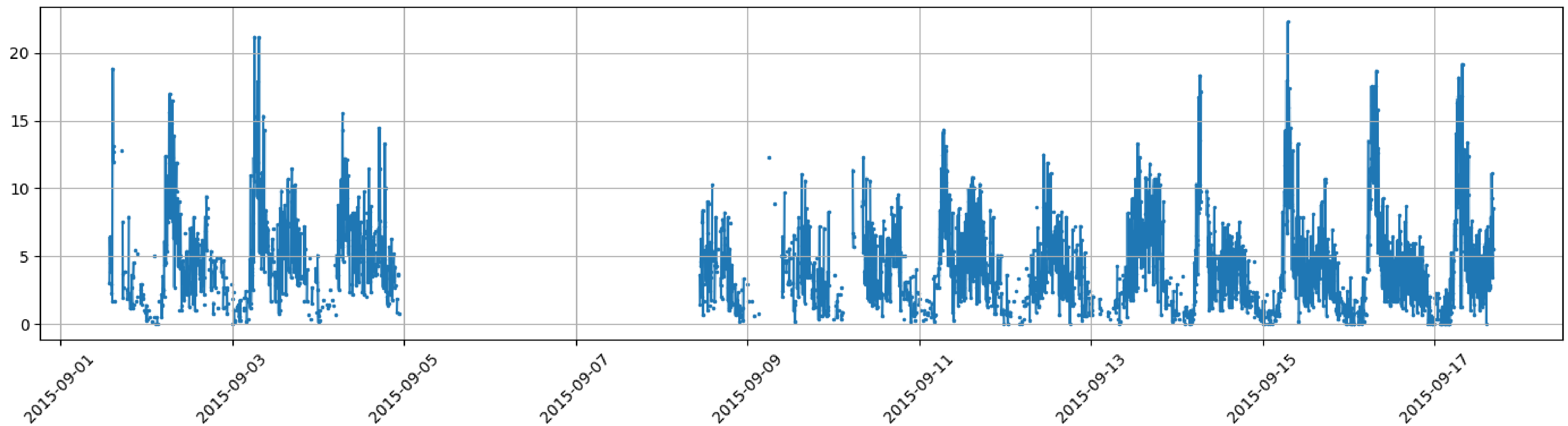
Filling Missing Values in Traffic Data

Back to the Traffic Data

We will try to use a Gaussian Process on our new traffic data

We will start directly from the dense series:

```
In [2]: util.plot_series(data_d, show_markers=True, figsize=figsize)
```



- There is a period, non-zero mean, local oscillations. And of course a huge gap

Time and Period

The input of the GP is going to be the time of the observation

Unfortunately, the GP in scikit-learn cannot handle `DateTime` objects

- Therefore, we will convert all time steps in numeric format
- We will use a simple time equivalent, namely 1 step = 1 time unit

In [3]:
```
data_dt = data_d.copy()
data_dt['time'] = np.arange(len(data_dt))
```

Before we start, it would be very useful to estimate the period

Due to the missing values, the series has a non-uniform sampling frequency

- Autocorrelation plots cannot be used in this case
- The standard FFT is also not applicable (we could use a non-uniform FFT)

Thankfully, this is traffic data! So we can bet there is a weekly period

Process Outline

We have no ground truth: how are we going to evaluate the kernels?

We will use the same trick we used before:

- We will focus on a portion of our sequence
  - ...One with relatively few missing values
- Then we will artificially remove part of the data points
  - This will form the ground truth for our evaluation

Main idea: use part of our data as a validation set

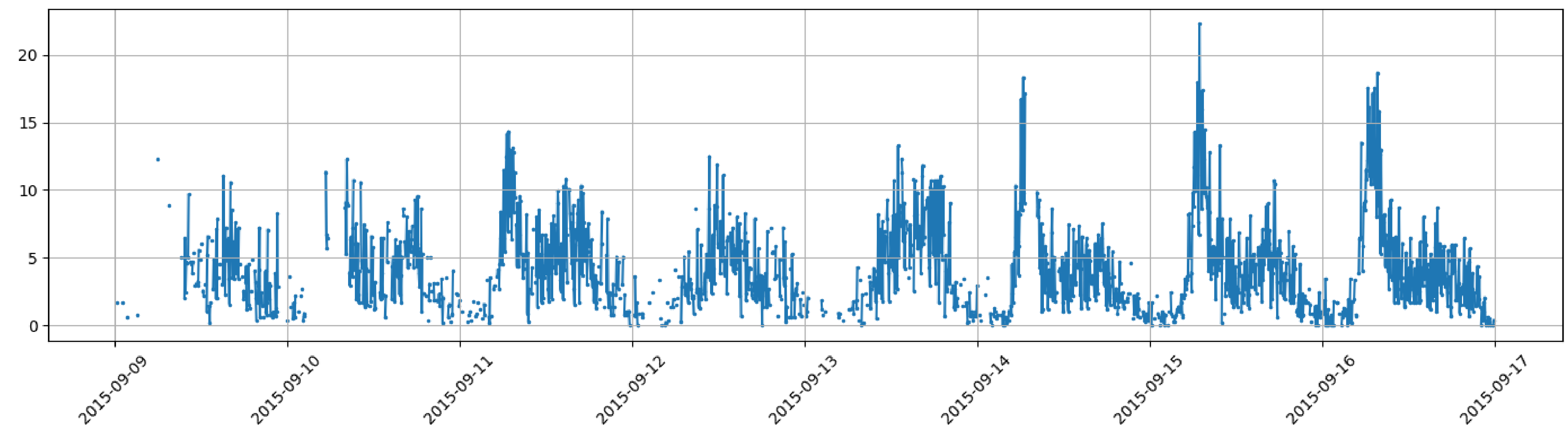
Which quality metric?

- Thanks to the availability of confidence intervals...
- ...We can compute the likelihood of our validation set!
- Using the MSE would do the same, only with more assumptions

Training and Validation Data

We will use for training (and validation) this stretch of the series

In [4]:
```
segment = data_dt[(data_dt.index >= '2015-09-09') & (data_dt.index < '2015-09-17')].copy()
util.plot_series(segment['value'], show_markers=True, figsize=figsize)
```



- We made sure to include at least one full week

Training and Validation Data

We can now separate training and validation data:

In [5]:
```
tmp = segment.dropna()

np.random.seed(42)
idx = np.arange(len(tmp))
np.random.shuffle(idx[1:-1]) # no not shuffle the first/last point
t = idx[1]; idx[1] = idx[-1]; idx[-1] = t # keep first/last points in the left half

sep = 2*len(idx) // 3
trdata = tmp.iloc[idx[:sep]]
tsdata = tmp.iloc[idx[sep:]]
```

- We are keeping 2/3 of the data for training
- Since we are using the dense series, we need to discard NaNs (`dropna`)
- Since we are doing interpolation...
- ...It's a good idea to keep the first and last point in the training set

A Starting Kernel

Let's try with a relatively simple kernel

```
In [6]: kernel = WhiteKernel(1e-3, (1e-4, 1e-1))
        kernel += ConstantKernel(1, (1e-2, 1e2)) * RBF(1, (1e-1, 1e1))

        np.random.seed(42)
        gp = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=3)
        gp.fit(trdata[['time']], trdata['value'])
        print(gp.kernel_)
```

```
WhiteKernel(noise_level=0.1) + 4.86**2 * RBF(length_scale=1.07)
```

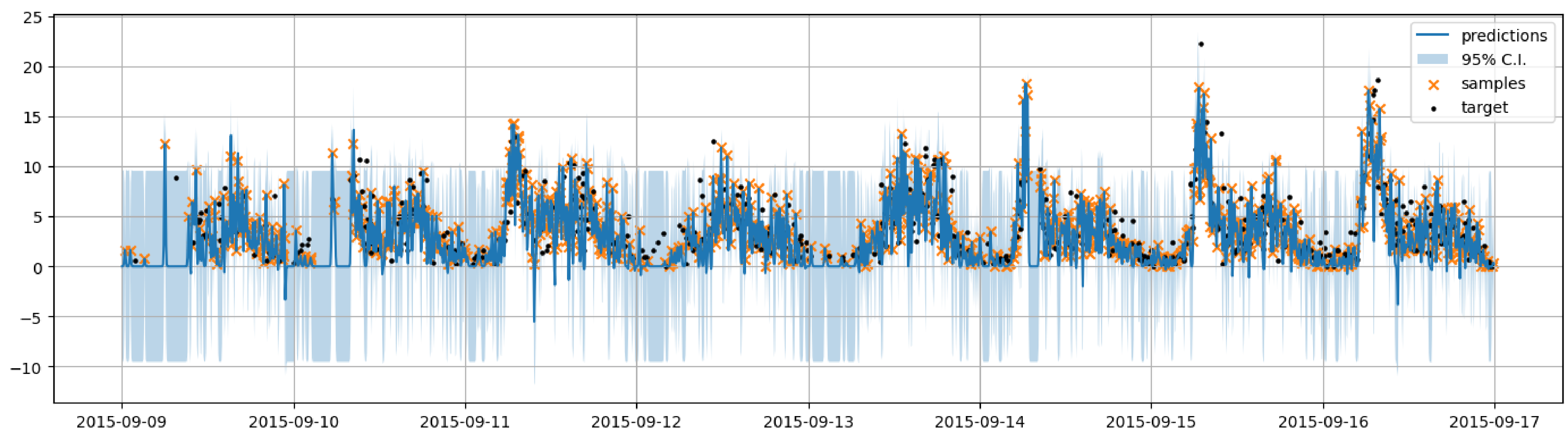
Then we obtain the predictions:

```
In [7]: pred, std = gp.predict(segment[['time']], return_std=True)
        pred = pd.Series(index=segment.index, data=pred)
        std = pd.Series(index=segment.index, data=std)
```

A Starting Kernel

Let's have a look at the predictions

```
In [8]: util.plot_gp(target_samples=tsdata['value'], samples=trdata['value'], pred=pred, std=std, fi
```



- Not so bad, but not so good either
- We have very wide confidence intervals!

A Starting Kernel

Let's compute the (log) likelihood of the validation data

In [9]:
```python
from scipy.stats import norm

# Obtain predictions for the validation data
pred_ts = pred[tsdata.index]
std_ts = std[tsdata.index]

ldens = norm.logpdf(tsdata['value'], pred_ts, std_ts)
ll = np.sum(ldens)
print(f'Log likelihood of the validation set: {ll:.2f}')
```

```
Log likelihood of the validation set: -1377.62
```

- This is our reference value
- We will try to beat it by improving the kernel

A Second Kernel

Let's add the period

We can choose the bounds so as to focus on a weekly period

```
In [10]: kernel = WhiteKernel(1e-3, (1e-4, 1e-1))
kernel += ConstantKernel(1, (1e-2, 1e2)) * RBF(1, (1e-1, 1e1))
kernel += ConstantKernel(1, (1e-2, 1e2)) * ExpSineSquared(1, 2000, (1e-1, 1e1), (1900, 2100))

np.random.seed(42)
gp = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=3)
gp.fit(trdata[['time']], trdata['value'])
print(gp.kernel_)
```

```
WhiteKernel(noise_level=0.0213) + 2.02**2 * RBF(length_scale=0.1) + 5.37**2 * ExpSineSquare
d(length_scale=0.1, periodicity=2.01e+03)
```

Then we obtain the new predictions:

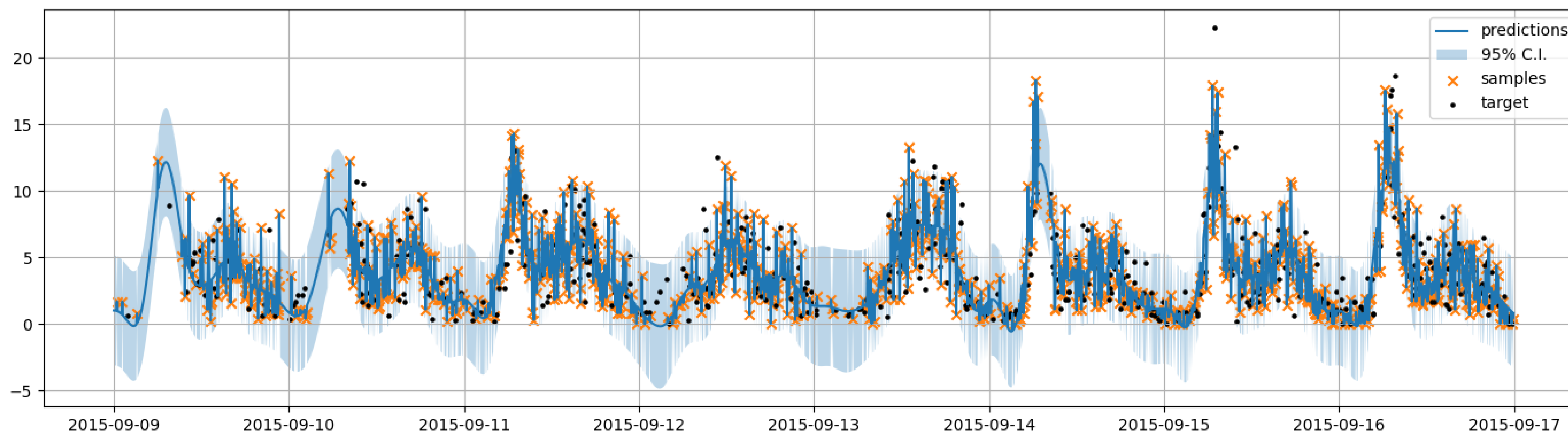
```
In [11]: pred, std = gp.predict(segment[['time']], return_std=True)
pred = pd.Series(index=segment.index, data=pred)
std = pd.Series(index=segment.index, data=std)
```

A Second Kernel

Both predictions and likelihood are now better

```
In [12]: util.plot_gp(target_samples=tsdata['value'], samples=trdata['value'], pred=pred, std=std, fi
         ldens = norm.logpdf(tsdata['value'], pred[tsdata.index], std[tsdata.index])
         print(f'Log likelihood of the validation set: {np.sum(ldens):.2f}')
```

```
Log likelihood of the validation set: -1110.69
```



- ...But the confidence intervals are still large

Transferring the Results

We now need to obtain predictions for the whole series

We would prefer to avoid training again the kernel parameters

- The large number of missing value may be problematic
- ...And the training time would be very large

...But we also really wish to use all available observations

- ...Not just those considered when training the kernel

With Gaussian Processes, we can do both

There is no need to train again the kernel every time new observations arrive

- We can build a new Σ matrix using the new observations and the old kernel

Transferring the Results

We reuse the kernel by passing it as argument when building a new GP:

```
In [13]: gp2 = GaussianProcessRegressor(kernel=gp.kernel_, optimizer=None)
```

Passing `optimizer=None` will disable optimization at training time

So that calling `fit` will just take into account a new set of observations

```
In [14]: tmp = data_dt.dropna() # The whole series (NaNs excluded)
         gp2.fit(tmp[['time']], tmp['value']);
```

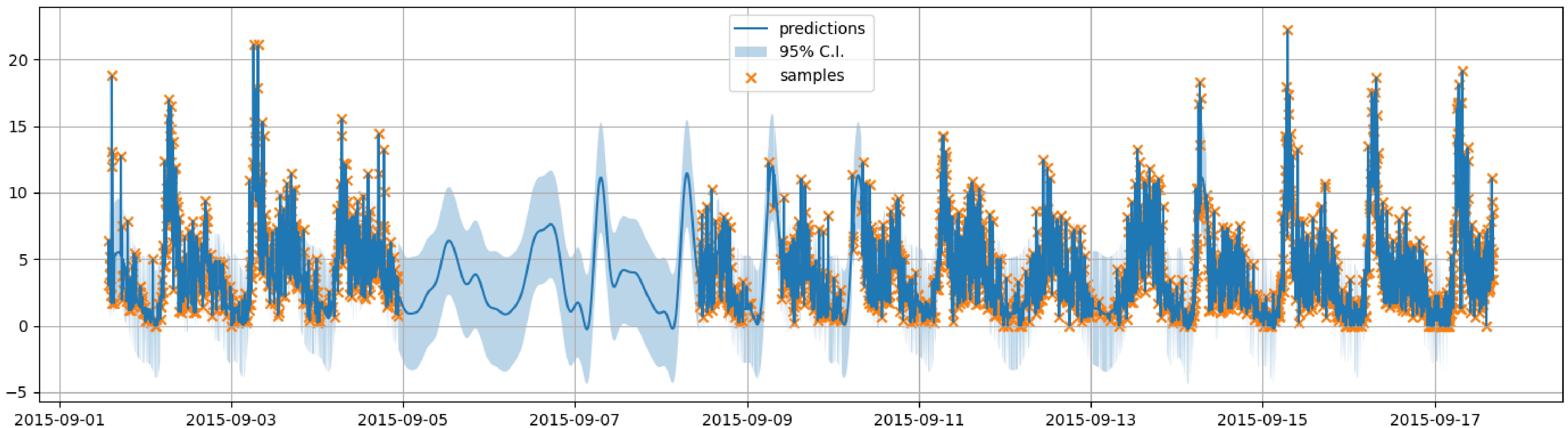
Now we can obtain predictions for the whole series:

```
In [15]: pred_all, std_all = gp2.predict(data_dt[['time']], return_std=True)
         pred_all = pd.Series(index=data_dt.index, data=pred_all)
         std_all = pd.Series(index=data_dt.index, data=std_all)
```

Transferring the Results

Let's have a look at all the predictions

In [16]:
```
util.plot_gp(samples=data_dt['value'], pred=pred_all, std=std_all, figsize=figsize)
```



- We actually managed to (partially) reconstruct even the large gap!
- ....But we still have those large confidence intervals

Transferring the Results

The confidence intervals are still very large

- This is in part understandable, give the presence of wide variations
- ...But at least one point is a bit strange

The confidence intervals are large even for the night hours!

There are two reasons:

- There are fewer samples at nighttime
  - As we get far from the samples the confidence drops (quickly, in our case)
- No traditional GP kernel can represent input-dependent variance
  - All kernels are about covariance, not variance
  - The lone exception is the `WhiteKernel`, which is not input dependent

Can we deal with this issues?

Standard Deviation Model

Multiplicative Ensemble

We can deal with the input-dependent variance in a separate model

We are going to build an ensemble of predictive models

- Classical ensembles (e.g. Random Forests, Gradient Boosting) are based on sums
- But that's not going to work with variance, since:

$$Var(x + \alpha) = Var(x)$$

However, variance can be scaled via multiplication:

In particular:

$$Var(\alpha x) = \alpha^2 Var(x)$$

- So we can use a "multiplicative" ensemble

Multiplicative Ensemble

Our model will become the product of two models

Formally, we will have:

$$g(x, \lambda) f(x, \theta)$$

- f, with parameters θ will be a Gaussian Process
- g, with parameters λ will be our variance model (or standard deviation model)

On the training set, we wish to have:

$$g(x_i, \lambda) f(x_i, \theta) \simeq y_i \quad \Rightarrow \quad f(x_i, \theta) \simeq \frac{y_i}{g(x_i, \lambda)}$$

- The Gaussian Process will need to learn a series with a variance altered by g
- The variance of each point y_i will be divided by $g(x_i, \lambda)^2$

Standard Deviation Model

We now need to choose our variance model g

- Since we have discrete time and a natural period (a week)
- ...We could use a simple map (time of the week $\rightarrow$ standard deviation)

Let's add a "hour of the week" information to our data:

The chosen time unit is actually irrelevant

In [17]:
```
data_dtw = data_dt.copy()
data_dtw['how'] = 24 * data_dt.index.weekday + data_dt.index.hour + data_dt.index.minute / 6
data_dtw.head()
```

Out[17]:

timestamp	value	time	how
2015-09-01 13:45:00	3.06	0	37.750000
2015-09-01 13:50:00	6.44	1	37.833333
2015-09-01 13:55:00	5.17	2	37.916667
2015-09-01 14:00:00	3.83	3	38.000000
2015-09-01 14:05:00	4.50	4	38.083333

Standard Deviation Model

Then we can compute the standard deviation via a pandas `groupby` operation:

```
In [18]: how_std = data_dtw.groupby('how').agg({'value': ['std', 'count']})
```

- `agg` allows to apply multiple aggregation functions to multiple columns

The resulting table has a hierarchical column index

Let's see some statistics about the value counts:

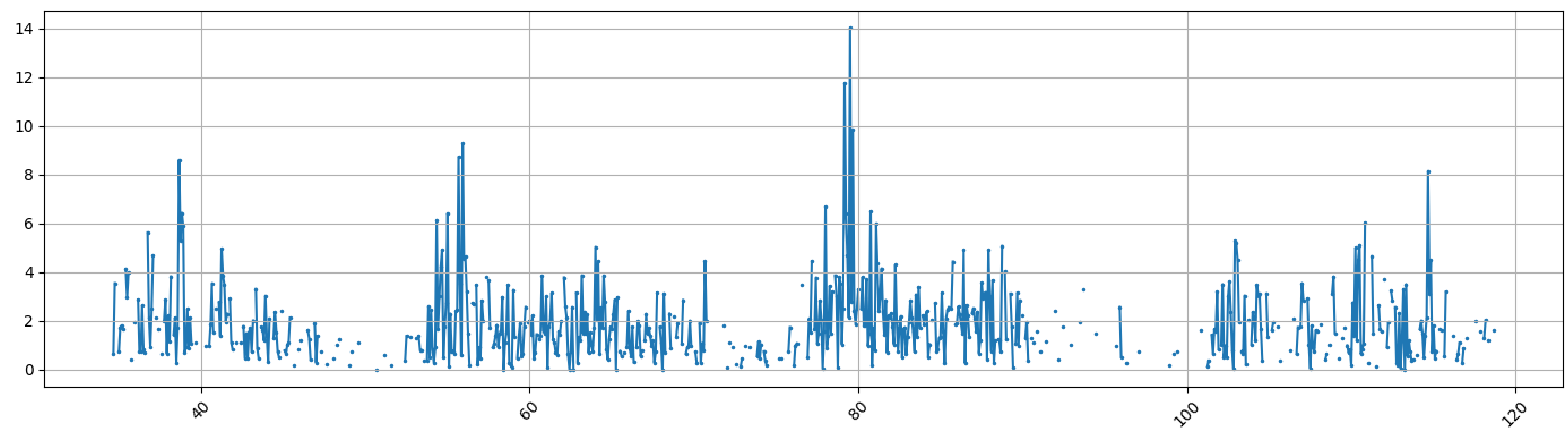
```
In [19]: how_std['value', 'count'].describe() # Notice the use of two names
```

```
Out[19]: count    2016.000000
         mean        1.177083
         std         0.850567
         min         0.000000
         25%         1.000000
         50%         1.000000
         75%         2.000000
         max         3.000000
         Name: (value, count), dtype: float64
```

Standard Deviation Model

Let's have a look at the standard deviation values

```python
In [20]: util.plot_series(how_std['value', 'std'], show_markers=True, figsize=figsize)
```



- There are many missing values (as expected from the counts)!
- Note: this is a time-to-stdev map, not our original series!

Choosing the Correct Interval

There are too many gaps in our data to compute σ with this granularity

There are a few possible solutions:

- Filling the gaps also in the standard deviation data
- ...Or using a coarser time unit
- ...Or choosing a shorter period (e.g. one day)

Let's try using hour-long intervals (rather than 5 minutes)

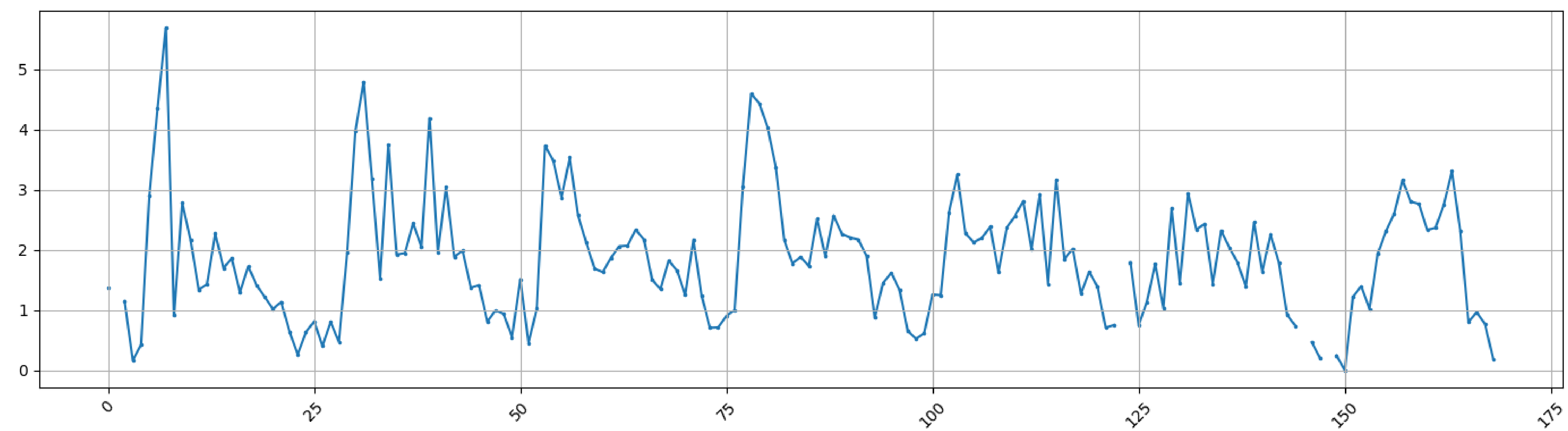
In [21]:
```
data_dtw = data_dt.copy()
data_dtw['how'] = np.round(24 * data_dt.index.weekday + data_dt.index.hour + data_dt.index.m
how_std = data_dtw.groupby('how').agg({'value': ['std', 'count']})
```

- We need to check that no std value is missing
- ...But also that the counts are large enough for a reliable computation

Choosing the Correct Interval

Let's look again at the standard deviation values

In [22]:
```
util.plot_series(how_std['value', 'std'], show_markers=True, figsize=figsize)
```

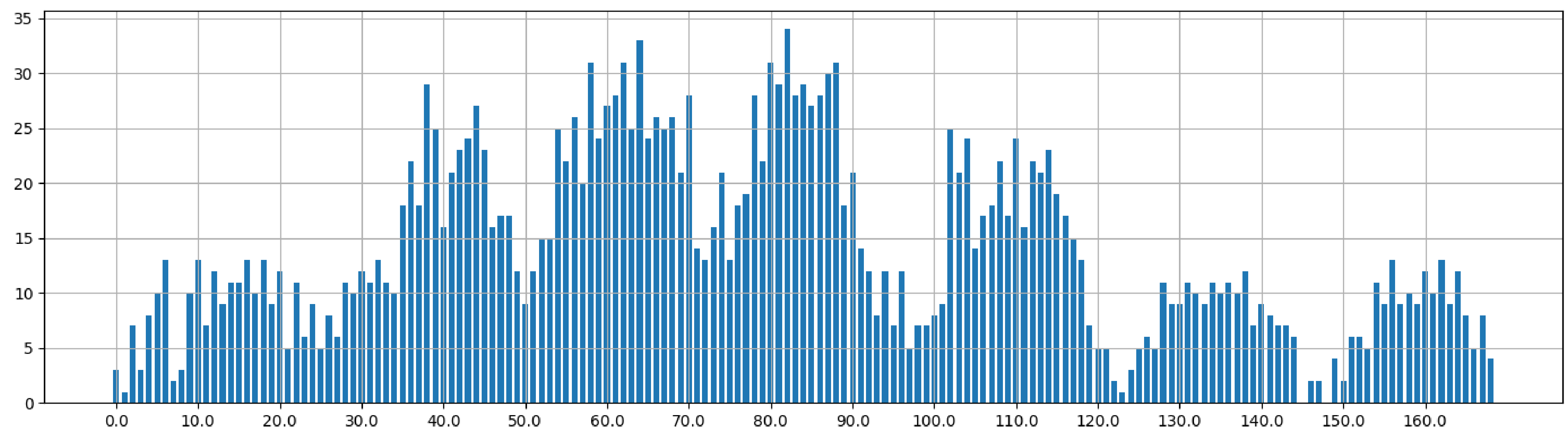


- There are still a few gaps

Choosing the Correct Interval

...And let's see the value counts

```
In [23]: util.plot_bars(how_std['value', 'count'], figsize=figsize)
```



- Several value counts are too low for σ to be reliable

Choosing the Correct Interval

We can try again with two-hour intervals

```
In [24]: data_dtw = data_dt.copy()
         data_dtw['how'] = 2*np.round(0.5*(24 * data_dt.index.weekday + data_dt.index.hour + data_dt.
         how_std = data_dtw.groupby('how').agg({'value': ['std', 'count']})
```

Let's check some information about the value counts:

- Ideally, we wish them at $\sim$ 30

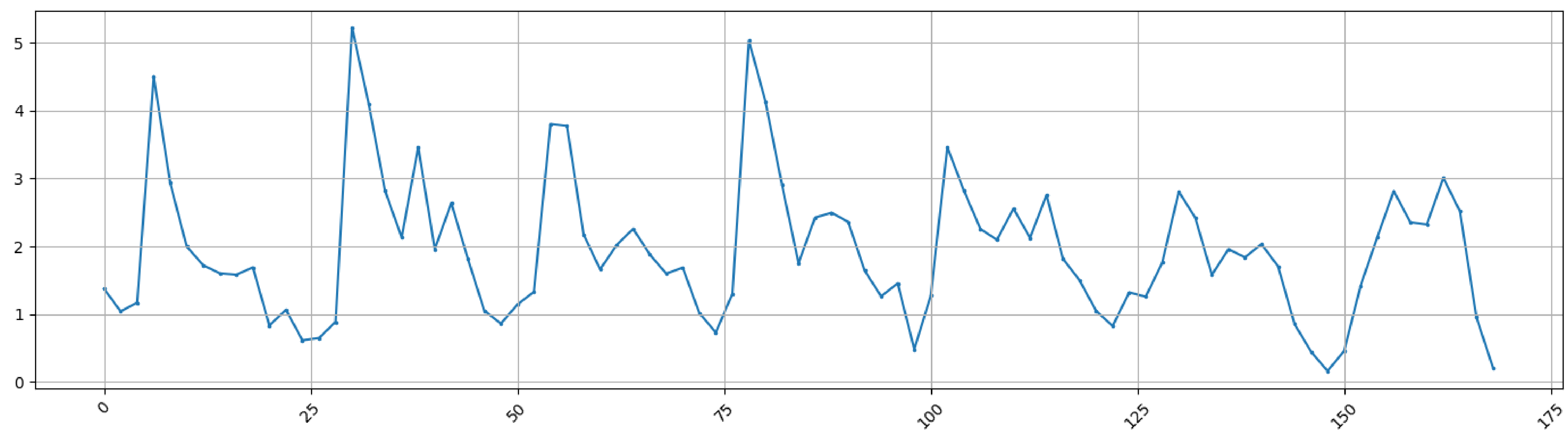
```
In [25]: how_std['value', 'count'].describe()
```

```
Out[25]: count    85.000000
         mean     27.917647
         std      16.132791
         min       3.000000
         25%      16.000000
         50%      22.000000
         75%      42.000000
         max      63.000000
         Name: (value, count), dtype: float64
```

Choosing the Correct Interval

Let's look the standard deviation with two-hour intervals

```
In [26]: util.plot_series(how_std['value', 'std'], show_markers=True, figsize=figsize)
```



- Finally, no more missing values and decently large counts

Upsampling and Smoothing

We managed to have reasonable standard deviation values..

...But out map/table has a very coarse time unit!

- Using it would lead to sharp variations in our predicted standard deviation

We will now proceed to mitigate the problem

We will start by upsampling, i.e. switching to a finer grain time unit:

```
In [27]: how_values = np.unique(24 * data_dt.index.weekday + data_dt.index.hour + data_dt.index.minut
         how_std_d = pd.DataFrame(index=sorted(how_values), columns=['std'], data=np.nan)
         how_std_d['std'] = how_std['value', 'std']
```

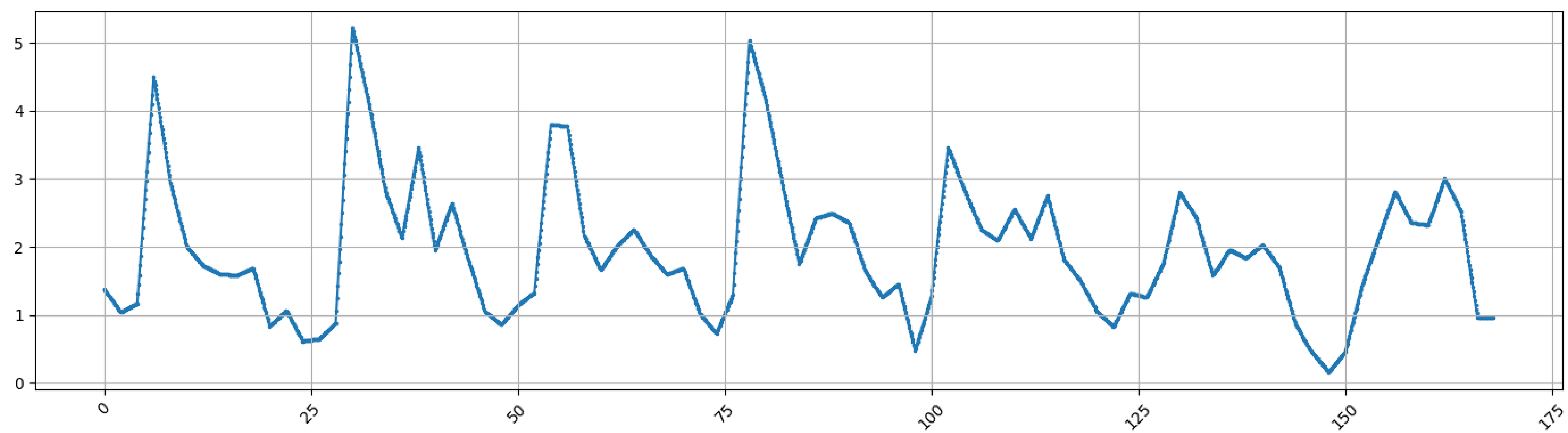
This process leads to many missing values, that we fill via linear interpolation:

```
In [28]: how_std_di = how_std_d.interpolate(method='linear')
```

Upsampling and Smoothing

Let's see the oversampled series

In [29]:
```
util.plot_series(how_std_di['std'], show_markers=True, figsize=figsize)
```



- The plot is the same as before, but there are more values on the x-axis

Upsampling and Smoothing

We will smooth the cuve via a simple low-pass filter

I.e. the Exponentially Weighted Moving Average

- This is a form of discrete filter, given by the recursion:

$$ss_i = \begin{cases} x_i & \text{if } i = 1 \\ \alpha x_i + (1 - \alpha) s_{i-1} & \text{otherwise} \end{cases}$$

- s_i is the i-th element of the output (smoothed) series
- α is called the smoothing factor and is equal to $1/(1 + \tau)$

Why not using a simple moving average?

- A moving average gives the same weigth to all observations...
- ...whereas in our case "recent" observations are more important
- I.e. the stdev from the original table should still be the dominant value

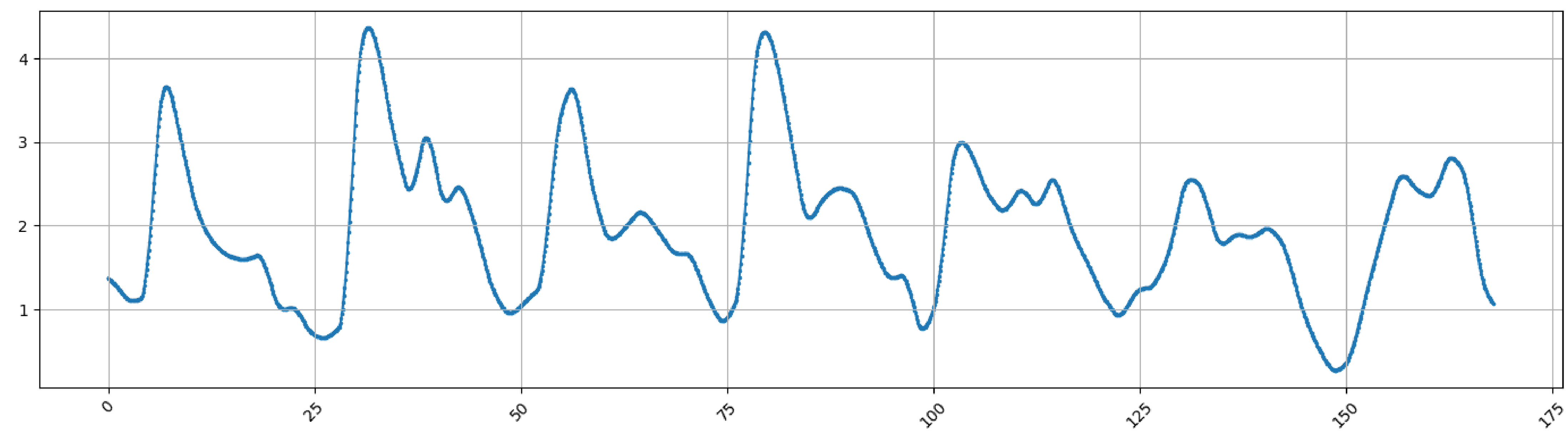
Upsampling and Smoothing

In pandas, we can use the `ewm` iterator, plus the `mean` aggregation function

```
DataFrame.ewm(com=None, ...).mean()
```

- The `com` parameter corresponds to τ

In [30]:
```
how_std_ds = how_std_di[['std']].ewm(com=12).mean()
util.plot_series(how_std_ds['std'], show_markers=True, figsize=figsize)
```



- We chose $\tau =$ the number of time steps in one hour

Gaussian Process for the Ensemble

Transforming the Dataset

We can now learn the Gaussian Process for our Ensemble

For this, we need to transform the original series using the stdev model

- We start by augmenting our dataset with the "hour of the week information"
- ...Then, we associate each data point to the predicted standard deviation

In [31]:
```
data_dt['how'] = 24 * data_dt.index.weekday + data_dt.index.hour + data_dt.index.minute / 60
data_dts = data_dt.join(how_std_ds, on='how')
data_dts.head()
```

Out[31]:

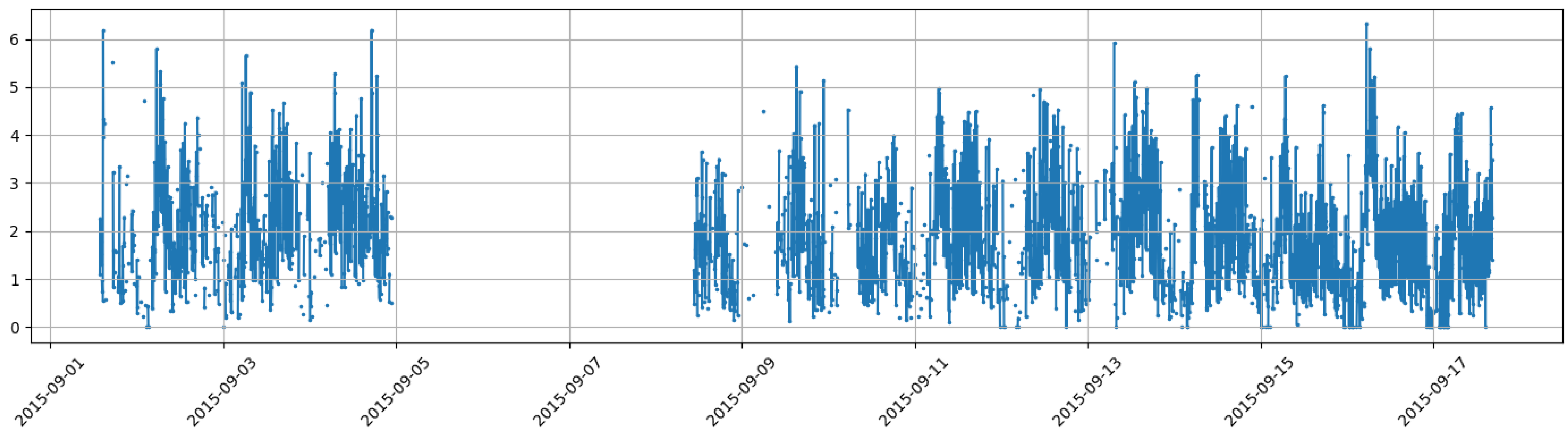
	value	time	how	std
timestamp				
2015-09-01 13:45:00	3.06	0	37.750000	2.822412
2015-09-01 13:50:00	6.44	1	37.833333	2.862934
2015-09-01 13:55:00	5.17	2	37.916667	2.904604
2015-09-01 14:00:00	3.83	3	38.000000	2.947336
2015-09-01 14:05:00	4.50	4	38.083333	2.981964

- We relied on the `join` method from `pandas`

Transforming the Dataset

Now we can actually transform the series values

```
In [32]: data_dts['value_tr'] = data_dts['value'] / data_dts['std']
         util.plot_series(data_dts['value_tr'], show_markers=True, figsize=figsize)
```



- The series has changed considerably: this is not a simple standardization

Training Data

We can now select a sub-sequence of the data for learning the kernel

...Which is necessary, since the data has changed!

```
In [33]: segment_s = data_dts[(data_dts.index >= '2015-09-09') & (data_dts.index < '2015-09-17')].cop
```

We separate training and validation data as we did before:

```
In [34]: tmp = segment_s.dropna()

np.random.seed(42)
idx = np.arange(len(tmp))
np.random.shuffle(idx[1:-1]) # no not shuffle the first/last point
t = idx[1]; idx[1] = idx[-1]; idx[-1] = t # keep first/last points in the left half

sep = 2*len(idx) // 3
trdata_s = tmp.iloc[idx[:sep]]
tsdata_s = tmp.iloc[idx[sep:]]
```

Learning the Kernel Parameters

We can now learn the kernel parameters

We can use the same starting parameters (priors) as before:

```
In [35]: kernel_s = WhiteKernel(1e-3, (1e-4, 1e-1))
         kernel_s += ConstantKernel(1, (1e-2, 1e2)) * RBF(1, (1e-1, 1e1))
         kernel_s += ConstantKernel(1, (1e-2, 1e2)) * ExpSineSquared(1, 2000, (1e-1, 1e1), (1900, 210

         np.random.seed(42)
         gp_s = GaussianProcessRegressor(kernel=kernel_s, n_restarts_optimizer=3)
         gp_s.fit(trdata_s[['time']], trdata_s['value_tr'])
         print(gp_s.kernel_)
```

```
WhiteKernel(noise_level=0.000153) + 0.91**2 * RBF(length_scale=0.447) + 1.66**2 * ExpSineSq
uared(length_scale=0.103, periodicity=2.01e+03)
```

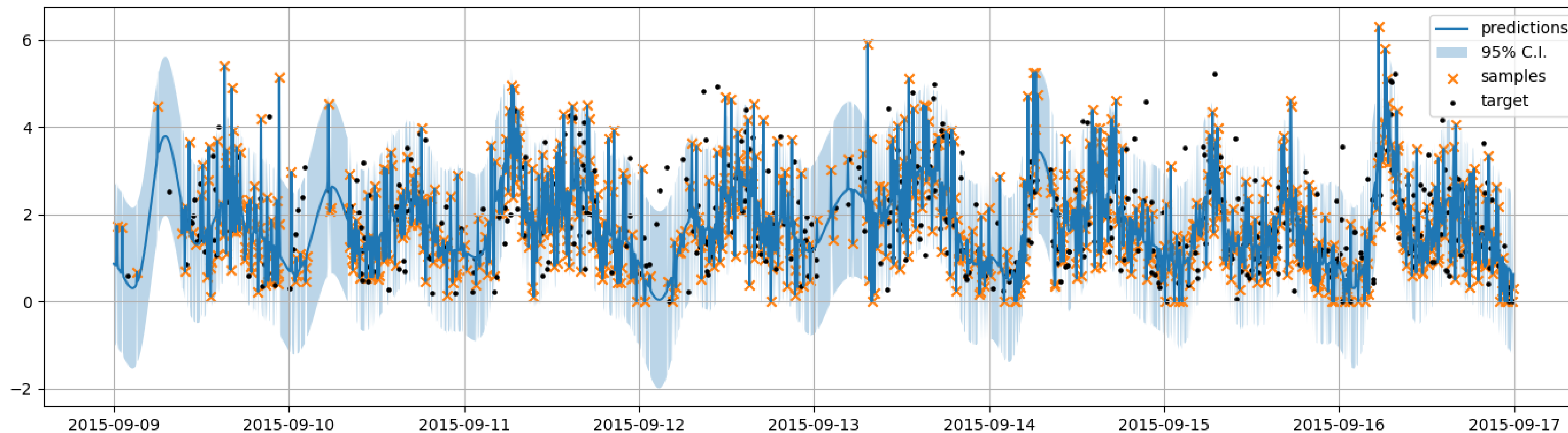
Then we obtain the predictions:

```
In [36]: pred_s, std_s = gp_s.predict(segment_s[['time']], return_std=True)
         pred_s = pd.Series(index=segment_s.index, data=pred_s)
         std_s = pd.Series(index=segment_s.index, data=std_s)
```

Learning the Kernel Parameters

Let's look at the predictions on the training data

```
In [37]: util.plot_gp(target_samples=tsdata_s['value_tr'], samples=trdata_s['value_tr'], pred=pred_s,
```



- For sake of simplicity, we will not try to improve the kernel

Transferring the Results

Now we obtain predictions for the missing values in the transformed series

Again, we reuse the kernel and add the observations:

In [38]:
```
gp2_s = GaussianProcessRegressor(kernel=gp_s.kernel_, optimizer=None)
tmp_s = data_dts.dropna() # The whole series (NaNs excluded)
gp2_s.fit(tmp_s[['time']], tmp_s['value_tr']);
```

Then we can obtain predictions (and confidence intervals) for the whole series

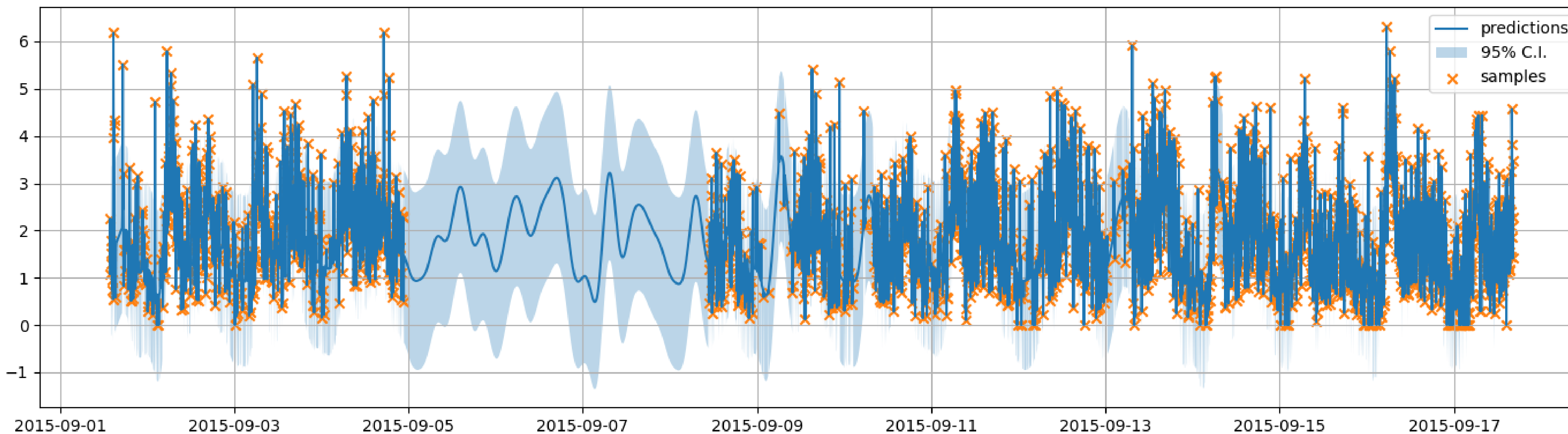
In [39]:
```
pred_all_s, std_all_s = gp2_s.predict(data_dts[['time']], return_std=True)
pred_all_s = pd.Series(index=data_dts.index, data=pred_all_s)
std_all_s = pd.Series(index=data_dts.index, data=std_all_s)
```

- Of course are still referring to the transformed series

Transferring the Results

Let's have a look at all the predictions

In [40]:
```
util.plot_gp(samples=data_dts['value_tr'], pred=pred_all_s, std=std_all_s, figsize=figsize)
```

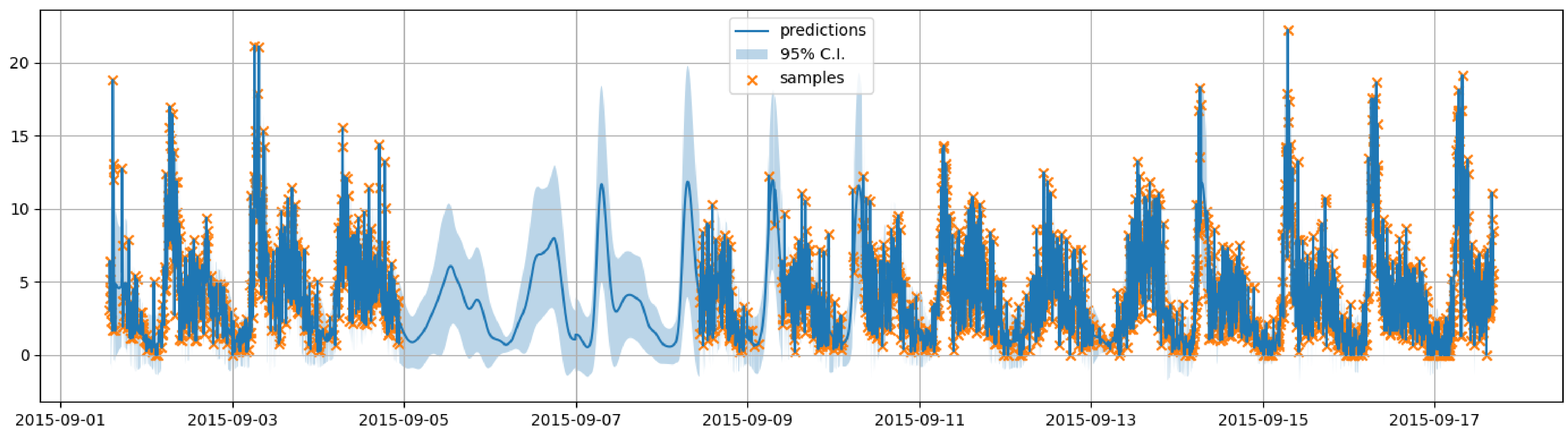


- They are not so easy to interpret, since they refer to the transformed series

Predictions for the Original Series

We obtain predictions for the original series by injecting back the variance

```
In [41]: pred_all2_s = pd.Series(index=data_dts.index, data=pred_all_s * data_dts['std'])
         std_all2_s = pd.Series(index=data_dts.index, data=std_all_s * data_dts['std'])
         util.plot_gp(samples=data_dt['value'], pred=pred_all2_s, std=std_all2_s, figsize=figsize)
```

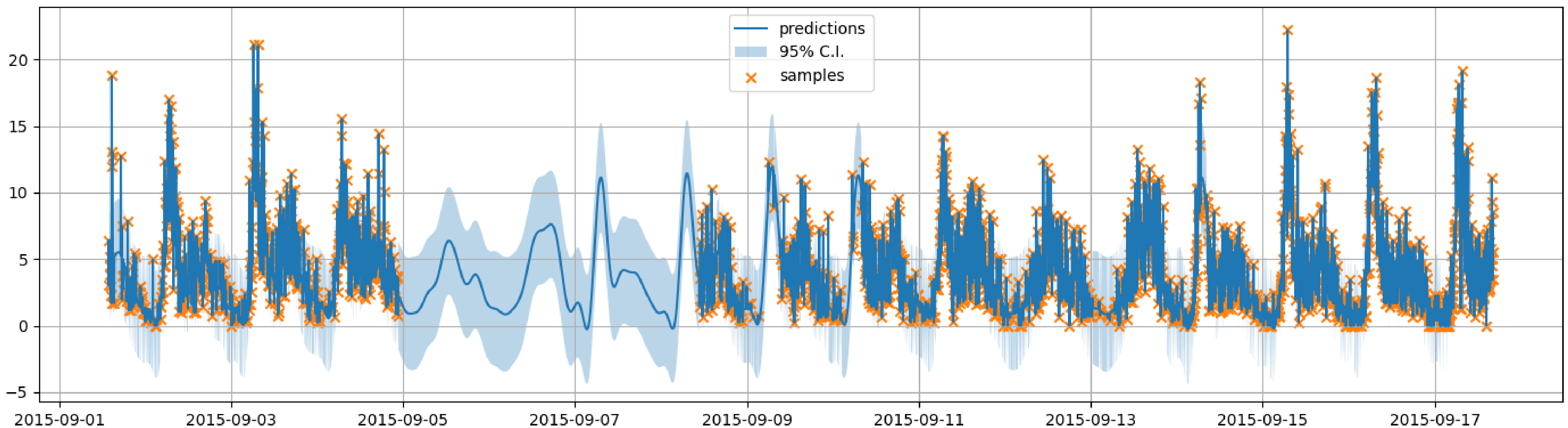


- Due to the properties of variance
- ...We can just multiply also the standard deviation

Predictions for the Original Series

For comparison, here are the results for the previous Gaussian Process

In [42]:
```
util.plot_gp(samples=data_dt['value'], pred=pred_all, std=std_all, figsize=figsize)
```



- The new confidence intervals are much tighter

Fill with Predictions and Samples

We can fill the missing values using the predictions

This will fill each missing value using the Maximum A Posteriori

In [43]:
```
mask = data_d['value'].isnull() # we need to fill only the NaNs
data_filled_pred = data_d.copy()
data_filled_pred.loc[mask, 'value'] = np.maximum(0, pred_all2_s[mask])
```

But with GPs, we can also sample from the distribution

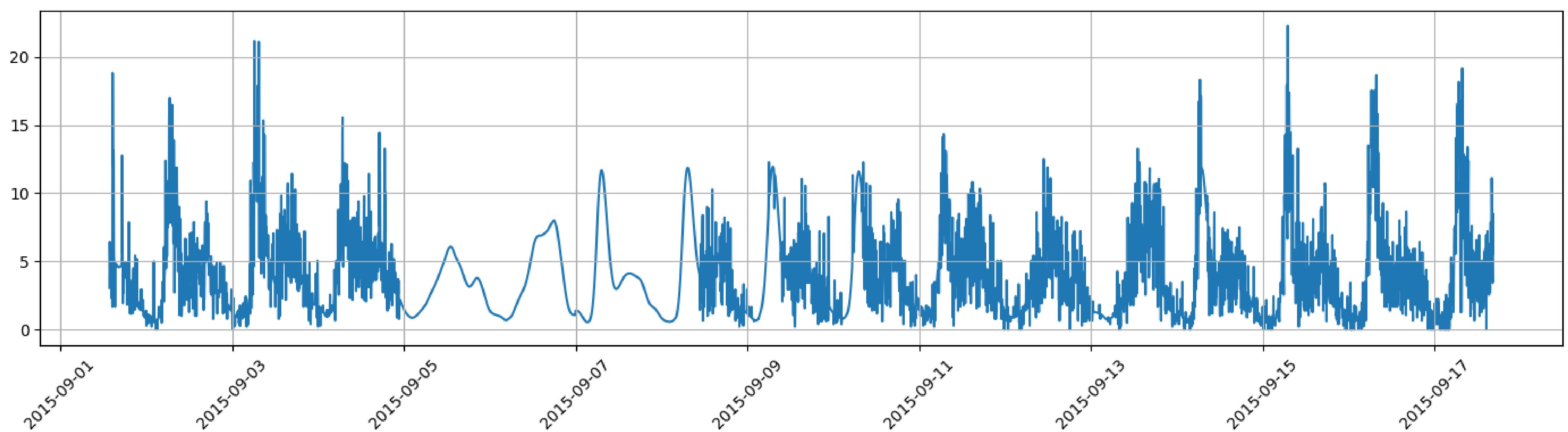
In [44]:
```
tmp = data_dts[mask]
sample_ms = gp2_s.sample_y(tmp[['time']], random_state=42).ravel()
data_filled_samples = data_d.copy()
data_filled_samples.loc[mask, 'value'] = np.maximum(0, sample_ms * tmp['std'])
```

- `sample_y` returns a matrix: we used `ravel` to have a single dimension
- In both cases, we clip values at zero (no less than 0 occupancy)

Filling with Predictions and Samples

Here's the series filled using predictions:

In [45]:
```
util.plot_series(data_filled_pred, figsize=figsize)
```

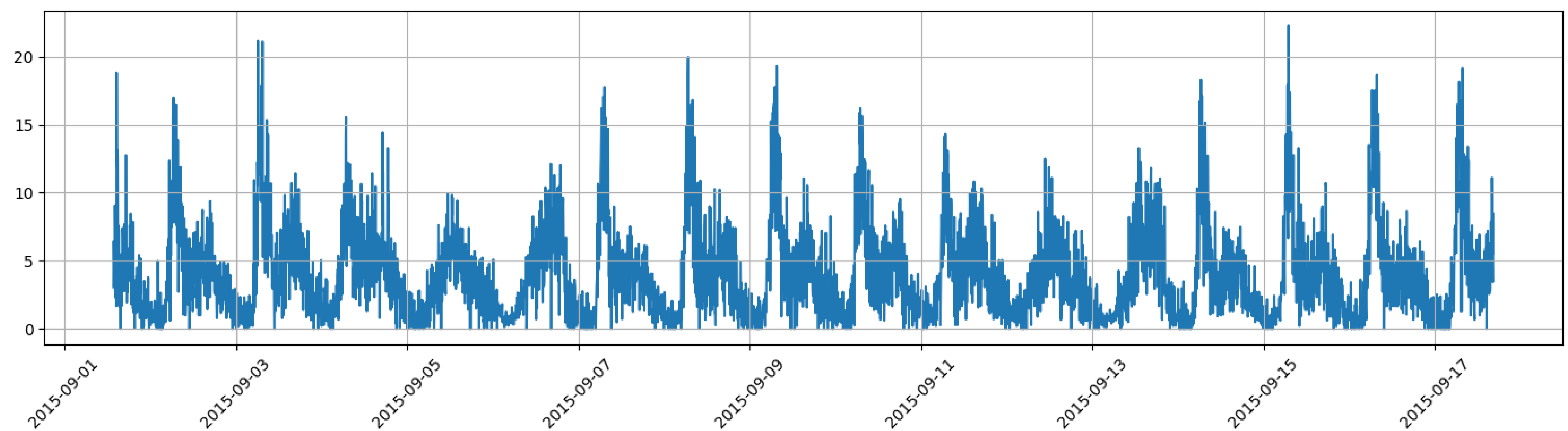


- The use of MAPs is evident in the large gap

Filling with Predictions and Samples

Here's the series filled using samples:

In [46]:
```
util.plot_series(data_filled_samples, figsize=figsize)
```



- There no evidently "fake" sections, now! ...Except for the effect of clipping at 0