Anomaly Detection and Kernel Density Estimation

Problem Formalization

How do we formalize this problem?

A possible approach: we know that anomalies are (often) unlikely

- If we can estimate the probability of every occurring observation x
- ...Then we can spot anomalies based on their low probability

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 [4]:
```
vmax = data['value'].max()
nab.plot_histogram(data['value'], vmax=vmax, bins=20)
```

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Problem Formalization

We can check our intuition on our data

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

In [8]:
```
w0_start, w0_end = windows.loc[0]['begin'], windows.loc[0]['end']
data_anomaly0 = data[(data.index >= w0_start) & (data.index < w0_end)]
nab.plot_histogram(data_anomaly0['value'], vmax=vmax, bins=30)
```

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- There seems to be a significant difference

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We turn a liability into a strength!

Formally, our detection condition can be stated as:

$$f(x) \leq \theta$$

- Where $f(x)$ is a Probability Density Function (PDF)
- ...And θ is a (scalar) threshold

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 $f(x, \omega)$ with the same input, and parameters $\boldsymbol{\omega}$

We want to make the two as similar as possible

Density Estimation

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- ...And a second function $f(x, \omega)$ with the same input, and parameters ω

We want to make the two as similar as possible

What about modeling that as supervised learning?

Given some suitable loss function $L(\mathbf{y}, \mathbf{y}^*)$, that would lead to:

$$\text{argmin}_\omega L(f(\hat{\mathbf{x}}, \omega), f^*(\hat{\mathbf{x}}))$$

- where $\hat{\mathbf{x}}$ 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

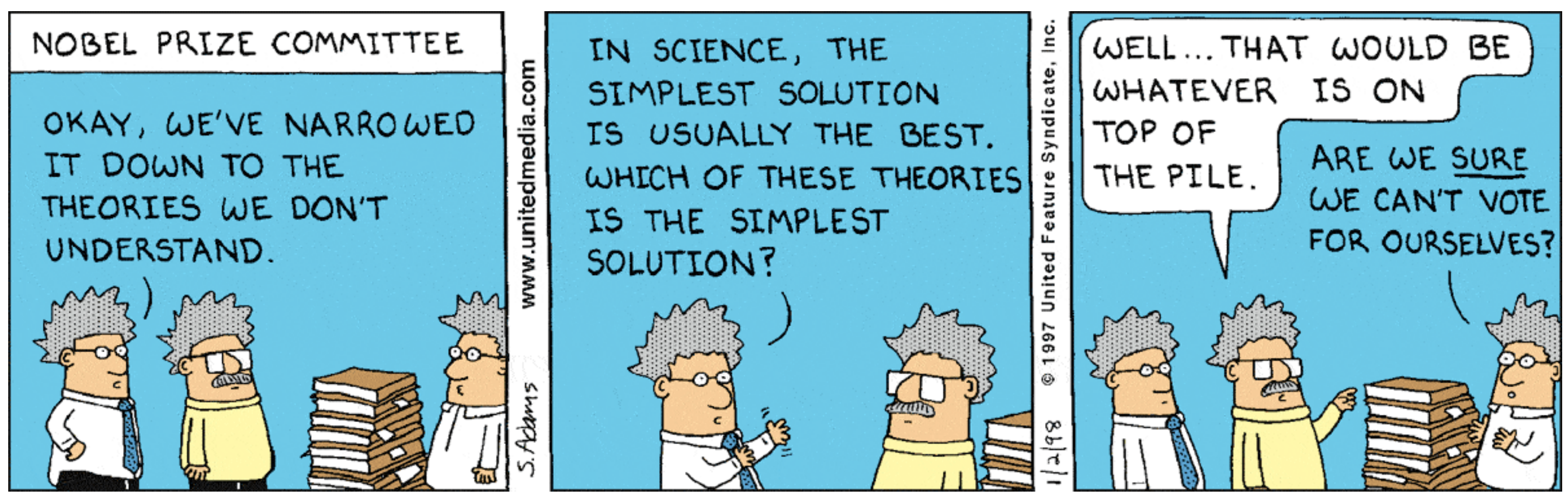
Which one shall we pick?

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



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

For its simplicity we will pick Kernel Density Estimation

- This will be returning principle in the course
- ...We will typically try simpler approaches first
- Especially at the beginning! Brace up for a slow start

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, the 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 [9]:
```
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
nab.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
```

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Kernel

An example with one sample and a Tophat kernel:

In [11]:
```
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
nab.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
```

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Kernel

An example with one sample and a linear kernel:

In [12]:
```
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
nab.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
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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") means that there is an implicit normalization constant
- The constant is handled by scikit-learn (in an efficient way)

All kernels in KDE:

- Are by default zero-centered (their mode is at 0)
- Can be relocated via an affine transformation (i.e. summing a constant to x)

In practice:

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

Kernel Density Estimation

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

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

- x is the input for which we want an estimate
- $\hat{\mathbf{x}}$ is the matrix with the training samples
  - The training samples are part of the model parameters
- $x - \hat{x}_i$ is the difference between x and the i-th training sample
  - I.e. the value at x of the kernel centered on $\hat{x}_i$

Changing the kernel function:

- Allows to adjust the properties of the distribution (e.g. smoothness)
- ...By exploiting our prior knowledge

Kernel Density Estimation

An example with two samples and a Guassian kernel:

In [13]:
```
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
nab.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
```

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Kernel Density Estimation

How do we tune the bandwidth?

A nice approach (in principle): minimize the Mean Integrated Squared Error:

$$MISE(h) = \int (f(x, \hat{x}, h) - f^*(x))^2 dx$$

- In practice, we can't use it (we don't have f^*)
- ...But we can use an approximation, i.e. the validation set (more about this later)

A rule of thumb for the univariate case:

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

- IQR is the inter-quartile range