A Formalization for Anomaly Detection

How do we formalize our problem?

Problem Formalization

A possible approach: we characterize the data distribution

If we can estimate the probability of every occurring observation x

- We can choose a size for the car pool
- ...Then we can spot anomalies based on their low probability

After all, anomalies are rare events, by definition

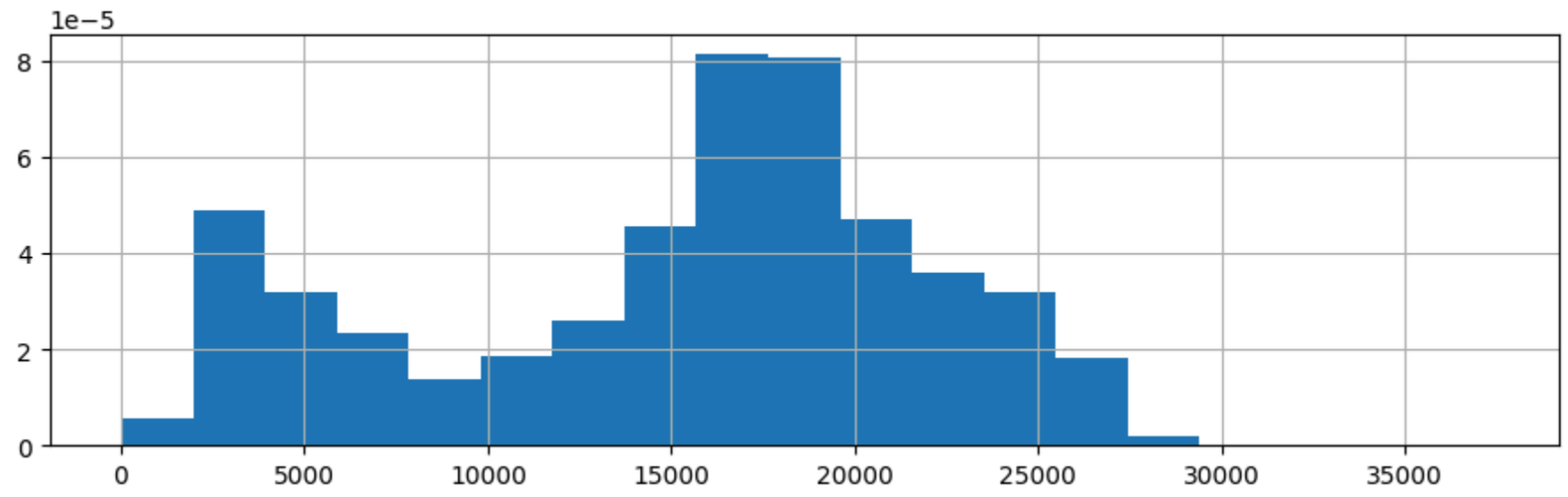
We turn a liability into a strenght!

Problem Formalization

We can check our intuition on our data

This is (roughly) the distribution over all the data

In [2]:
```
vmax = data['value'].max()
util.plot_histogram(data['value'], vmax=vmax, bins=20)
```

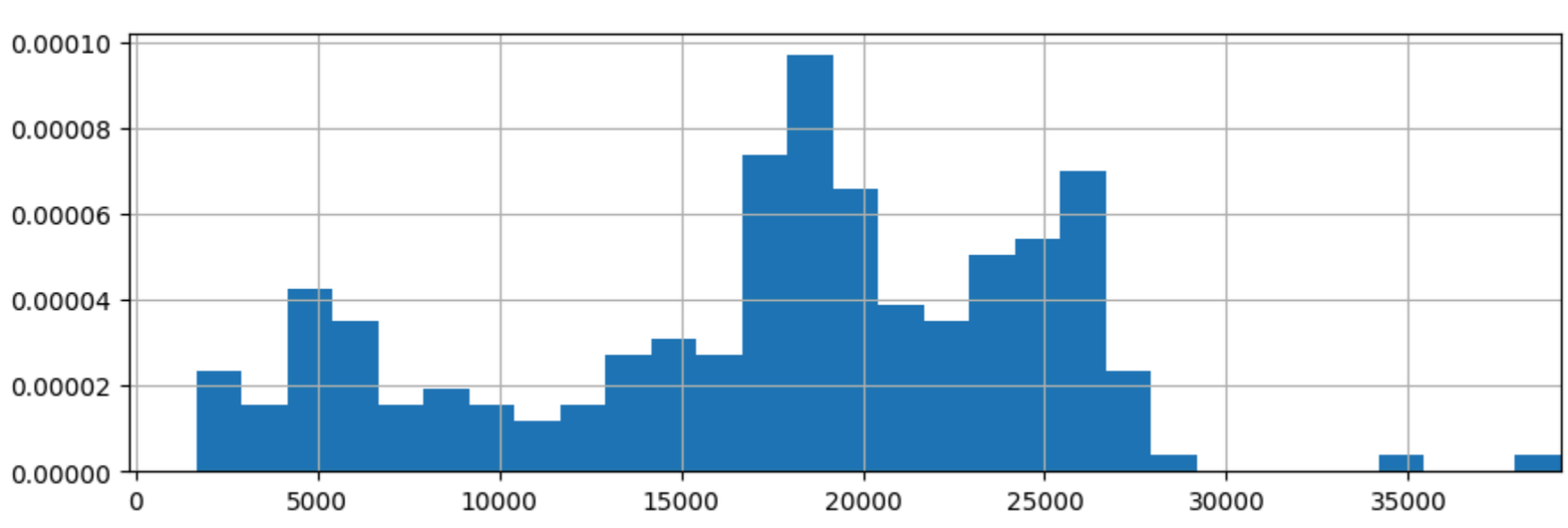


Problem Formalization

We can check our intuition on our data

This is (roughly) the distribution around the first anomaly:

In [3]:
```
w0_start, w0_end = windows.loc[0]['begin'], windows.loc[0]['end']
data_anomaly0 = data[(data.index >= w0_start) & (data.index < w0_end)]
util.plot_histogram(data_anomaly0['value'], vmax=vmax, bins=30)
```



- It seems indeed that there's a significant difference

What is the next step?

Problem Formalization

When we reach this stage, it's a good idea for formalize our problem

We can characterize a continuous distribution via its density

- Given a random variable X with values x
- ...We care about its Probability Density Function $f(x)$

Since anomalies are assumed to be unlikely

...Our detection condition can be stated as:

$$f(x) \leq \varepsilon$$

- Where ε is a (scalar) threshold

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What do we need to make this work?

Density Estimation

We need one way to estimate probability densities

For some random process with n-dimensional variable $\boldsymbol{x}$:

- Given the true density function $f(\boldsymbol{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^+$
- ...And a second function $\hat{f}(\boldsymbol{x}, \boldsymbol{\theta})$ with the same input, and parameters $\boldsymbol{\theta}$

We want to make the two as similar as possible

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Can we obtain that using supervised learning?

Given some suitable loss function $L(y, \hat{y})$, we would need to solve:

$$\text{argmin}_\theta L(\hat{f}(x, \theta), f(x))$$

- where $\boldsymbol{x}$ represents the training data

Density Estimation

Unfortunately, this approach cannot work

...Because typically we do not have access to the true density f^*

Density estimation is an unsupervised learning problem

It can be solved via a number of techniques:

- Simple histograms
- Kernel Density Estimation
- Gaussian Mixture Models
- Normalizing Flows
- Non Volume Preserving (NVP) transformations

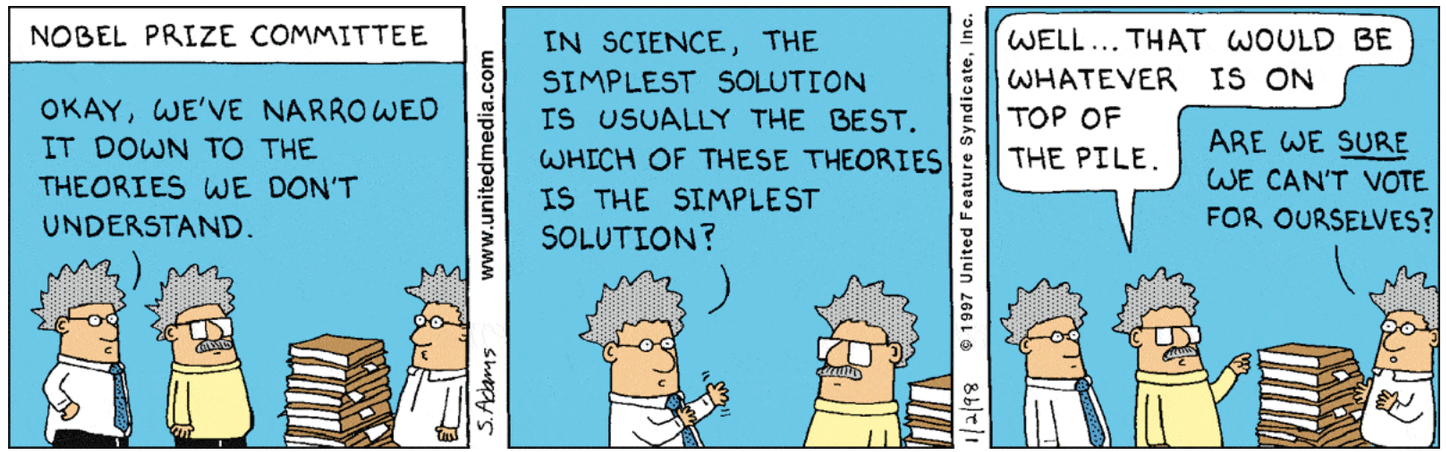
Which one shall we pick?

Our Friend, Occam's Razor

We will go with Occam's razor

It's a philosophical principle stating that:

Between two hypotheses, the simpler one is usually correct



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In practice, it's often a good idea to start with a simple approach

- If it works well, then you have a solution
- If it does not, they you have a baseline

In both cases, you win!

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For this example, we will pick Kernel Density Estimation

Kernel Density Estimation

Kernal Density Estimation

In Kernel Density Estimation (KDE), the main idea is that:

- Wherever (in input space) there is a sample
- ...It's likely that there are more

So, we assume that each training sample is the center for a density "kernel"

Formally, suck kernel $K(x, h)$ is just a valid PDF:

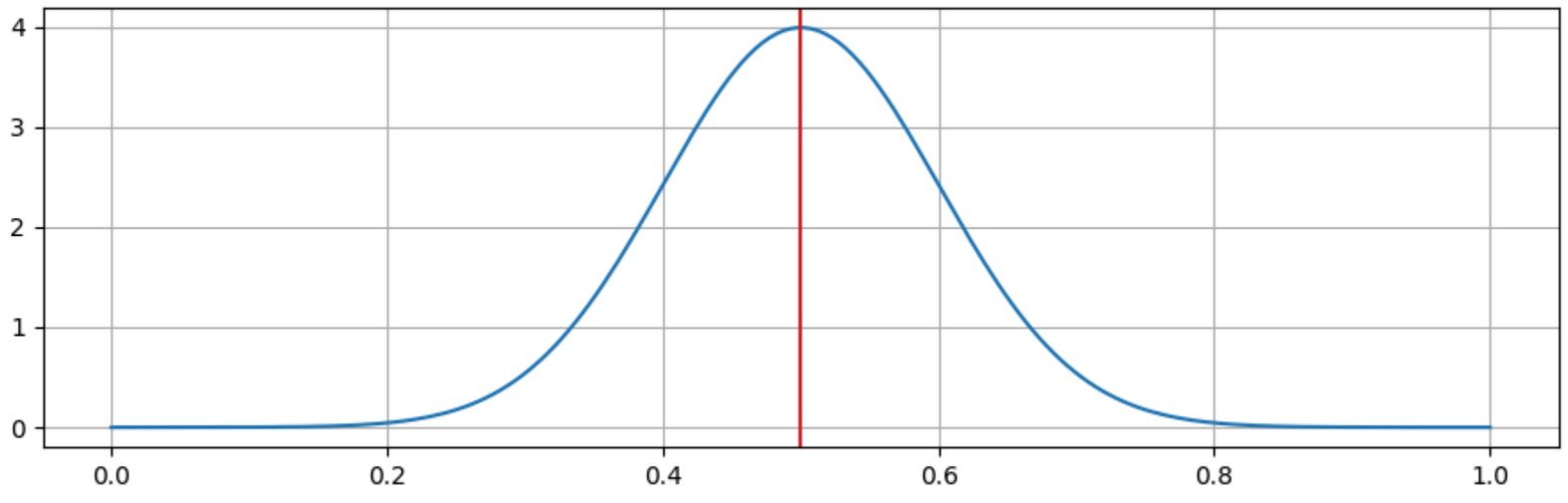
- x is the input variable (scalar or vector)
- h is a parameter (resp. scalar or matrix) called bandwidth

Typical kernels: Gaussian, exponential, cosine, linear...

Kernels

An example with one sample and a Guassian kernel:

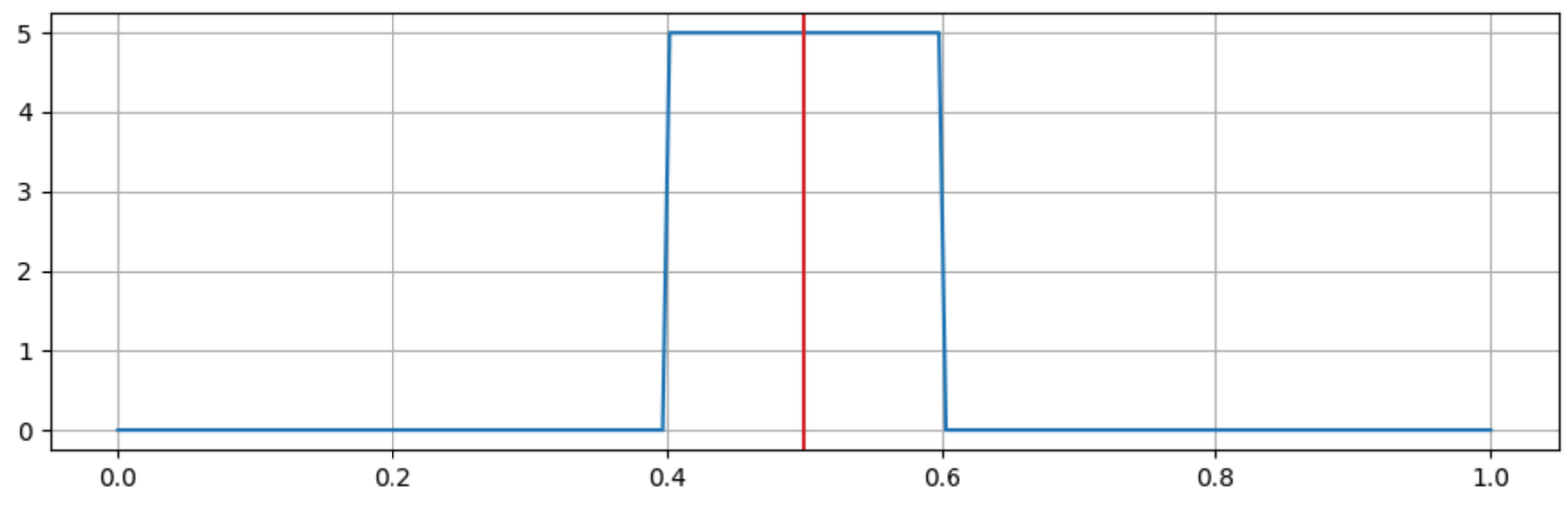
In [4]:
```
x = np.array(0.5).reshape(1,1) # single sample
kde = KernelDensity(kernel='gaussian', bandwidth=0.1) # build the estimator
kde.fit(x) # fit the estimator on the data
# We use a plotting function from our module
util.plot_density_estimator_1D(kde, xr=np.linspace(0, 1, 200))
ymin, ymax = plt.ylim()
plt.vlines(x, ymin, ymax, color='tab:red')
plt.ylim((ymin, ymax)); # ; = suppress output
```



Kernels

An example with one sample and a Tophat kernel:

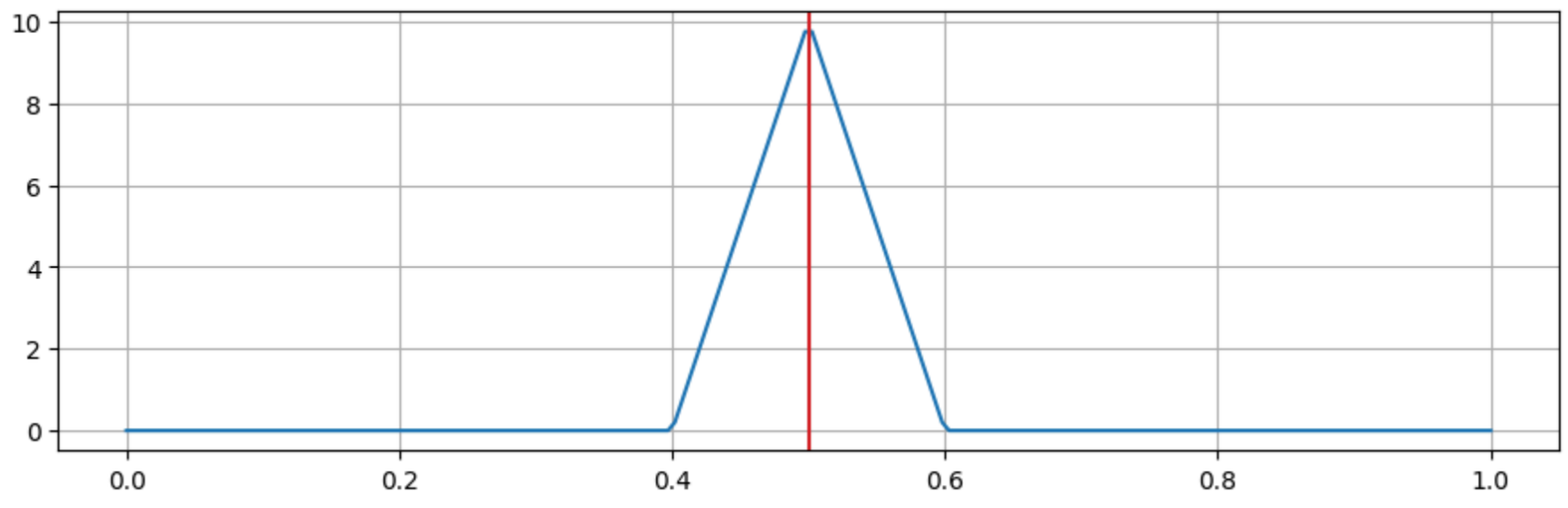
In [5]:
```
x = np.array(0.5).reshape(1,1) # single sample
kde = KernelDensity(kernel='tophat', bandwidth=0.1) # build the estimator
kde.fit(x) # fit the estimator on the data
# We use a plotting function from our module
util.plot_density_estimator_1D(kde, xr=np.linspace(0, 1, 200))
ymin, ymax = plt.ylim()
plt.vlines(x, ymin, ymax, color='tab:red')
plt.ylim((ymin, ymax)); # ; = suppress output
```



Kernel

An example with one sample and a linear kernel:

In [6]:
```
x = np.array(0.5).reshape(1,1) # single sample
kde = KernelDensity(kernel='linear', bandwidth=0.1) # build the estimator
kde.fit(x) # fit the estimator on the data
# We use a plotting function from our module
util.plot_density_estimator_1D(kde, xr=np.linspace(0, 1, 200))
ymin, ymax = plt.ylim()
plt.vlines(x, ymin, ymax, color='tab:red')
plt.ylim((ymin, ymax)); # ; = suppress output
```



Kernels

As an example, a Gaussian kernel in sklearn is given by:

$$K(x, h) \propto e^{-\frac{x^2}{2h^2}}$$

- The $\propto$ ("proportional to")

The function is similar to a the PDF of the Normal distribution:

- The mean can be interpreted as 0
- h plays the role of the standard deviation
- ...And scikit learn handles normalization

Kernel Re-centering

Since the "mean" is 0, the kernel is centered on 0

All kernels in KDE are by default zero-centered

- ...But we need to place then over each sample
- How can this be done?

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- ...But we need to place then over each sample
- How can this be done?

We can use an affine transformation (like in the scale/location trick)

In practice, the expression:

$$K(x - \mu, h)$$

- ...Gives the value the value of a kernel centered on μ
- ...Computed for the value x

Kernel Density Estimation

The estimated density of any point is obtained as a kernel average:

$$f(x, \bar{x}, h) = \frac{1}{m} \sum_{i=0}^{m} K(x - \bar{x}_i, h)$$

- $\boldsymbol{x}$ is the input for which we want an estimate
- $\bar{\boldsymbol{x}}_{\boldsymbol{i}}$ is sequence of the $\boldsymbol{m}$ training samples
- $\boldsymbol{x} - \bar{\boldsymbol{x}}_{\boldsymbol{i}}$ is the difference between $\boldsymbol{x}$ and the i-th training sample

By changing the kernel function:

- We can adjust the properties of the distribution (e.g. smoothness)
- Typically, the choice is based on prior domain knowledge

Kernel Density Estimation

KDE models are not trained in the usual sense

...But they store internally all the training samples

- I.e. the training set is part of the model parameters
- This is a property common to most kernel models

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There is one thing that we need to train, i.e. the bandwidth h

- We will see a general approach later in the course
- ...But in the univariate case we can apply a rule of thumb:

$$h = 0.9 \min\left(\hat{\sigma}, \frac{IQR}{1.34}\right) m^{-\frac{1}{5}}$$

Where IQR is the inter-quartile range

Kernel Density Estimation

An example with two samples and a Guassian kernel:

In [7]:
```
x = np.array([0.25, 0.75]).reshape(-1,1) # two sample, univariate
kde = KernelDensity(kernel='gaussian', bandwidth=0.1) # build the estimator
kde.fit(x) # fit the estimator on the data
util.plot_density_estimator_1D(kde, xr=np.linspace(0, 1, 200))
ymin, ymax = plt.ylim()
plt.vlines(x, ymin, ymax, color='tab:red')
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