In [2]:
```python
# ============================================================
# Notebook setup: run this before everything
# ============================================================

%load_ext autoreload
%autoreload 2

# Control figure size
figsize=(14, 4)

from sklearn.neighbors import KernelDensity
from util import util
import numpy as np
from matplotlib import pyplot as plt
import pandas as pd
import os

data_folder = os.path.join('..', 'data', 'nab')
file_name = os.path.join('realKnownCause', 'nyc_taxi.csv')
data, labels, windows = util.load_series(file_name, data_folder)
```

```
The autoreload extension is already loaded. To reload it, use:
  %reload_ext autoreload
```

KDE for Our Anomaly Detection Case Study

A Few Tweaks

We will work with *log probabilities*

- This is what sklearn does by default
- ...And simplifies some operations
- I.e. products become sums

Additionally, we will work with *negated* (log) probabilities

- They can be interpreted as *alarm signals*
- ...Which is the customary approach in anomaly detection

Overall, our anomaly detection condition becomes:

$$-\log f(x, \theta) \geq \varepsilon$$

...Which is equivalent to the previous formulation

Training and Testing

We will split our data in two segments

A *training set*:

- This will include only data about the *normal* behavior
- Ideally, there should be no anomalies here (we do not want to learn them!)
- We will use it to fit a KDE model

A *test set*:

- To assess how well the approach can generalize

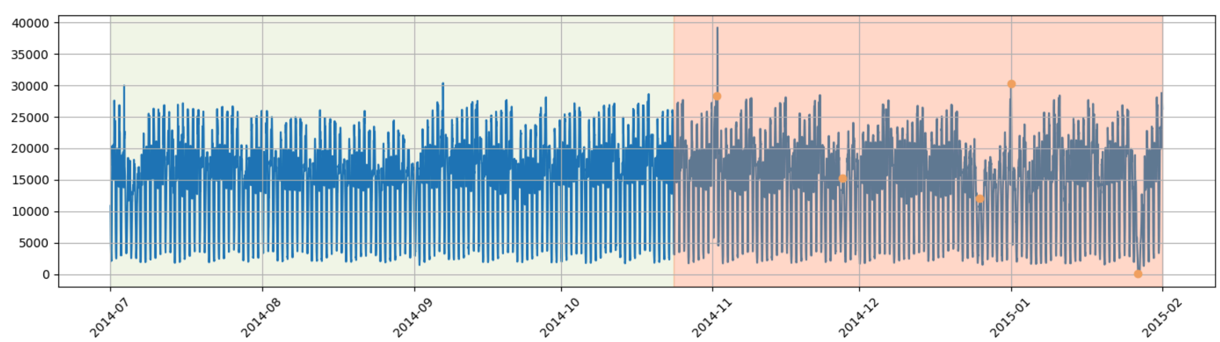
If the training set contains some anomalies

- Things may still be fine, as long as they are very *infrequent*
- ...Since we will still learn that they have low probability

Training and Testing

In time series data sets are often split chronologically:

In [3]:
```
train_end = pd.to_datetime('2014-10-24 00:00:00')
util.plot_series(data, labels, test_start=train_end, figsize=figsize)
```



- Green: training set, orange: test set

Fitting the Estimator

Now, we can separate the training set

...And estimate the bandwidth by using the rule of thumb:

In [4]:
```
data_tr = data[data.index < train_end]
q1 = data_tr['value'].quantile(0.25)
q3 = data_tr['value'].quantile(0.75)
sigma = data_tr['value'].std()
m =  len(data_tr)
h = 0.9 * min(sigma, (q3-q1)/ 1.34) * m**(-0.2)
print(f'The estimated bandwidth is {h:.3f}')
```

```
The estimated bandwidth is 1056.061
```

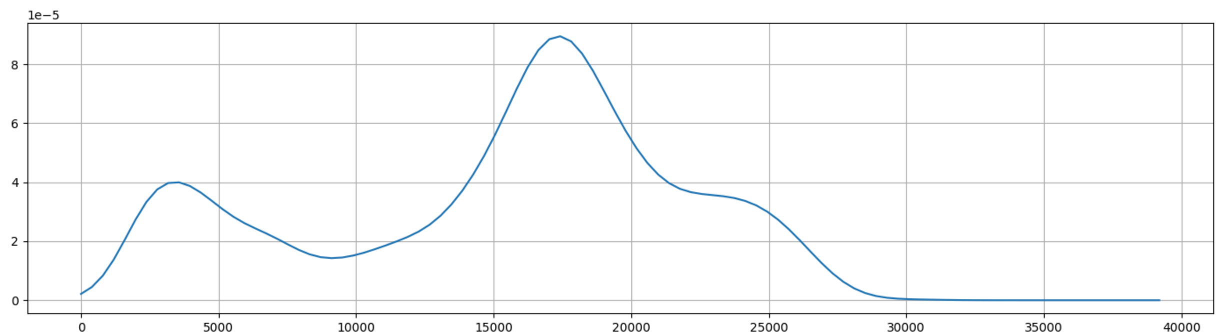
Then we fit a univariate KDE estimator (using scikit-learn)

In [5]:
```python
kde = KernelDensity(kernel='gaussian', bandwidth=h)
kde.fit(data_tr.values);
```

Fitting the Estimator

Let's have a look at the estimate distribution:

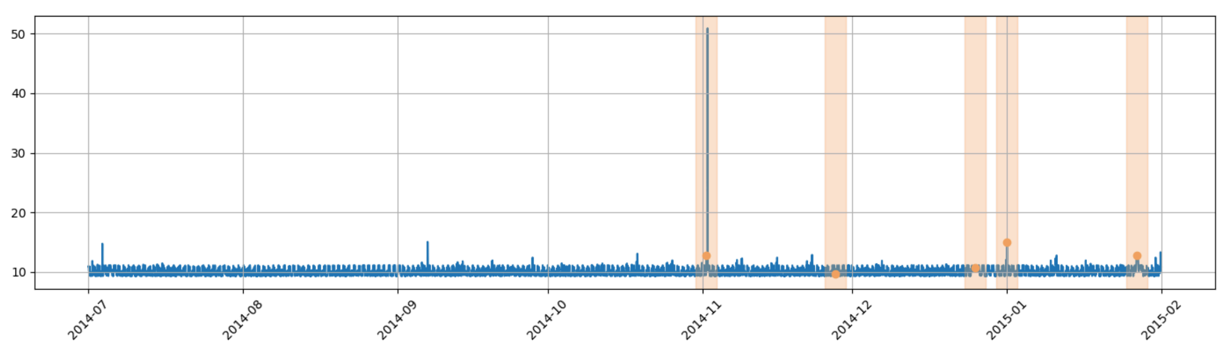
In [6]:
```python
vmax = data['value'].max()
xr = np.linspace(0, vmax, 100)
util.plot_density_estimator_1D(kde, xr, figsize=figsize)
```



Alarm Signal

We can now obtain (and plot) our *alarm signal*:

In [7]:
```python
ldens = kde.score_samples(data.values) # Obtain log probabilities
signal = pd.Series(index=data.index, data=-ldens) # Build series with neg. p
util.plot_series(signal, labels=labels, windows=windows, figsize=figsize) #
```



- Notice how the the process (inference) is noticeably slower than training
- Can you tell why this was the case?

Detecting Anomalies

Let us pick a threshold (at random, for now) and try to detect some anomalies:

In [8]:
```python
thr = 13
pred = pd.Series(signal.index[signal >= thr])
print(pred.head(), f'#anomalies: {len(pred)}')
```

```
0   2014-07-03 19:00:00
1   2014-09-06 22:30:00
2   2014-09-06 23:00:00
3   2014-10-18 23:30:00
4   2014-11-02 01:00:00
Name: timestamp, dtype: datetime64[ns] #anomalies: 15
```

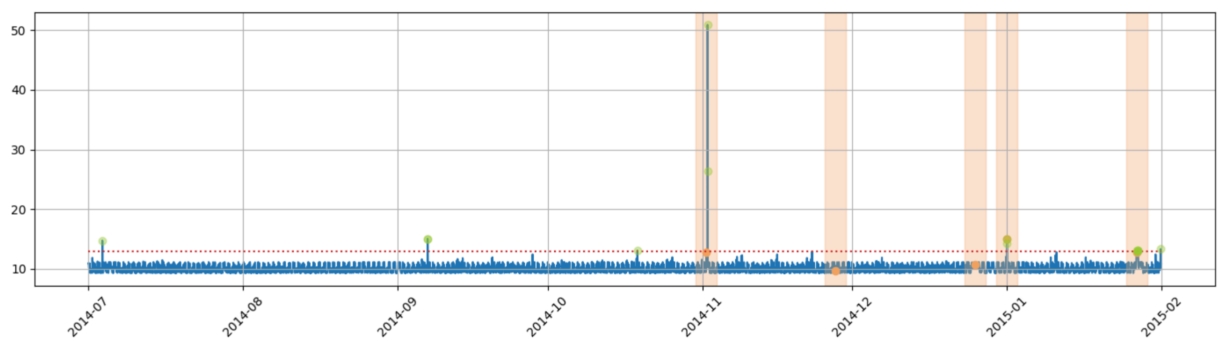
- We just apply the filter `signal >= thr` to the signal index
- This yields a number of (predicted) anomalous timestamps
- Our module contains a function to perform this step:

```python
def get_pred(signal, thr)
```

Detecting Anomalies

Let us plot our predictions on the series:

In [9]:
```python
util.plot_series(signal, labels=labels, windows=windows, predictions=pred, t
```



- Not very good, but the threshold *is* random
- There are a many false positives, which are *very common* in anomaly detection

Metrics for Anomaly Detection

How do we evaluate the quality of our system?

Metrics for Anomaly Detection

Evaluating the quality of an Anomaly Detection system can be tricky

- Usually, we do not need to match the anomalies exactly
- Sometimes we wish to anticipate anomalies
- ...But sometimes we just want to detect them in past data

There is no "catch-all" metric, like accuracy in classification

It is much better to devise a *cost model*

- We evaluate the cost and benefits of our predictions:
- By doing this, we focus on *the value for our customer*

> **This is important *for all industrial problems!***

A Simple Cost Model

We will use a simple cost model

Remember that our goals are:

- Analyzing anomalies
- Anticipating anomalies

First, we define:

- *True Positives* as windows for which we detect at least one anomaly
- *False Positives* as detected anomalies that do not fall in any window
- *False negatives* as anomalies that go undetected
- *Advance* as the time between an anomaly and when first we detect it

A Simple Cost Model

They can be computed using a function in our module:

```python
def get_metrics(pred, labels, windows)
```

In [10]:
```python
tp, fp, fn, adv = util.get_metrics(pred, labels, windows)
print('True Positives', tp.head(), f'#true positives: {len(tp)}')
```

```
True Positives 0   2014-11-01 19:00:00
1   2015-01-01 01:00:00
2   2015-01-27 00:00:00
dtype: datetime64[ns] #true positives: 3
```

In [11]:
```python
print('Advance', adv.head(), 'For each true positive')
```

```
Advance 0   -1 days +18:00:00
1     0 days 00:30:00
2   -1 days +22:00:00
dtype: timedelta64[ns] For each true positive
```

A Simple Cost Model

They can be computed using a function in our module:

```python
def get_metrics(pred, labels, windows)
```

In [12]:
```python
print('False Positives', fp.head(), f'#false positives: {len(fp)}')
```

```
False Positives 0   2014-07-03 19:00:00
1   2014-09-06 22:30:00
2   2014-09-06 23:00:00
3   2014-10-18 23:30:00
4   2015-01-31 19:00:00
dtype: datetime64[ns] #false positives: 5
```

In [13]:
```python
print('False Negatives', fn.head(), f'#false negatives: {len(fn)}')
```

```
False Negatives 0   2014-11-27 15:30:00
1   2014-12-25 15:00:00
dtype: datetime64[ns] #false negatives: 2
```

A Simple Cost Model

Then we introduce:

- A cost c_{alarm} for loosing time in analyzing false positives
- A cost c_{missed} for missing an anomaly
- A cost c_{late} for a late detection (partial loss of value)

Our cost model (simple, but serviceable) is then given by:

In [14]:
```python
c_alrm = 1 # Cost of investigating a false alarm
c_missed = 10 # Cost of missing an anomaly
c_late = 5 # Cost for late detection

# A simple cost model
cost = c_alrm * len(fp) + \
       c_missed * len(fn) + \
       c_late * (len([a for a in adv if a.total_seconds() <= 0]))
print(f'The cost with the current predictions is: {cost}')
```

```
The cost with the current predictions is: 35
```

Of course, in a real problem the cost model should be *discussed with the stakeholders*

Threshold Choice

Refactoring the Cost Model

We will use this cost model for *choosing our threshold*

With this aim, we encapsulate the formula in a Python class in our module:

```
class ADSimpleCostModel:
    def __init__(self, c_alrm, c_missed, c_late):
        # Store cost parameters
        ...

    def cost(self, signal, labels, windows, thr):
        # Compute the cost
        ...
```

Refactoring the Cost Model

We can now evaluate our cost by:

- Instantiating the class with our values for $c_{alarm}, c_{missed}, c_{late}$
- Calling the `cost` function with different threshold values

In [15]:
```
cmodel = util.ADSimpleCostModel(c_alrm, c_missed, c_late)
cost = cmodel.cost(signal, labels, windows, thr)
print(f'The cost with the current predictions is: {cost}')
```

```
The cost with the current predictions is: 35
```

The process is rather efficient:

- When we change the threshold
- ...We *do not need to rebuild* the alarm signal

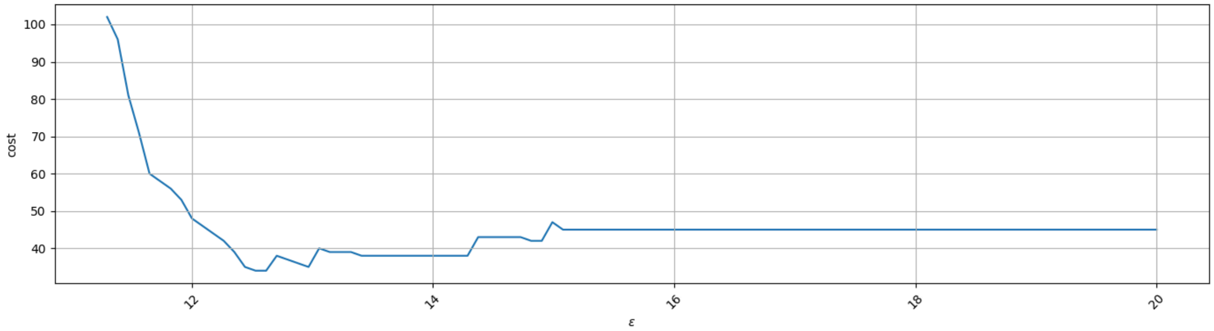
So, no need to repeat either training or inference

Effect of the Threshold

We can now look at the effect of changing the threshold:

First, we'll do this for an *idealized problem* (i.e. over all the data)

In [16]:
```
cmodel = util.ADSimpleCostModel(c_alrm, c_missed, c_late)
thr_range = np.linspace(11.3, 20, 100)
cost_range = pd.Series(index=thr_range, data=[cmodel.cost(signal, labels, wi
util.plot_series(cost_range, figsize=figsize, xlabel=r'$\varepsilon$', ylabe
```



Choosing the Threshold

Ideally, we wish to choose *the best threshold*

However, we have two problems:

- We cannot really use all the data
- ...we need to keep some away to test generalization
- The threshold-to-cost function is non-smooth and non-differentiable

Luckily, both are easy to address

We can:

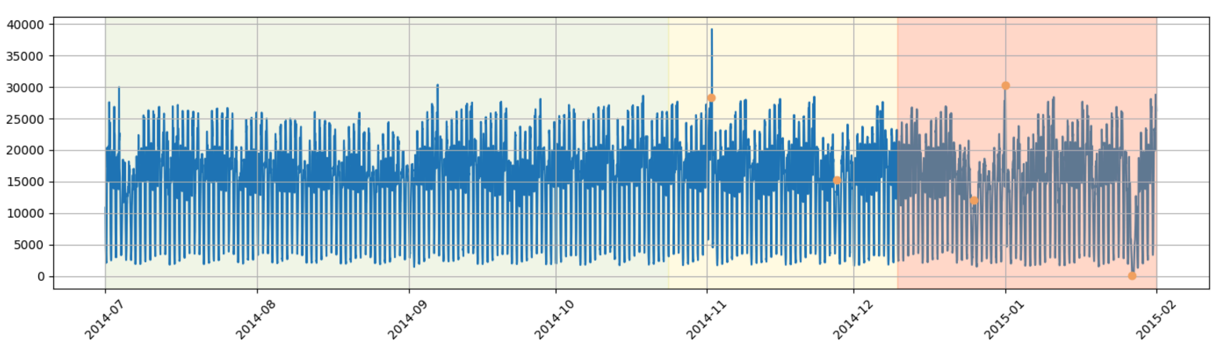
- Define a *validation set* to use when optimizing the threshold
- Use a simple *line search approach*, since ε is a scalar

Define a Validation Set

First, we define our validation set:

- It should contain some anomalies
- ...But some should be left our (for testing)

In [17]:
```
val_end = pd.to_datetime('2014-12-10 00:00:00')
util.plot_series(data, labels, val_start=train_end, test_start=val_end, figs
```



Optimize the Threshold

We will use a line sampling approach:

We build the validaton set and define a range of "sampled" thresholds:

In [18]:
```
signal_opt = signal[signal.index < val_end]
labels_opt = labels[labels < val_end]
windows_opt = windows[windows['end'] < val_end]
```

Then, we use a function from our module to pick the best one:

```
def opt_thr(signal, labels, windows, cmodel, thr_range):
    costs = # compute costs as before
    best_idx = np.argmin(costs)
    return thr_range[best_idx], costs[best_idx]
```

Validation Set?

Did you notice how we included the training data in the validation set?

> **Is that good or bad?**

It's definitely not standard, but reasonable in this case!

The reason is that our "validation set"

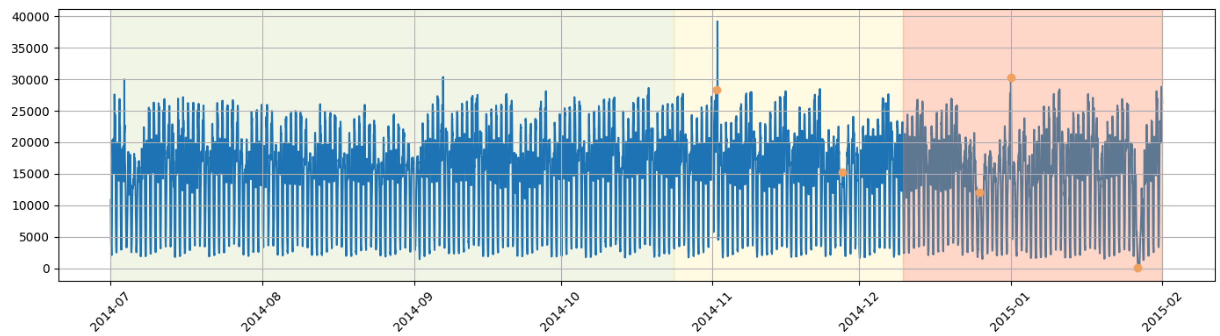
- ...Is *not needed to ward off against overfitting*
- ...But just to optimize one more parameter (i.e. θ)

It is actually *part of the training data*

Get Accustomed to Drift

One more thing: see how the anomaly frequency changes over time?

In [19]:
```
util.plot_series(data, labels, val_start=train_end, test_start=val_end, figs
```



- In time series, the data distribution often *drifts over time*
- When this happens, it is usually good to split the series in contiguous chunks
- I.e. the training, validation, and test set should be sequences

Optimize the Threshold

Let's see the results of threshold optimization

In [20]:
```
best_thr, best_cost = util.opt_thr(signal_opt, labels_opt, windows_opt,  cmc
print(f'Best threshold: {best_thr:.3f}, corresponding cost: {best_cost:.3f}'
```

```
Best threshold: 15.079, corresponding cost: 15.000
```

- The reported cost is on the training and validation set

For all the data (yes, we are cheating a bit) we have:

In [21]:
```
ctst = cmodel.cost(signal, labels, windows, best_thr)
print(f'Cost on the whole dataset {ctst}')
```

```
Cost on the whole dataset 45
```

- This is, as expected, *suboptimal*
- ...But it works! We have our *first complete anomaly detection approach*