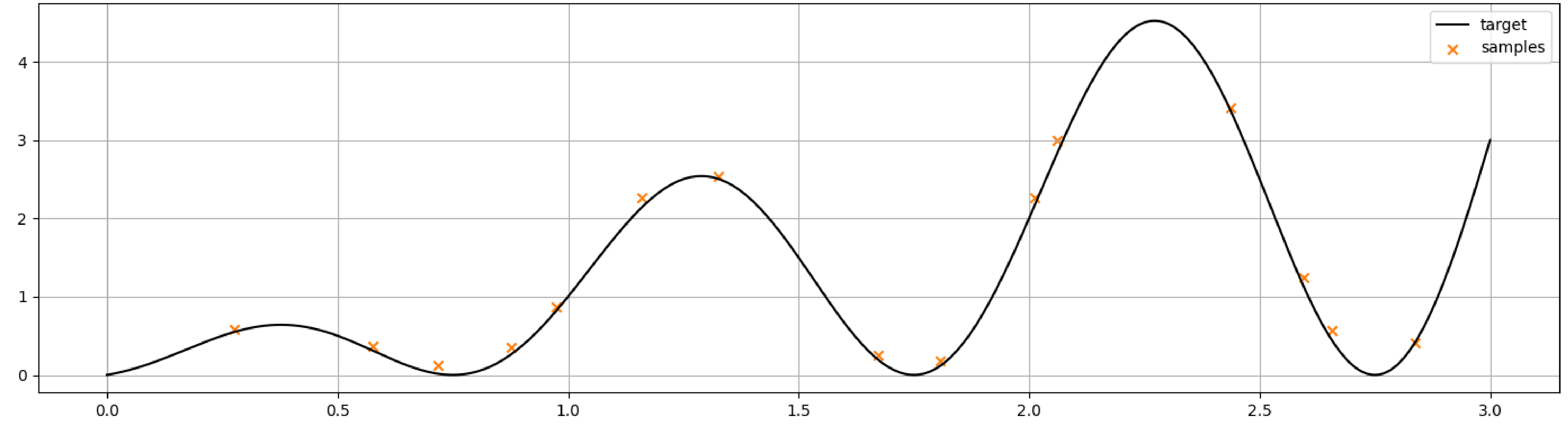
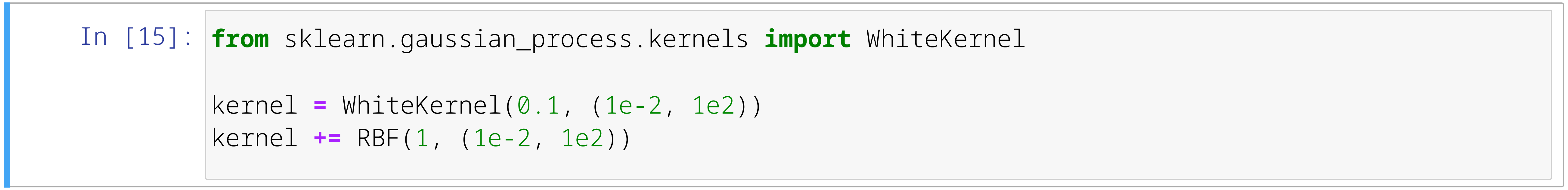


We have some noise, a period, and a trend

How to Improve the Model

So, let us deal with the noise first



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

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

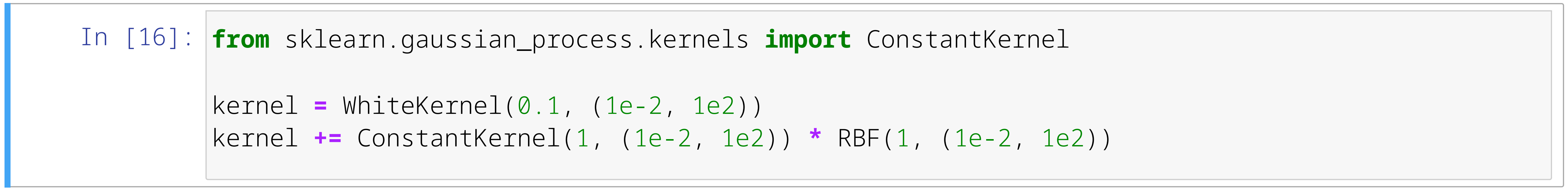
`WhiteKernel` captures the presence of noise in the data

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

- The only parameter of `WhiteKernel` represents the noise level σ^2
- A small noise level prevents overfitting
- ...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 [16]:
```python
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

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```

`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:

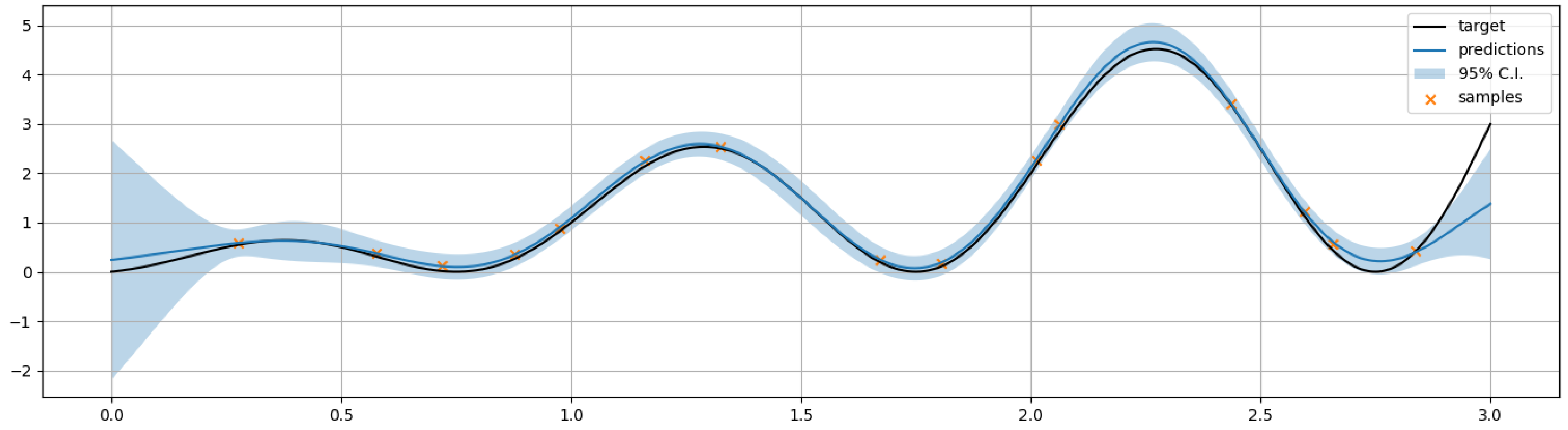
```
In [17]: gp = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
gp.fit(y_tr.index.values.reshape(-1,1), y_tr.values) # needs 2D input
print(gp.kernel_)
```

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

How to Improve the Model

Let us see the new predictions

In [18]:
```
xp, std = gp.predict(x.reshape(-1,1), return_std=True)
util.plot_gp(target=y, samples=y_tr, pred=pd.Series(index=y.index, data=xp),
             std=pd.Series(index=y.index, data=std), figsize=figsize)
```



- Better, since the black curve is mostly in the confidence interval
- ...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 [19]: 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-1, 1e1), (1e-1, 1e1))
```

`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 if the distance is close to a multiple of the period p
- The scale parameter l controls 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 [20]: 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-1, 1e1), (1e-1, 1e1))
         kernel += DotProduct(1, (1e-2, 1e2))
```

`DotProduct` (somewhat) captures the trend:

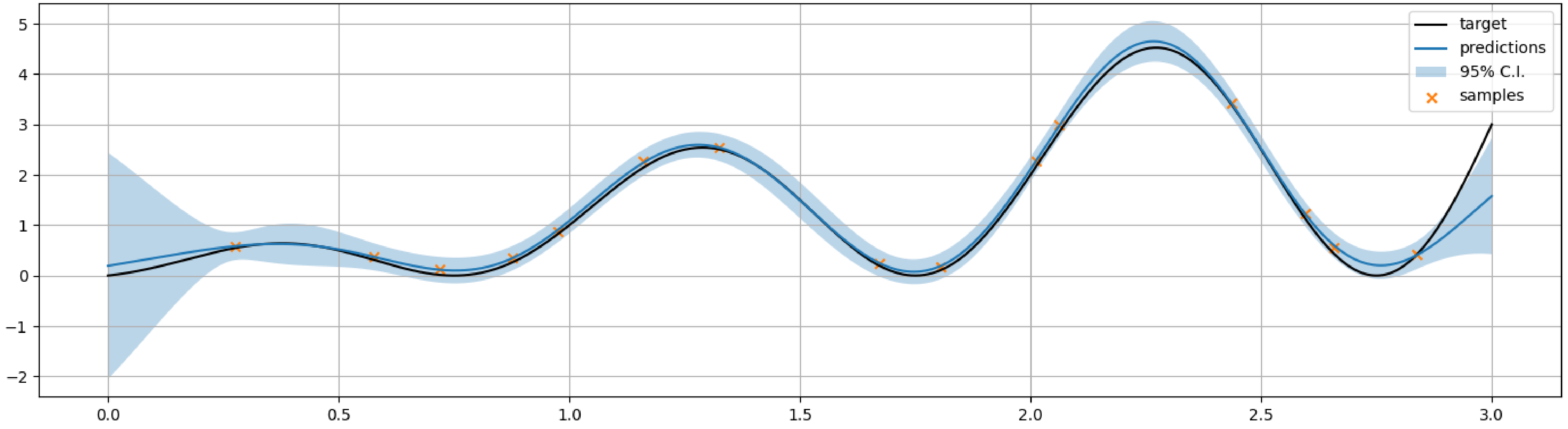
$$K(x_i, x_j) = \sigma^2 + x_i x_j$$

- 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

How to Improve the Model

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

In [21]:
```
gp = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
gp.fit(y_tr.index.values.reshape(-1,1), y_tr.values) # needs 2D input
xp, std = gp.predict(x.reshape(-1,1), return_std=True)
util.plot_gp(target=y, samples=y_tr, pred=pd.Series(index=y.index, data=xp),
             std=pd.Series(index=y.index, data=std), figsize=figsize)
```



- Notice how the C.I. grows close to the sides?
- GPs tend to interpolate well and extrapolate poorly