

Problem and Data

# **Anomaly Detection on Taxi Calls**

# Let's considere a Taxi company:



# **Anomaly Detection on Taxi Calls**

### Some context information:

- There's historical data about taxi calls in NYC (number of taxi calls over time)
- A major decision for the company is choosing the size of the car pool
- This depends on how many calls are expected
- Strong deviations from the usual patterns may also cause issues
- The company is mostly interested in detecting such "anomalies"
- Anticipating them would be a welcome addition, but it is not essential

# **Anomaly Detection on Taxi Calls**

### Some context information:

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- This depends on how many calls are expected
- Strong deviations from the usual patterns may also cause issues
- The company is mostly interested in detecting such "anomalies"
- Anticipating them would be a welcome addition, but it is not essential

### How can we tackle this problem?

# **Getting Started**

### A couple of good ideas:

Trying to understand the context:

- The company priorities and how their business works
- Any expectation on the data

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...And also inspecting the data

- ...So that we get a "feel" of how it works
- Formally: until we understand better its statistical distribution

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- Formally: until we understand better its statistical distribution

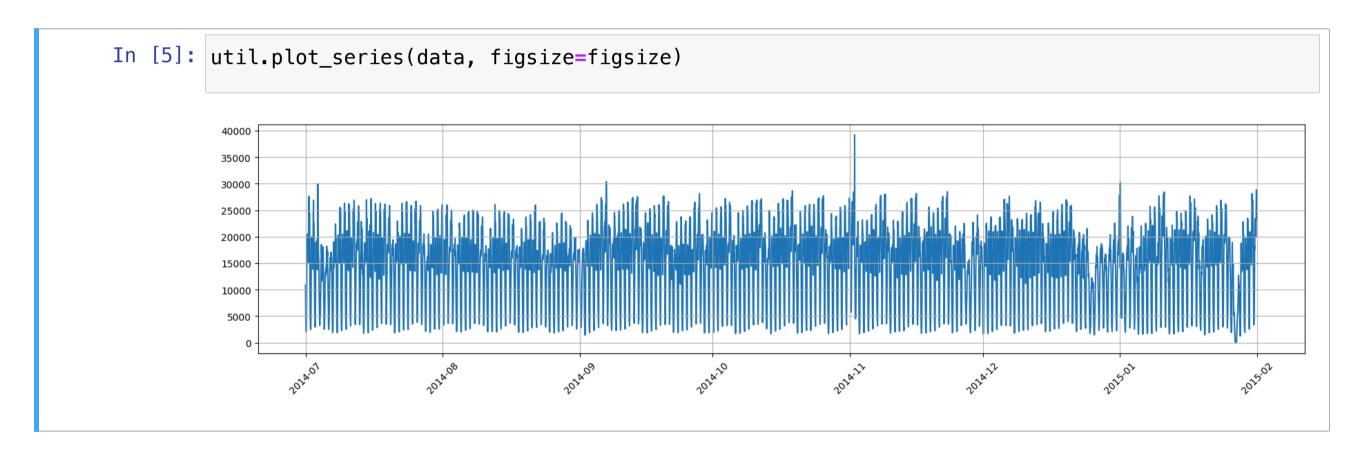
Doing both these things early is always a good idea

### Let's have a look at the available data

- data is a pandas DataFrame object
- It is essentially a table, in this case representing a time series
- There are well defined column names (here "value")
- There is a well defined row index (here "timestamp")

### Time series are quite easy to visualize

The most direct approach is using a Cartesian plot



■ If are curious, all use case code is available as part of the course material

#### We can now move to other data structures

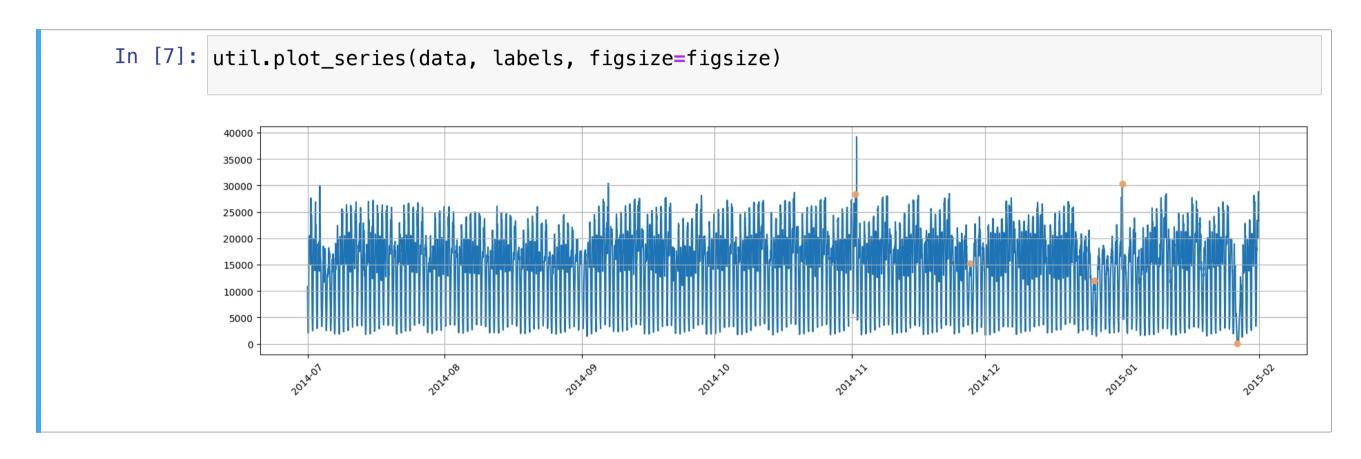
### labels is a pandas Series object

You can think of that as a one-column table

### This series contains the timestamp of all known anomalies

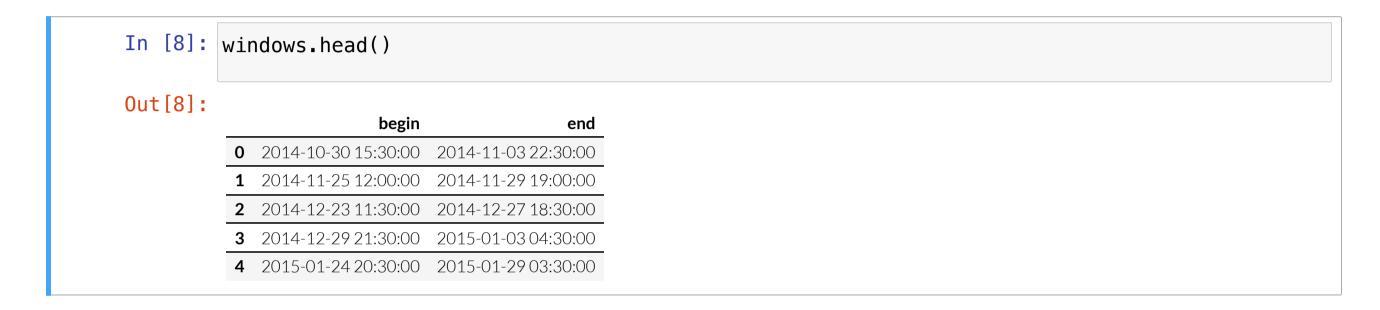
- There are just a few of them
- ...and they are all hand-labeled

### We can plot the call and anomalies together



- Most anomalies in the second part of the series
- ...But that's just a coincidence

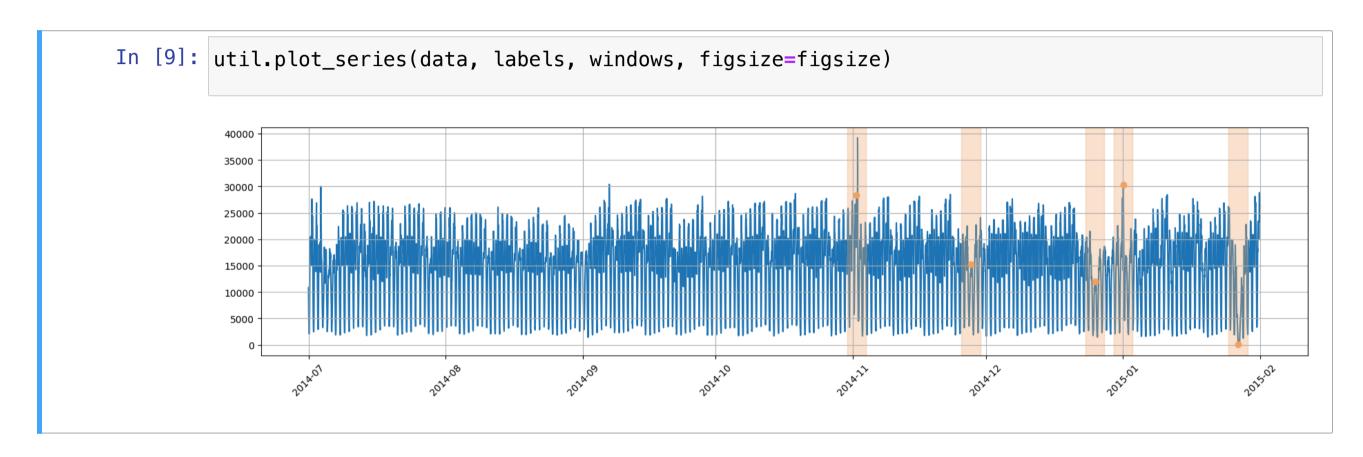
### Now we can check the "windows" data structure



windows is another a pandas DataFrame object (a table)

- It contains the start/end of windows containing anomalies
- Detections within the window are useful and count as "hits"
- Detections outside the windows are false alarms

### Let's plot all the information together



Detections that occur too early/late count as misses



Formalizing the Problem

Let's start with a question

What is our biggest difficulty right now?

# On the Importance of Formalization

### Right now, the problem we are tackling is too vaguely defined

This makes it much harder to think about:

- Solution approaches
- Evaluation procedures
- Key Performance Indicators

### **Eventually, we'll need to formally specify:**

- The input and output of our solution system
- ...And a set of quality metrics

But first, we need a formal way just to reason on the system

# **System Formalization**

### Let's attempt to formalize the system, first

We can view the number of taxi call as a random variable

$$X \sim P(X)$$

- lacksquare X is a source of random data
- D(X) is its support, i.e. the set of possible outcomes
- $lackbox{P}(X)$  is its distribution, i.e. the probability of every outcome

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Can we use this to define our car pool size, or to detect anomalies?

# **Anomaly Detection and Car Pool Sizing**

### Formally, we could size the car pool via a rule like

$$\underset{q \in D(X)}{\operatorname{argmin}} F(q) \ge \alpha$$

- F(x) tells use the probability that  $X \leq x$  (Cumulative Distribution Function)
- lacktriangleright lpha is the total probability of the scenario we want to cover with our pool

### ...And we could detect anomalies via a rule like:

$$P(x) \le \varepsilon$$

- $\bullet$  is a threshold value
- If the probability of observing x call is below  $\theta$ , we say we have an anomaly

We've already made good progress!

# What do we need to use this idea in practice?

# **Density Estimation**

### The main issue we have now is that we really don't know P(X)

...But we can learn it from our data

- Given a dataset  $\{x_i\}_{i=1}^m$  containing observed numbers of taxi calls
- ...We can try to approximate P(X) with a parametric function  $\hat{f}(x;\theta)$

### This is the gist of density estimation

In practice,  $\hat{f}(x;\theta)$  is often trained for maximum likelihood estimation

- This is a very common training method based on the idea that a good model
- ...Should assign a high-probability to real data

# **MLE Training**

### Formally, MLE training consists in solving:

$$\underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{m} \hat{f}(x_i; \theta)$$

- Given our dataset  $\{x_i\}_{i=1}^m$ ...
- ...We choose the model parameters  $\theta$ ...
- ...So that the estimated probability is as high as possible

### Now we need to define two things:

- Which data we should use for training
- Which function (i.e. model) to use as an estimator



**Data and Model** 

# **Training and Testing**

### We will split our data in two segments

A training set, used for learning the estimator:

- This will include only data about the normal behavior
- Ideally, there should be no anomalies here (we do not want to learn them!)

A test set, use for evaluation

We should never optimize anything on this

# **Training and Testing**

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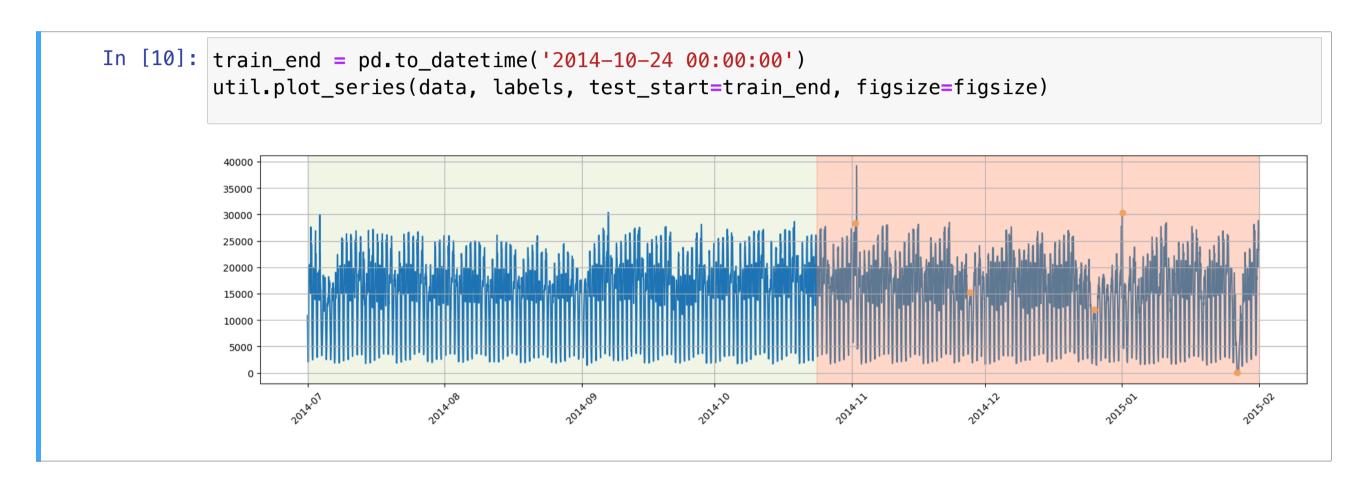
We should never optimize anything on this

### If the training set contains some anomalies

- Things are still mostly fine!
- ...As long as they are very infrequent

# **Training and Testing**

In time series data sets are often split chronologically:



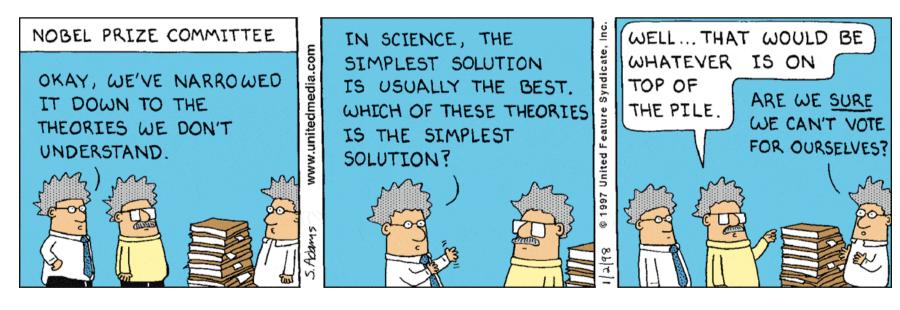
■ Green: training set, orange: test set

# **Choosing an Estimator**

### Which estimation model should we use?

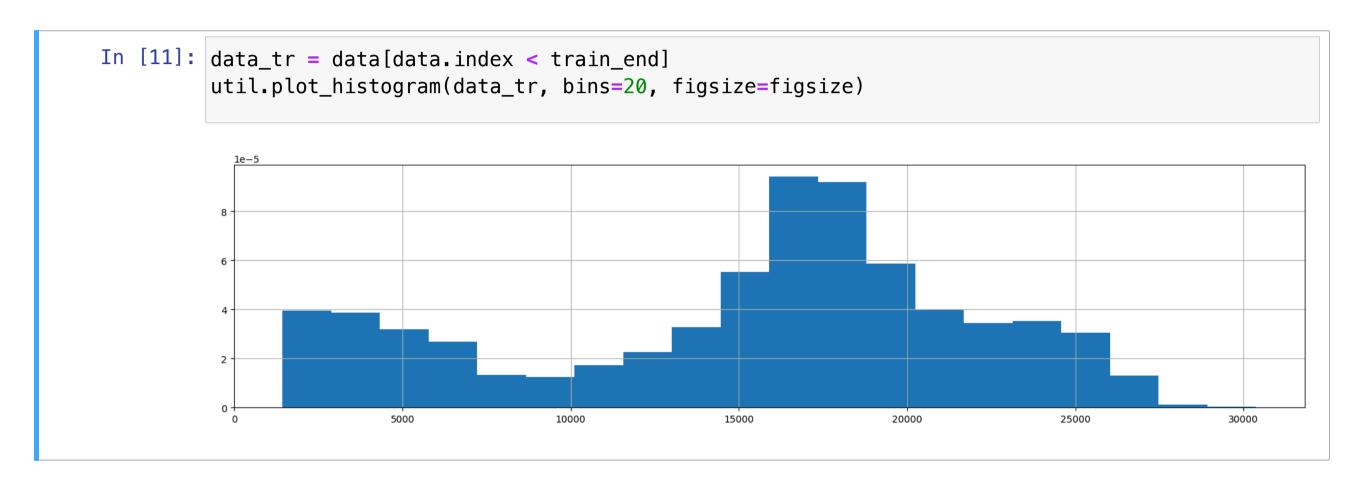
- Lacking any strong reason for doing otherwise
- Using Occam's razor is usually a good idea

### So, we'll go for a simple approach



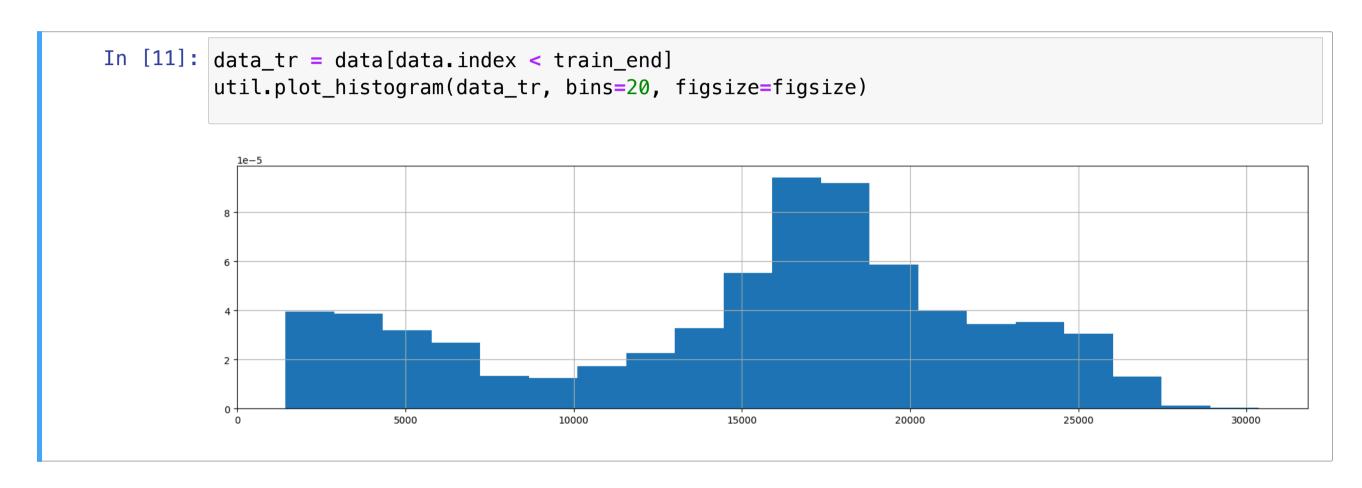
# **Histograms as Density Estimators**

### A histogram is a (very) simple density estimator



# **Histograms as Density Estimators**

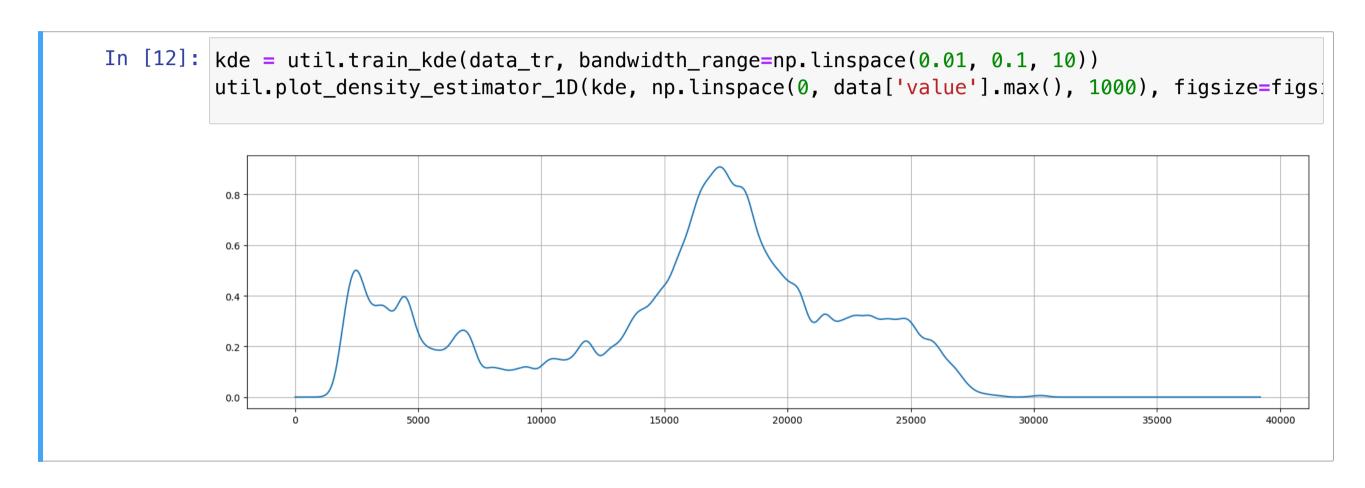
### A histogram is a (very) simple density estimator



- It gives us a probability for every value
- lacktriangle The model parameters  $oldsymbol{ heta}$  are in this case the bins

# **Kernel Density Estimation**

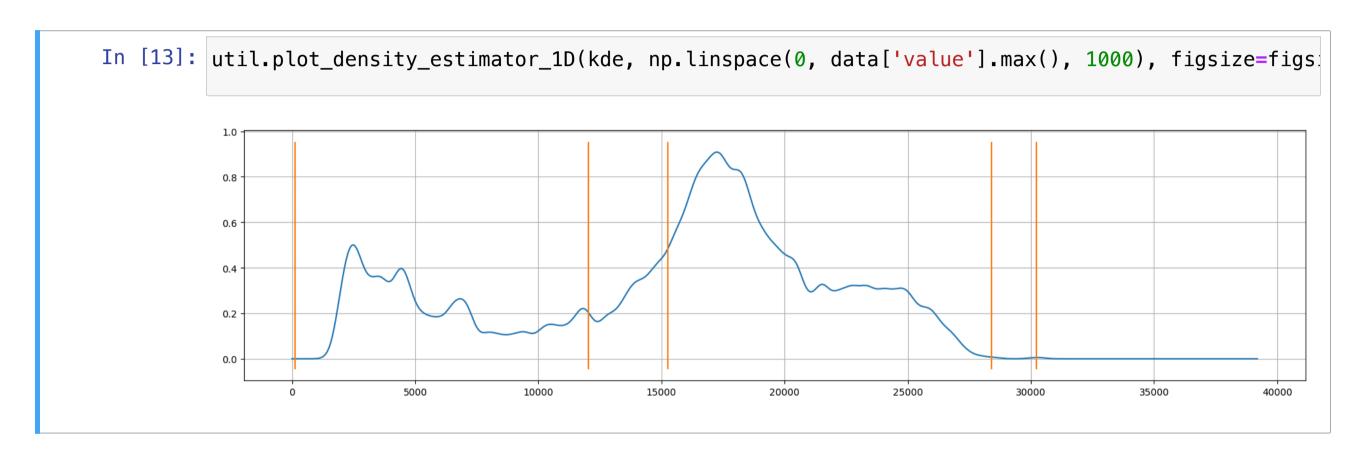
### **Another simple approach is Kernel Density Estimation**



- KDE plances one small kernel (e.g. a Gaussian) on every training point
- A distribution is the obtained by averaging

# **Density Estimation for Anomaly Detection**

We can test our idea by checking the probability of anomalous points



Several of the anomalous points have very low estimated probabilities

# **Alarm Signal**

### In anomaly detection, it is actually customary to work with alarm signals

- Rather than checking for low probabilities
- ...We check for a high "alarm"

### We can obtain an alarm signal from our estimator as:

$$-\log \hat{f}(x;\theta) \ge \varepsilon$$

- We use log probabilities (to reduce a bit the scale)
- ...And we change the sign to interpret them as an "alarm"

It is still equivalent to the previous formulation

# **Alarm Signal**

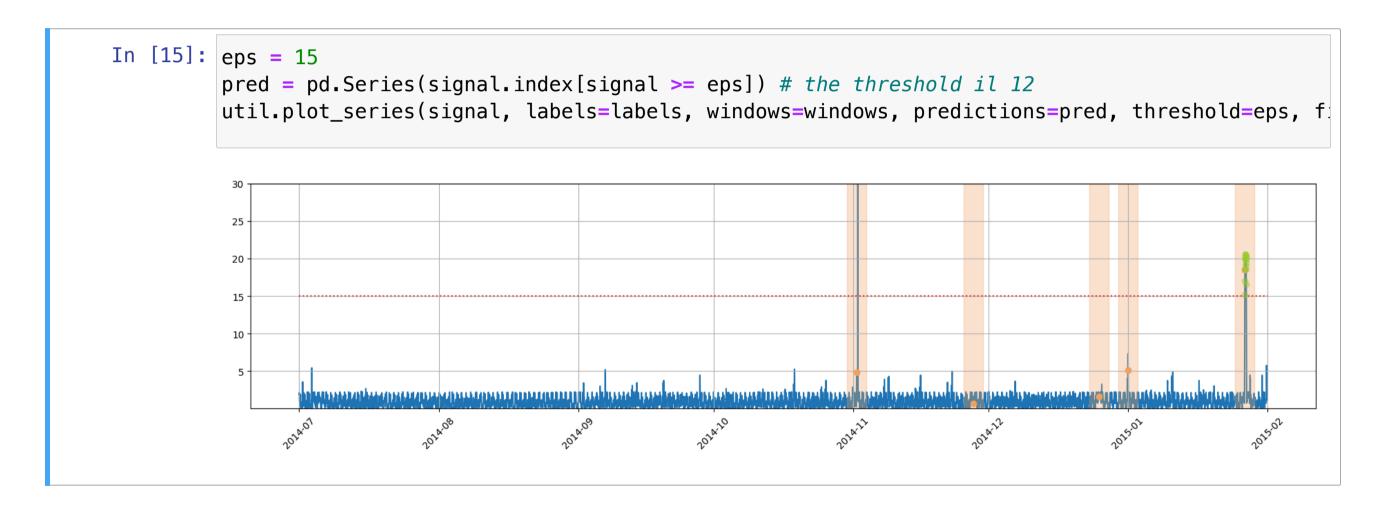
### We can now obtain (and plot) our alarm signal:

```
In [14]: | ldens = kde.score_samples(data.values) # Obtain log probabilities
       signal = pd.Series(index=data.index, data=-ldens) # Build series with neg. prob.
       util.plot_series(signal, labels=labels, windows=windows, figsize=figsize, y_cap=30) # Plot
        25
        20
        15
        10
```

Again, some anomalies stand out

# **Detecting Anomalies**

# By picking a threshold, we can simulate the operation of our anomaly detector



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

# **Anomaly Detection in Taxi Calls**

**Metrics and Threshold Choice** 

For choosing a threshold, we need to determine its quality

# ...But how do we evaluate a system like this?

# **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

## We will use a simple model based on:

- 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
- Late detections as windows where a detection was correct, but late

# A Simple Cost Model

### In our example, we'll assign a somewhat arbitrary cost to every error

## This is just an example, but the idea of focusing on acutal cost is important

In general, our goal is to find some kind of cost function  $c(\{x_i\}_{i=1}^m, \theta, \varepsilon)$  depending on:

- An evaluation dataset  $\{x_{i=1}\}^m$
- lacktriangle The estimator parameters  $oldsymbol{ heta}$
- lacksquare The threshold  $oldsymbol{arepsilon}$

# **Choosing the Threshold**

## Ideally, we wish to choose the best threshold

For that, we need a dataset to evaluate  $c(\{x_i\}_{i=1}^m, \theta, \varepsilon)$ 

- ...But we cannot use the test data!
- ...Since that would lead to overfitting

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# Most data-driven AI approaches have both parameters and hyperparameters

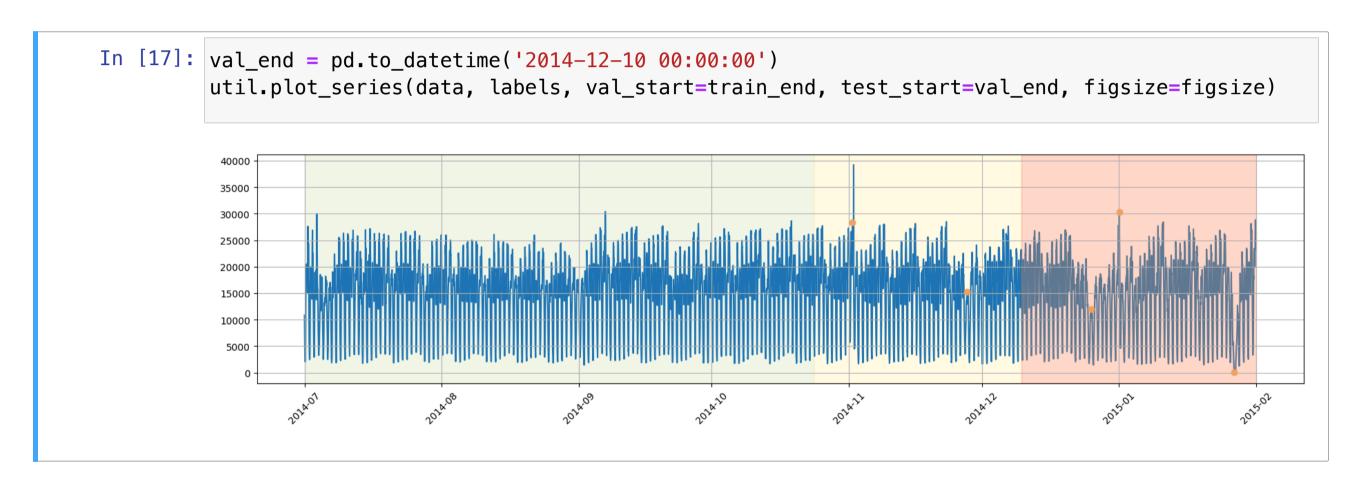
- In our case,  $\theta$  represents the parameter
- ...And  $\boldsymbol{\varepsilon}$  is a hyper-parameter

Neither should be optimized on the test data

## **Define a Validation Set**

# We can however define a separate validation set

We need a fraction of the data containing anomalies



# **Effect of Changing the Threshold**

We can visualize the cost associated to different thresholds on the validation set

```
In [18]: signal_opt = signal[signal.index < val_end]</pre>
         labels_opt = labels[labels < val_end]</pre>
         windows_opt = windows[windows['end'] < val_end]</pre>
         thr_range = np.linspace(3, 1000, 1000)
         cost_range = pd.Series(index=thr_range, data=[cmodel.cost(signal_opt, labels_opt, windows_or
         util.plot_series(cost_range, figsize=figsize, xlabel=r'$\varepsilon$', ylabel='cost')
          cost
                                                           ε
```

# **Threshold Optimization**

We can now define our threshold  $\varepsilon$  by optimizing over the validation set:

$$\underset{\varepsilon}{\operatorname{argmin}} c(\{x_i\}_{i=1}^m, \theta, \varepsilon)$$

```
In [19]: best_thr, best_cost = util.opt_thr(signal_opt, labels_opt, windows_opt, cmodel, thr_range)
    print(f'Best threshold: {best_thr:.3f}, corresponding cost: {best_cost:.3f}')

Best threshold: 5.994, corresponding cost: 15.000
```

Then we can check how our detector performed on the test data:

```
In [20]: signal_test = signal[signal.index >= val_end]
    labels_test = labels[labels >= val_end]
    windows_test = windows[windows['begin'] >= val_end]
    ctst = cmodel.cost(signal_test, labels_test, windows_test, best_thr)
    print(f'Cost on the test data {ctst}')
```

Cost on the test data 10



Improving the Results

### **Reassess and Plan**

## Let's recap our current situation

- We have a formalization for our anomaly detector
- ...And one for threshold optimization

Which means that we have a full problem formalization

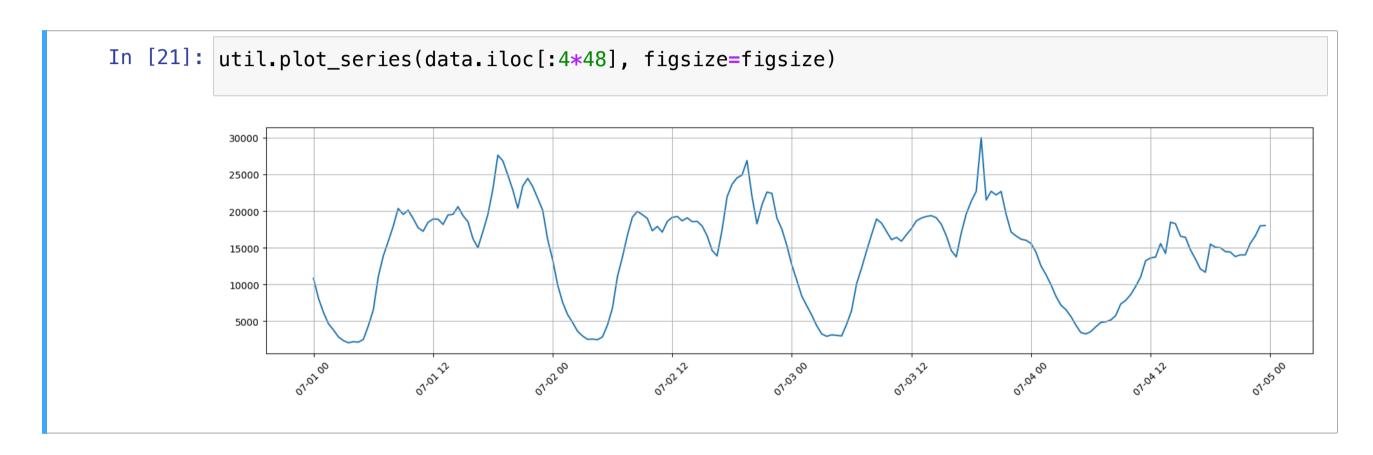
## We also have a simple prototype

- KDE is used for density estimation
- Grid search for threshold optimization

Can we do better?

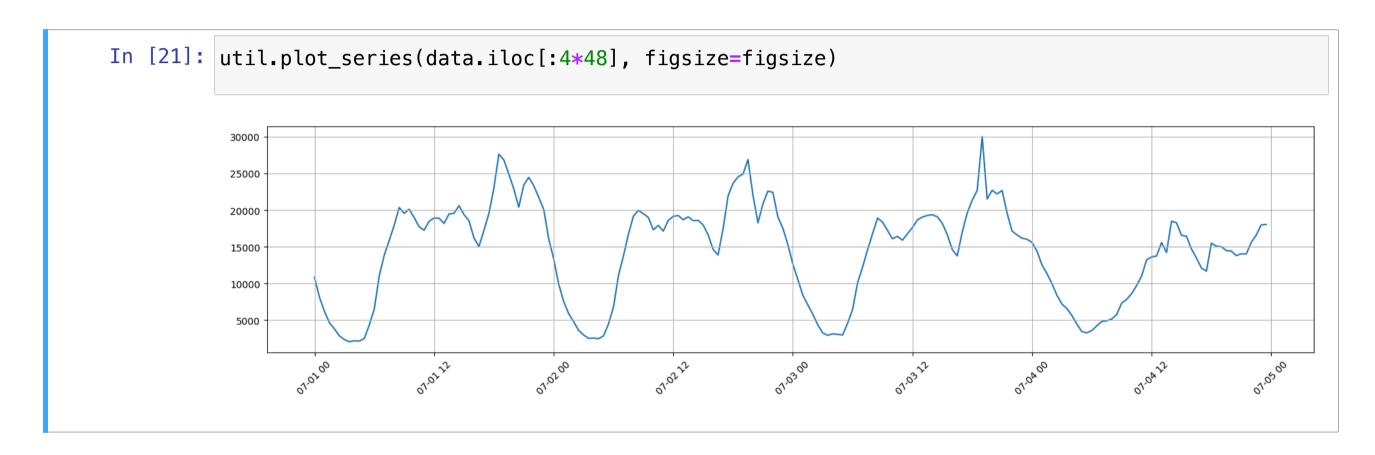
# A Closer Look at Our Data

#### Let's have a closer look at our series



## A Closer Look at Our Data

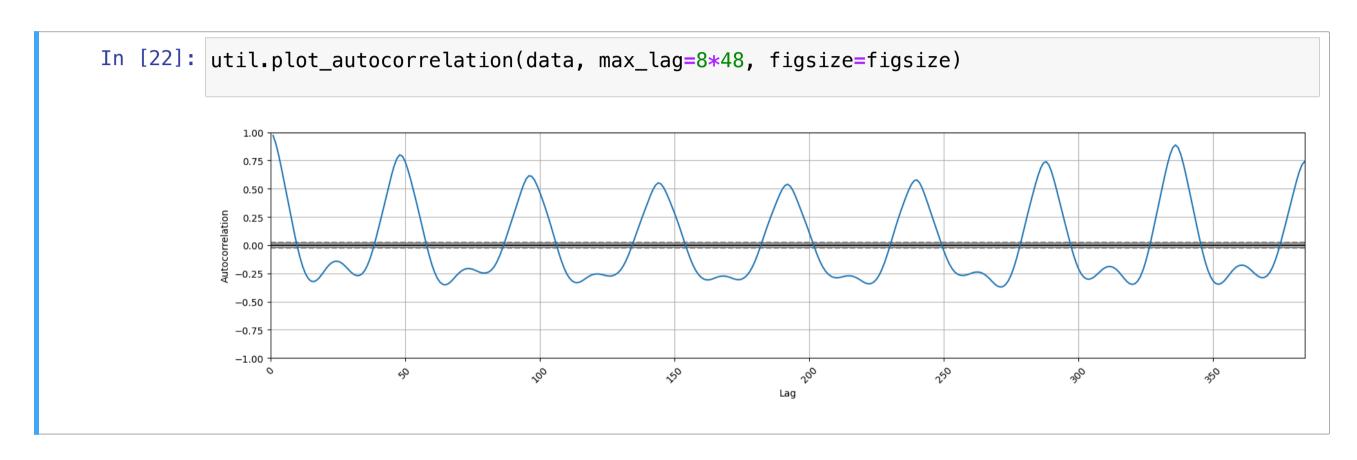
#### Let's have a closer look at our series



- The number of calls seems to be roughly following a period
- Which is quite normal, given that it's a local, human, activity

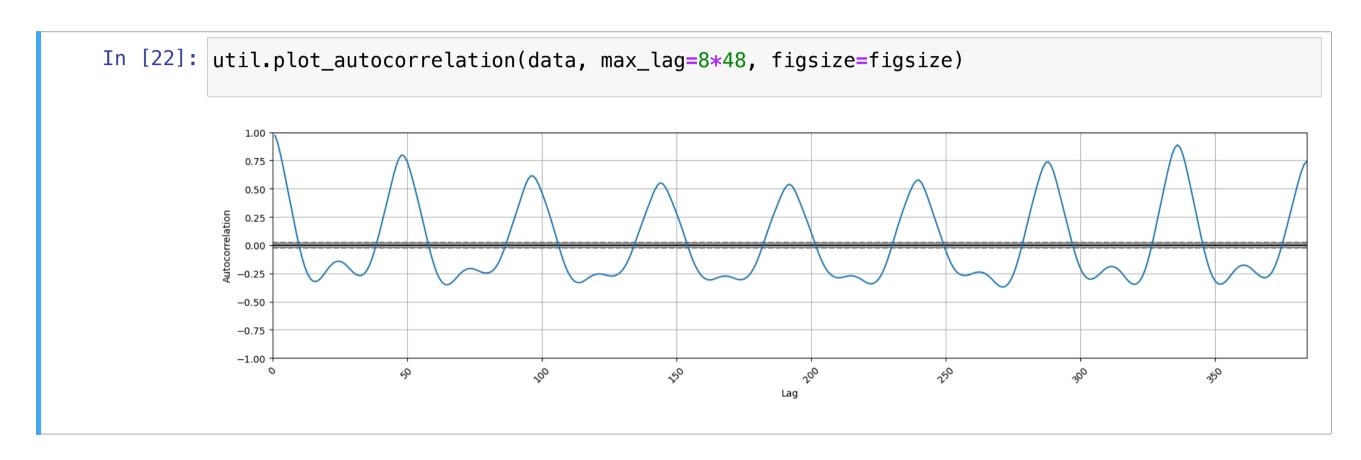
## **Determine the Period**

This is even clearer if we draw an autocorrelation plot



### **Determine the Period**

# This is even clearer if we draw an autocorrelation plot



- There are peaks every 48 time steps (a time step is 30 minutes)
- And the peak at  $7 \times 48$  steps (one week) is particularly tall

# Time as an Additional Input

#### One way to look at that

...Is that the distribution depends on the position within the period

- lacktriangle Therefore, we should consider the number of taxi calls  $oldsymbol{x}$
- ...And the time of the week *t* together

### Let us extract (from the index) the time information information:

```
In [23]: hour_of_week = (24 * data.index.weekday + data.index.hour + data.index.minute / 60)
```

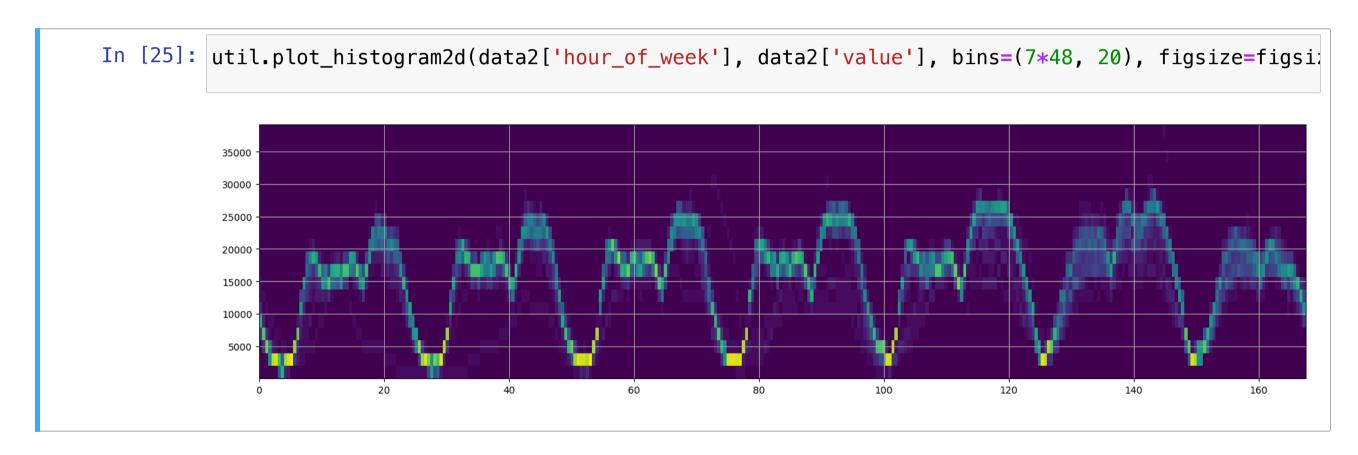
We can then add it as a separate column to the data:

```
In [24]: data2 = data.copy()
  data2['hour_of_week'] = hour_of_week
```

## **Multivariate Distribution**

# Let us examine the resulting multivariate distribution

We can use a 2D histogram:



x = time, y = value, color = frequency of occurrence

# **Training a Density Estimator**

### We can train a KDE model for this new dataset, too

```
In [26]: data2_tr = data2[data2.index < train_end]
  kde2 = util.train_kde(data2_tr, bandwidth_range=np.linspace(0.01, 0.1, 10))</pre>
```

The model will now estimate a joint distribution (calls & time):

$$\hat{f}(X,T) \simeq P(X,T)$$

We can use this model for anomaly detection just like in the previous case

$$\hat{f}(X,T) \le \varepsilon$$

■ In truth, things are bit more complicated, but we'll skip the details

# **Alarm Signal**

# We can obtain an alarm signal like in the previous case

```
In [27]: ldens2 = kde2.score_samples(data2.values) # Obtain log probabilities
         signal2 = pd.Series(index=data2.index, data=-ldens2) # Build series with neg. prob.
         util.plot_series(signal2, labels=labels, windows=windows, figsize=figsize, y_cap=30) # Plot
          25
          20
          15
          10 -
```

■ There are not several peaks around some of the previously missed anomalies

## **Threshold Selection**

# The cost surface we get for $\varepsilon$ is also more varied

```
In [28]: signal_opt2 = signal2[signal2.index < val_end]</pre>
         thr_range2 = np.linspace(4, 40, 1000)
         cost_range2 = pd.Series(index=thr_range2, data=[cmodel.cost(signal_opt2, labels_opt, windows
         util.plot_series(cost_range2, figsize=figsize, xlabel=r'$\varepsilon$', ylabel='cost')
          to 17.5
            12.5
             7.5
                                                           ε
```

### **Evaluation**

## Let's see which kind of costs we get for the new model

We'll start from the training and validation data

- ullet This is the data for which  $oldsymbol{arepsilon}$  is directly optimized
- So, improvement can be taken almost for granted here

```
In [29]: best_thr2, best_cost2 = util.opt_thr(signal_opt2, labels_opt, windows_opt, cmodel, thr_range print(f'Best threshold: {best_thr:.3f}, corresponding cost: {best_cost2:.3f}')

Best threshold: 5.994, corresponding cost: 6.000
```

But we also get better results on the test data!

```
In [30]: signal_test2 = signal2[signal2.index >= val_end]
   ctst = cmodel.cost(signal_test2, labels_test, windows_test, best_thr2)
   print(f'Cost on the test data {ctst}')
Cost on the test data 9
```