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

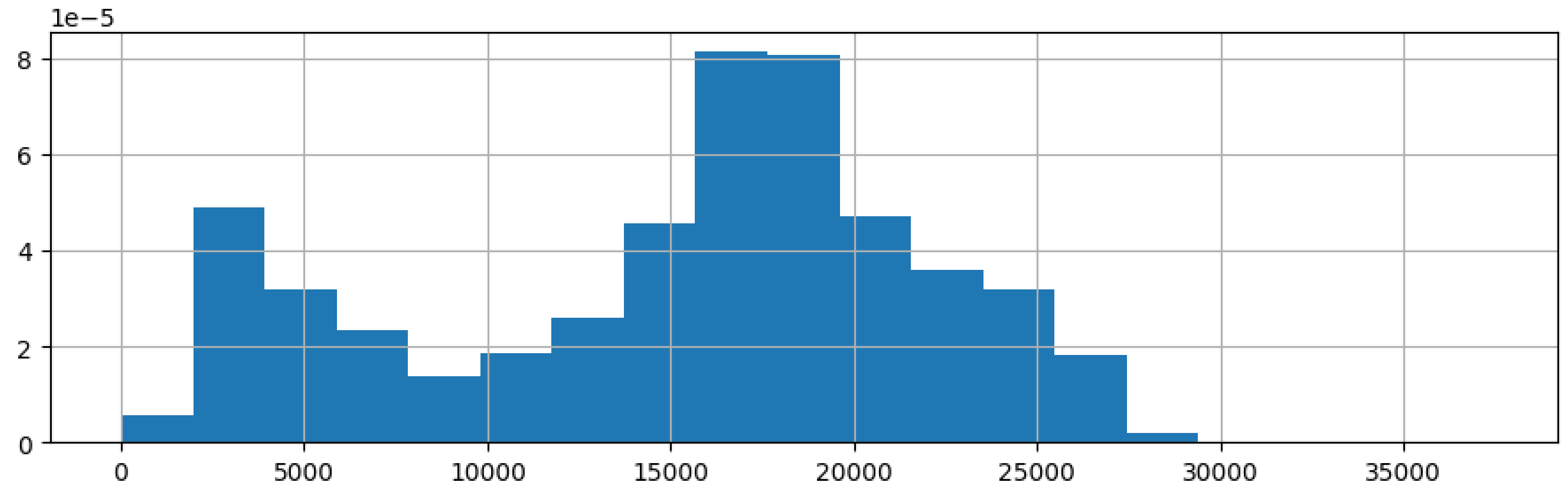
We turn a liability into a strenght!

Problem Formalization

We can check our intuition on our data

This is (roughly) the distribution over all the data

```
In [3]: vmax = data['value'].max()
        util.plot_histogram(data['value'], vmax=vmax, bins=20)
```

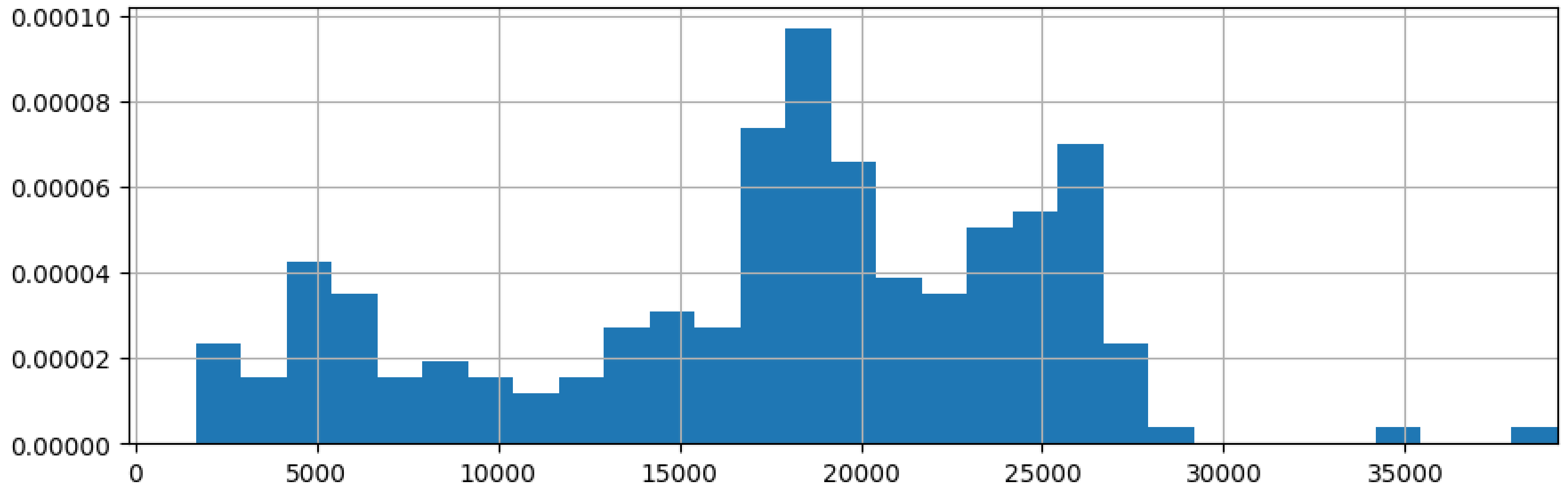


Problem Formalization

We can check our intuition on our data

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

```
In [4]: 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

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 $f(x) : \mathbb{R}^n \rightarrow \mathbb{R}^+$
- ...And a second function $\hat{f}(x, \theta)$ 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 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

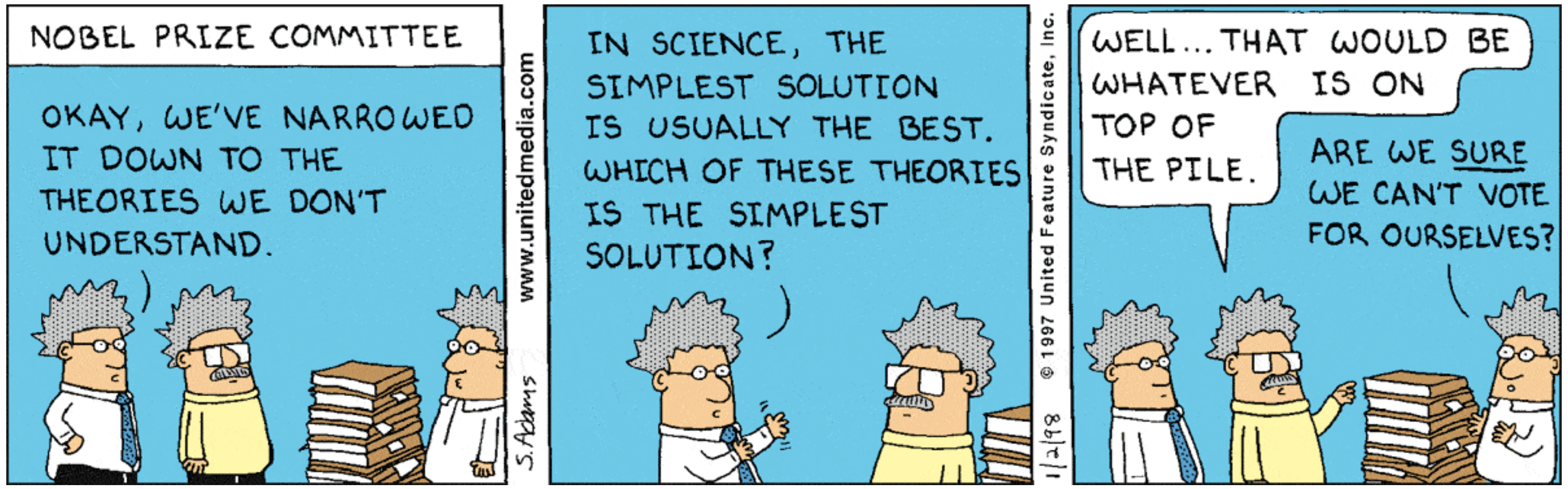
Which one shall we pick?

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


NOBEL PRIZE COMMITTEE
OKAY, WE'VE NARROWED IT DOWN TO THE THEORIES WE DON'T UNDERSTAND.
www.unitedmedia.com
S. Adams
IN SCIENCE, THE SIMPLEST SOLUTION IS USUALLY THE BEST. WHICH OF THESE THEORIES IS THE SIMPLEST SOLUTION?
© 1997 United Feature Syndicate, Inc.
1/2/98
WELL... THAT WOULD BE WHATEVER IS ON TOP OF THE PILE.
ARE WE SURE WE CAN'T VOTE FOR OURSELVES?

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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:

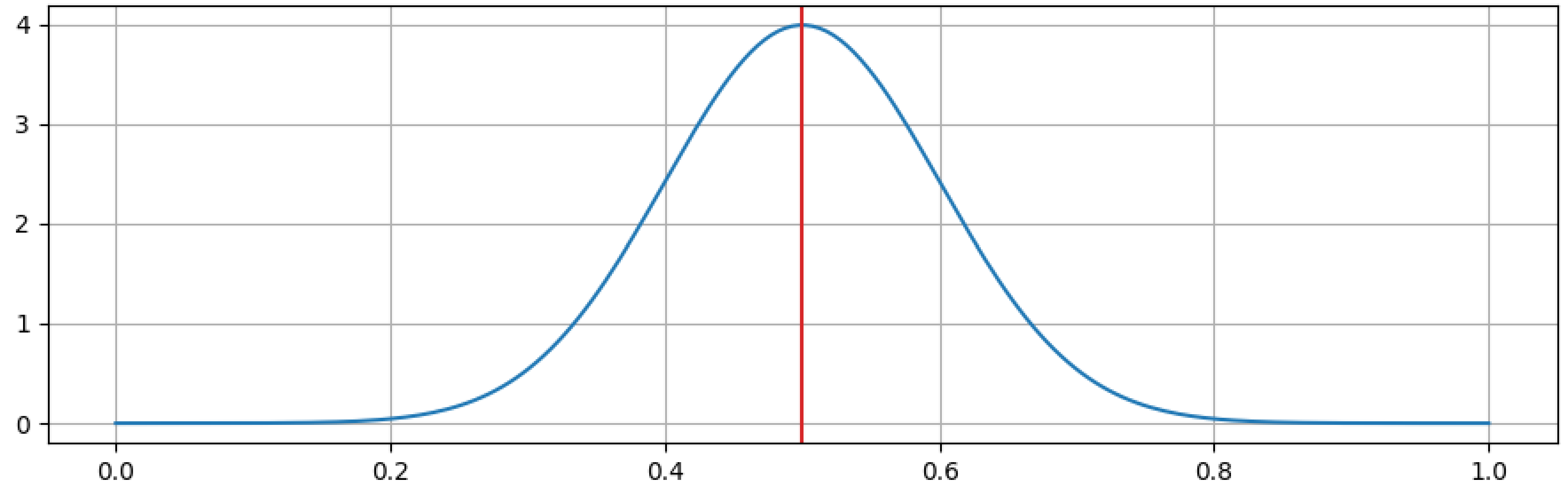
- x is the input variable (scalar or vector)
- h is a parameter (resp. scalar or matrix) called bandwidth

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

Kernels

An example with one sample and a Guassian kernel:

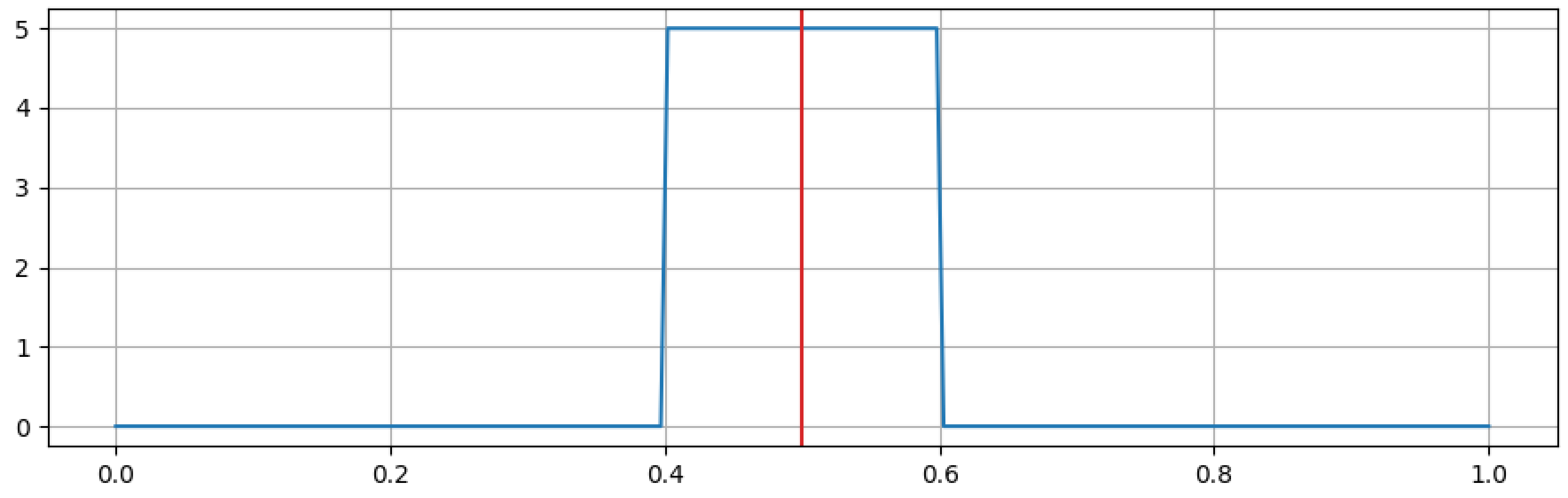
```
In [6]: x = np.array(0.5).reshape(1,1) # single sample
        kde = KernelDensity(kernel='gaussian', bandwidth=0.1) # build the estimator
        kde.fit(x) # fit the estimator on the data
        # We use a plotting function from our module
        util.plot_density_estimator_1D(kde, xr=np.linspace(0, 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:

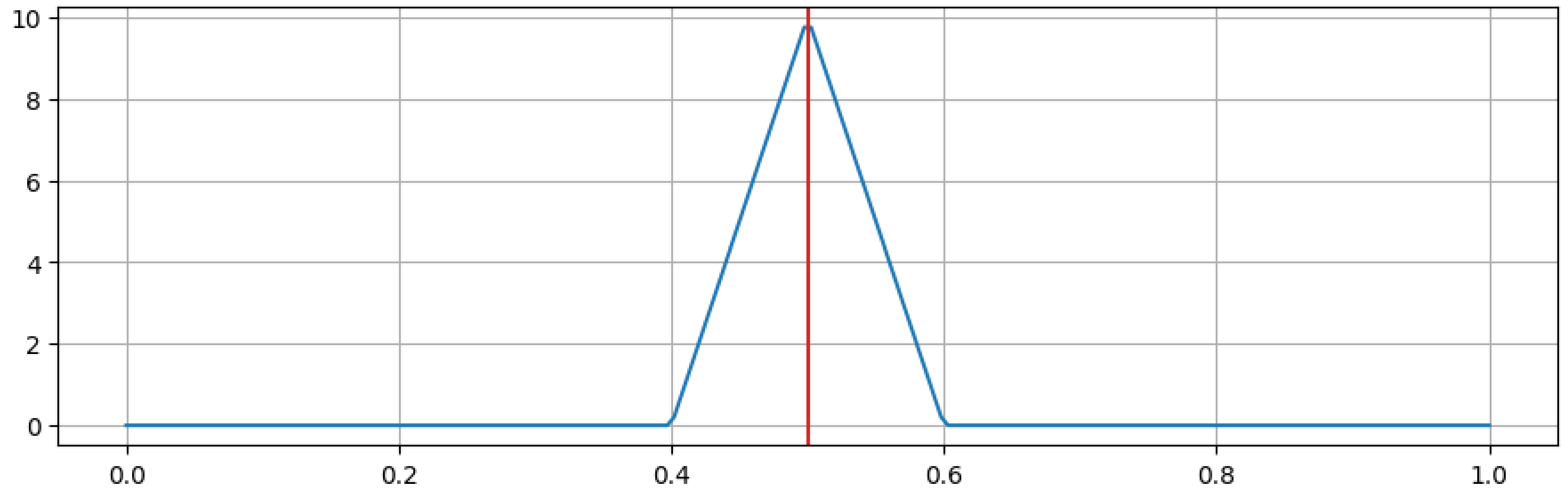
```
In [7]: x = np.array(0.5).reshape(1,1) # single sample
        kde = KernelDensity(kernel='tophat', bandwidth=0.1) # build the estimator
        kde.fit(x) # fit the estimator on the data
        # We use a plotting function from our module
        util.plot_density_estimator_1D(kde, xr=np.linspace(0, 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 [8]: 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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- 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:

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

- x is the input for which we want an estimate
- $\bar{x}_i$ is sequence of the m training samples
- $x - \bar{x}_i$ is the difference between 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:

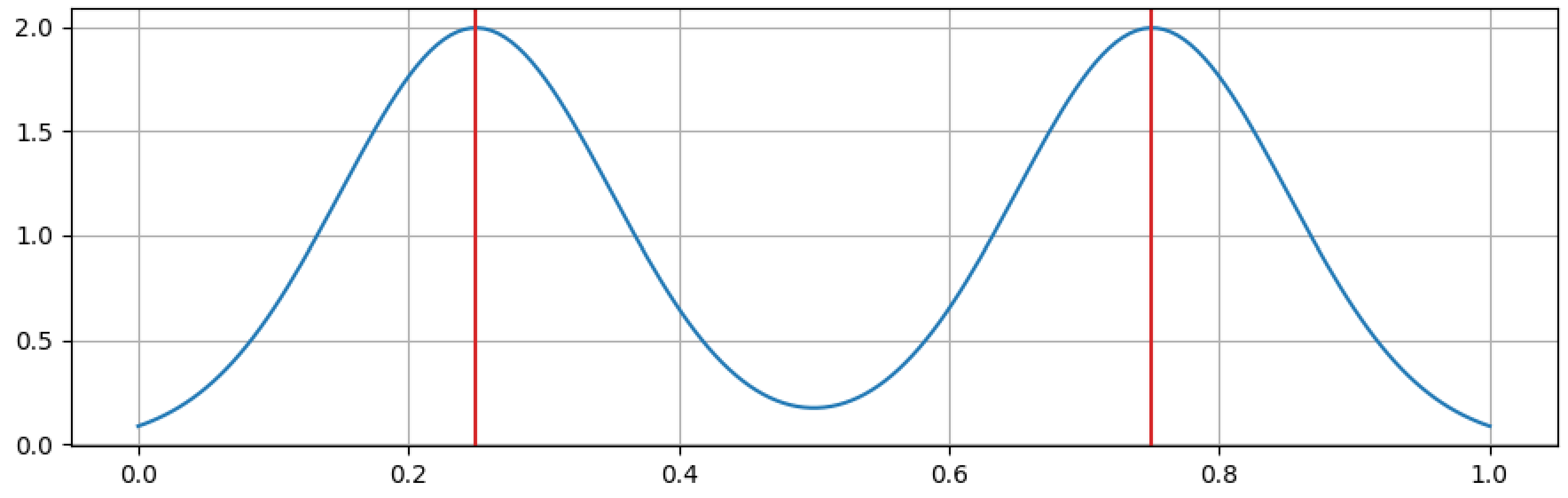
$$h = 0.9 \min\left(\hat{\sigma}, \frac{IQR}{1.34}\right) m^{-\frac{1}{5}}$$

Where IQR is the inter-quartile range

Kernel Density Estimation

An example with two samples and a Guassian kernel:

```
In [9]: 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')
        plt.ylim((ymin, ymax)); # ; = suppress output
```


2.0
1.5
1.0
0.5
0.0
0.0
0.2
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0.6
0.8
1.0