[1]:
```
%matplotlib inline
# make figures better for projector:
import matplotlib
font = {'size':18}
matplotlib.rc('font', **font)
#matplotlib.rc('figure', figsize=(9.0, 6.0))

import warnings
warnings.filterwarnings('ignore')
```

[2]:
```
%config InlineBackend.figure_format = 'retina'
```

DS1 Lecture 10

Jim Bagrow

Last time:

1. Data cleaning:
    - Rejecting bad data, combining data, filtering and processing data
2. Histograms as data "microscopes"
    - See the distribution of the data
    - Binning is key!
    - "broad" and log-vs-linear scales

Today's plan:

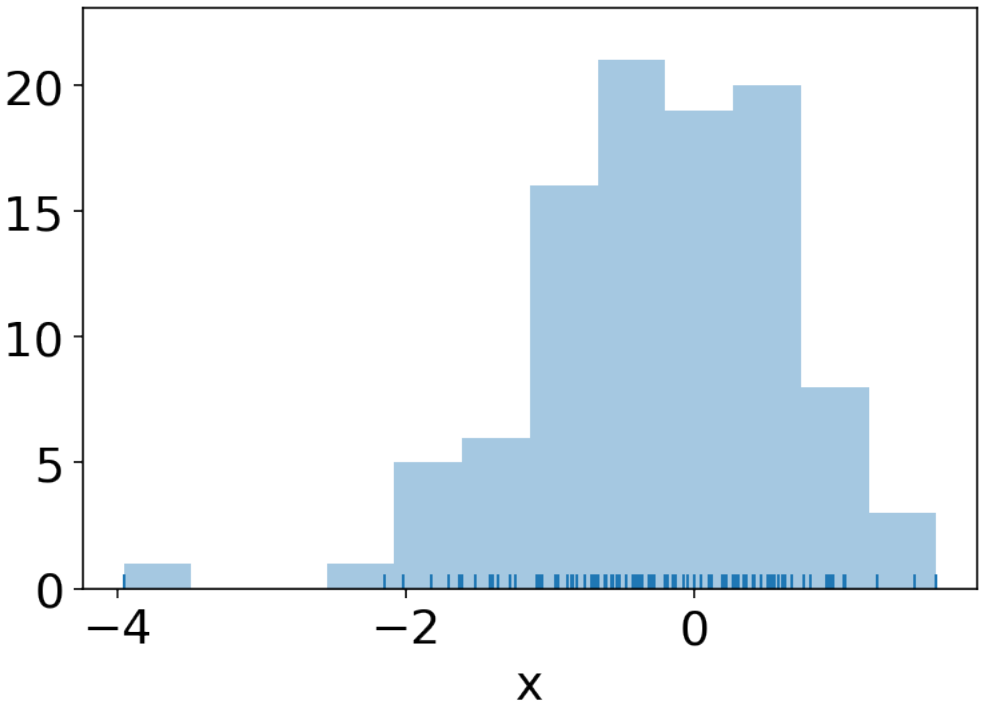
1. More on histograms
    - box plots
    - $\rightarrow$ tools for *distributions*
2. Scatter plots

Recall, last time we used histograms on some **fish mass data** to reveal that (probably) three species of fish were being caught.

- For distributions of numeric data (or what I call "X-data"), histograms are an amazing and powerful tool!

The idea behind a histogram is to take the *domain* of your data, chop it into bins, and count how many data points fall into each bin. This brings out the underlying distribution:

[3]:
```
import numpy as np
import seaborn as sns # another plotting library


x = np.random.randn(100)
ax = sns.distplot(x, bins='auto', rug=True, kde=False)
#                                  ^^^^^^^^  ^^^^^^^^^
plt.xlabel("x")
plt.show()
```



Dealing with many histograms

Histograms are one of the most important EDA (exploratory data analysis) tools.

Often you want to explore larger datasets, meaning you may want to visualize many histograms.

As a data scientist working away, you may find yourself looking at histogram after histogram after histogram ad nauseum.

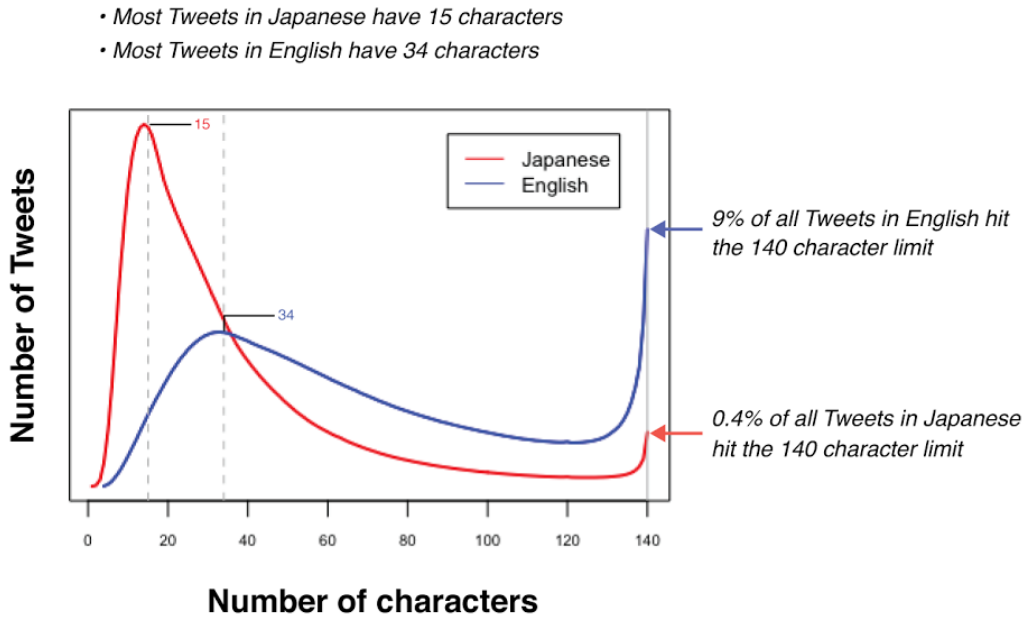
But how to compactly summarize many histograms for an audience? (This is getting more into *presentation* than exploration.)

Sometimes we have **multiple collections** of X-data (e.g., X-data by age: for subjects in their 20s, their 30s, 40s, etc.) We want to compare these different distributions to see if something in the X-data is changing as the (e.g.) age changes.

A great example is the Twitter tweet-length data science question, looking at English and Japanese tweets:

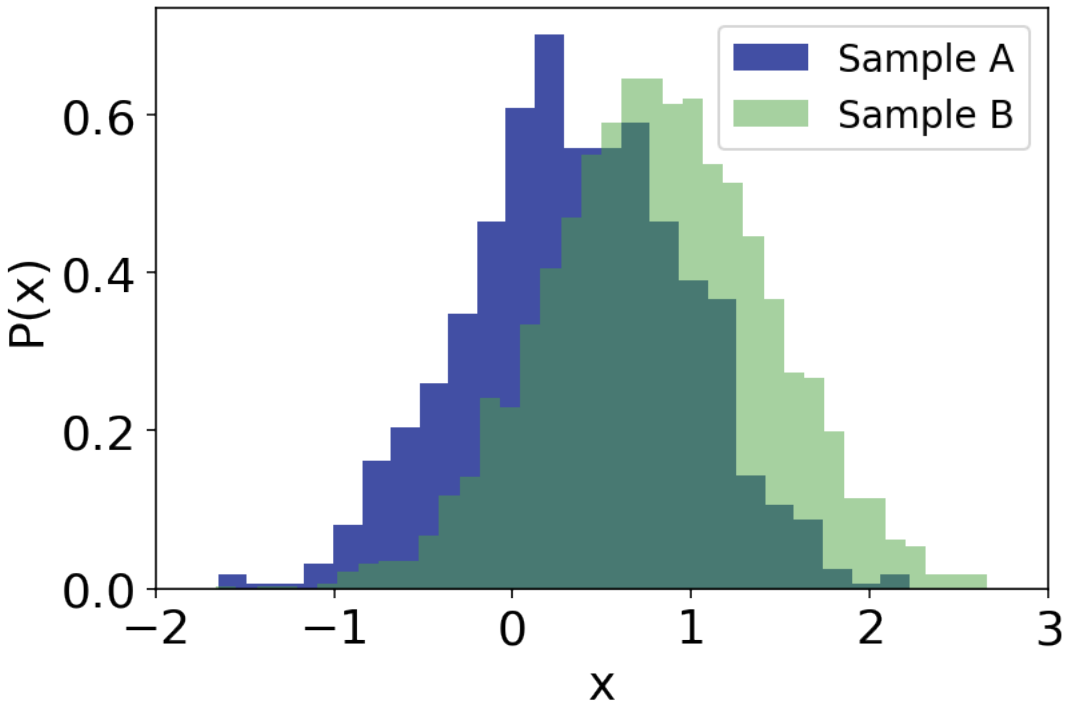
[4]:
```
from IPython.display import Image
Image("figures/more-chars-1.png", width=700)
```

[4]:



Two-ish histograms

[5]:
```
data_A = [ np.random.randn()*0.6 + 0.34 for _ in range(1000) ]
data_B = [ np.random.randn()*0.6 + 0.82 for _ in range(3000) ]

plt.hist(data_A,bins='auto', density=True,
         color="#424FA4")

plt.hist(data_B,bins='auto', density=True,
         color="#4FA442",
         alpha=0.5) # ***
plt.xlim(-2,3)

plt.xlabel("x");
plt.ylabel("P(x)");
plt.legend(["Sample A", "Sample B"], fontsize=14)
plt.show()
```



This may work, but consider plotting the histograms as just lines instead of filled curves, as the visual intersection of the two shapes may cause confusion.

More than two histograms

Transparency can help visualize the overlap (similarity/difference) of two distributions.

We can draw multiple histograms but too much overlap will make it hard to read.

- This can be visually confusing if you need to show many histograms at once.
- Transparency can introduce **artifacts** (people will confuse the overlapping segment as a third histogram).

Histogram curves can get complicated and you can only cram so much information into one plot!

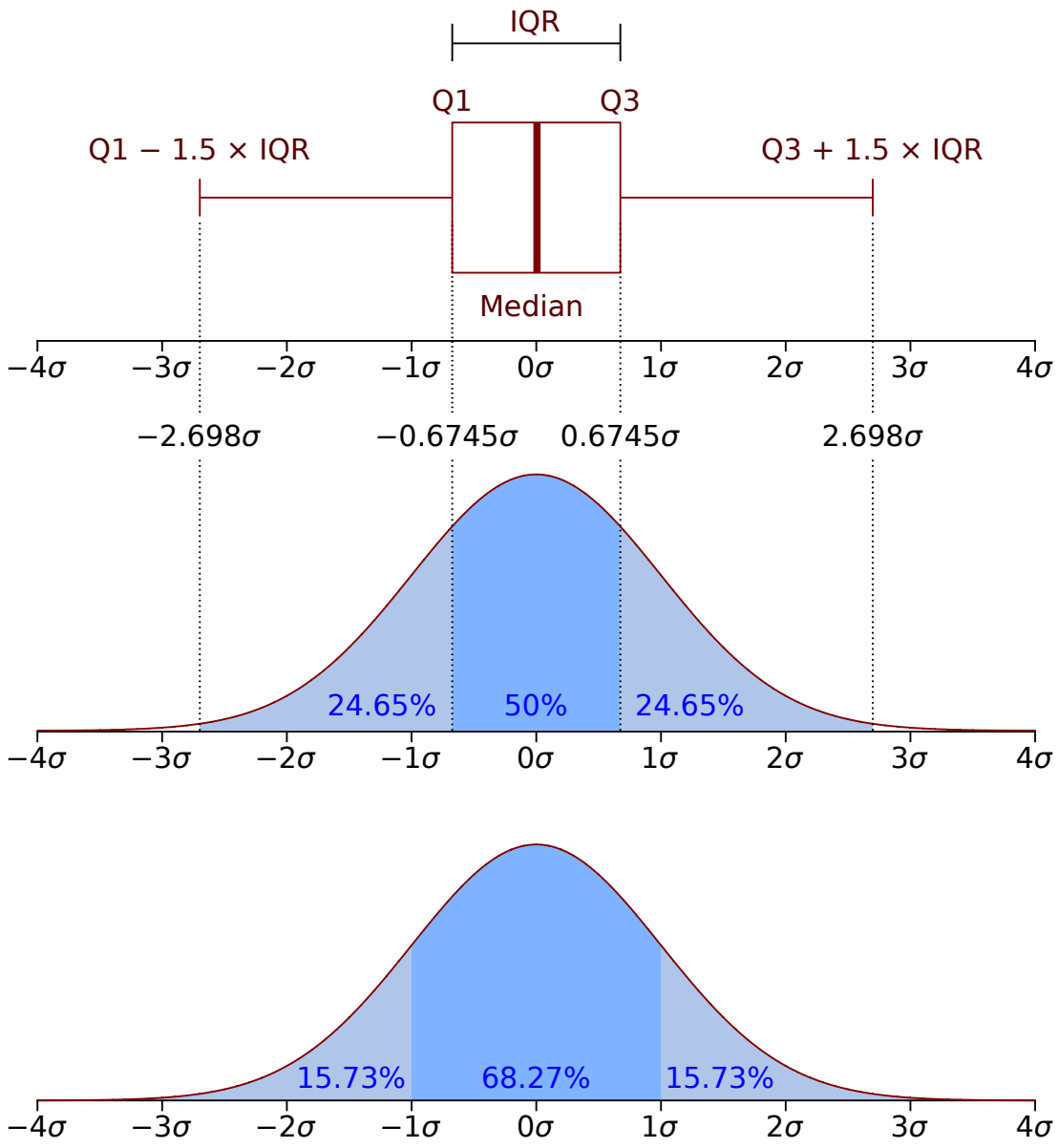
Another idea is to **further reduce the information about the distribution**

Box plots

A boxplot is just a simple way to summarize the center of a distribution of data and its width. A picture is worth a thousand words:

[6]:
```
#Image("figures/Boxplot_vs_PDF.svg", width=700)
from IPython.core.display import SVG
SVG(filename='figures/Boxplot_vs_PDF.svg')
```

[6]:



A Boxplot (top) compared to the underlying gaussian distribution.

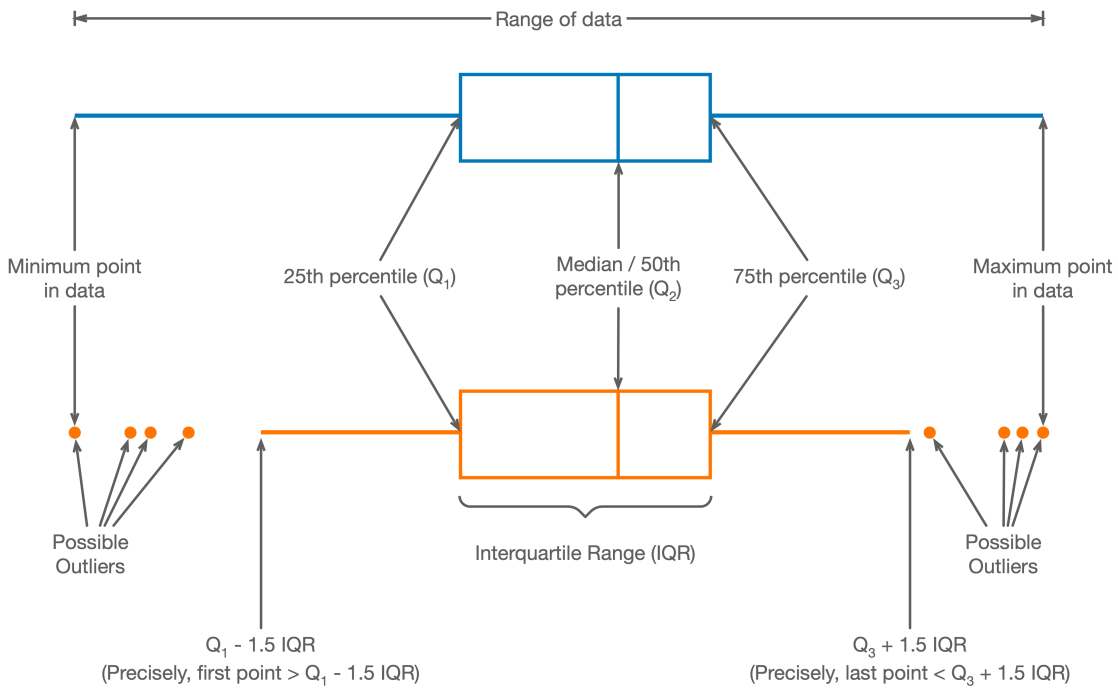
Boxplots illustrate in a reduced schematic the:

1. Median (center stripe)
2. IQR (width of box)
3. 1.5 IQR $\pm$ the outer quartiles, using error bars
   - sometimes the errorbars denote the 5th and 95th percentile or other features
4. **Outliers** are sometimes drawn as individual points beyond the error bars

Box plot "anatomy":

[7]:
```
Image("figures/boxplots-annotated.png", width=750)
```

[7]:

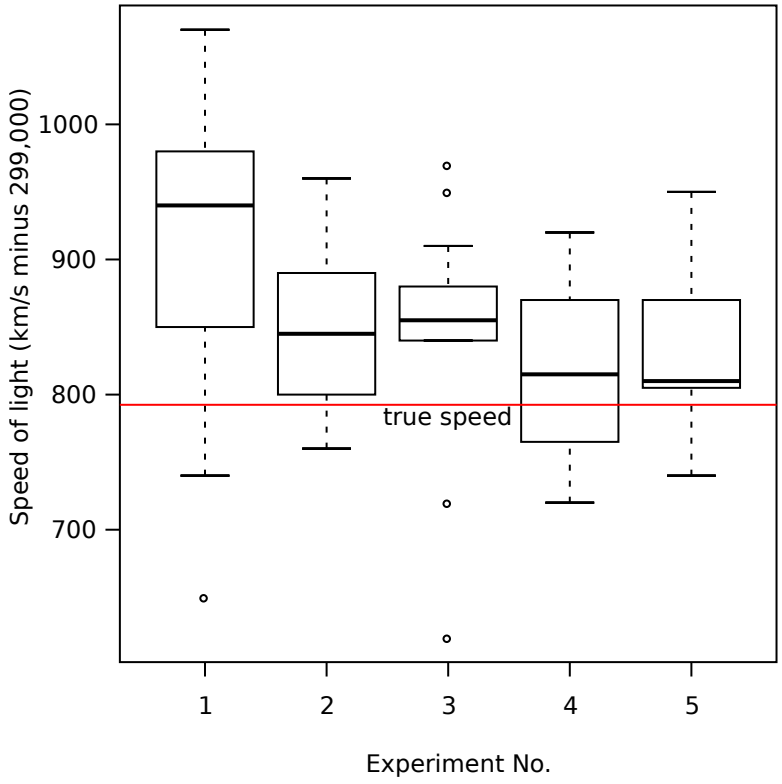


- The definition of the *whiskers* hanging off the central box is not as standardized as the central box itself.

By simplifying the full shape of the distribution, boxplots let us compactly **compare and contrast** distributions:

[8]:
```
SVG(filename="figures/Michelsonmorley-boxplot.svg")
```

[8]:



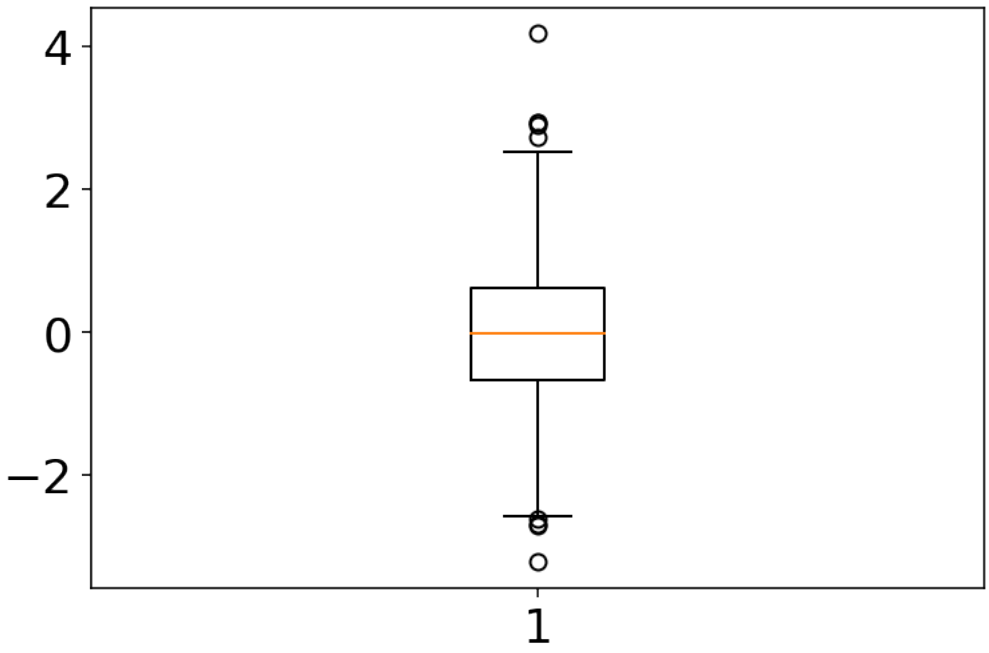
(Try fitting those five distributions into one plot using histograms.)

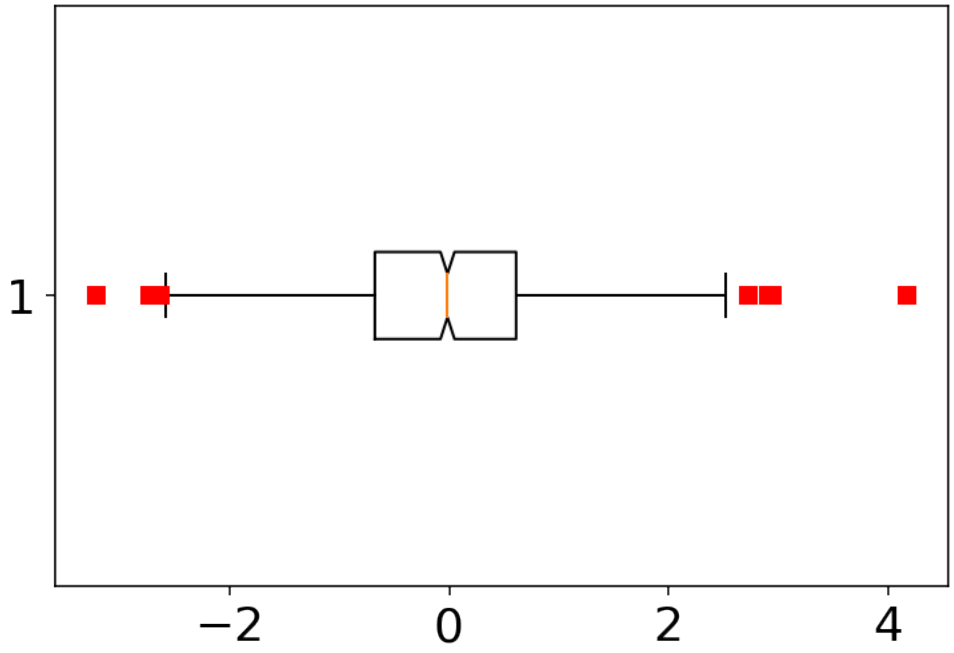
Boxplots are an ***old-fashioned idea*** from a time when computers were not used to visualize data. Instead, graphics were drawn by hand! But they can still be useful now, when multiple overlapping histograms become too crowded to display!

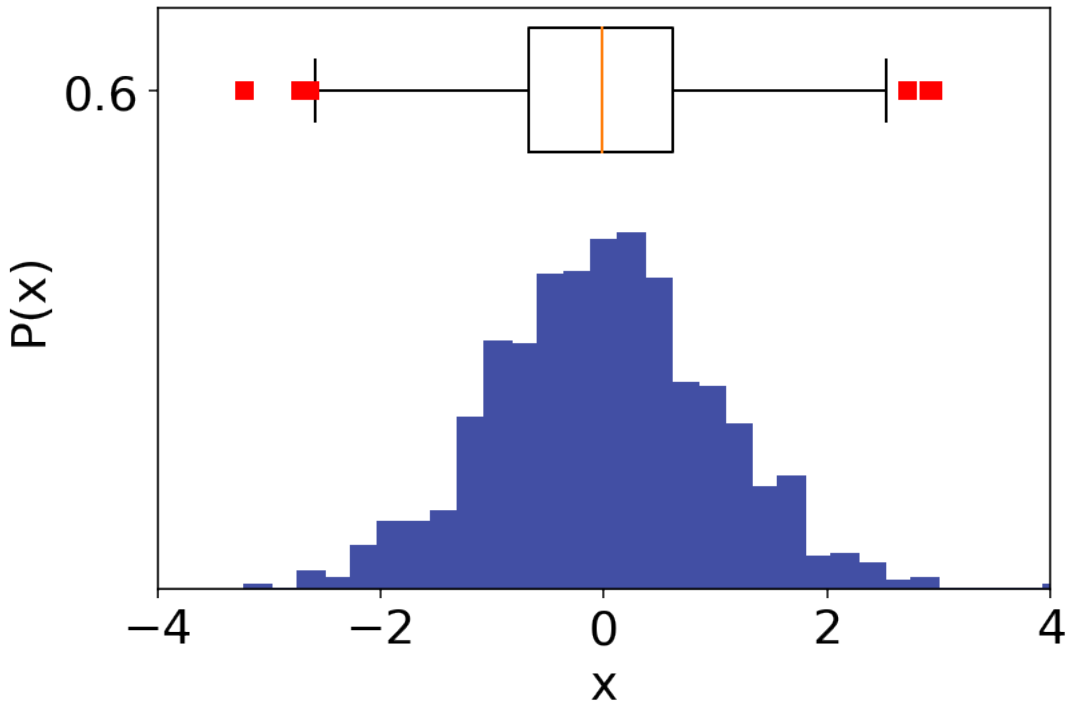
How to make boxplots in Python:

[9]:
```
data = [ np.random.randn() for _ in range(1000) ]
numbins =  int(np.sqrt(len(data))) # int is floor?


# default box plot
plt.boxplot(data)

# horizontal box plot with red squares for outliers...
plt.figure() # newfigure
plt.boxplot(data,notch=True,sym='rs',vert=False)


# compare histogram to boxplot on same plot:
plt.figure() # new figure
plt.hist(data,numbins, density=True, facecolor="#424FA4",edgecolor="#424FA4")
plt.boxplot(data,notch=False,sym='rs',vert=False, positions=[0.6])
```

```
plt.xlim(-4,4); plt.ylim(0,0.7)
plt.xlabel("x"); plt.ylabel("P(x)")
plt.show()
```



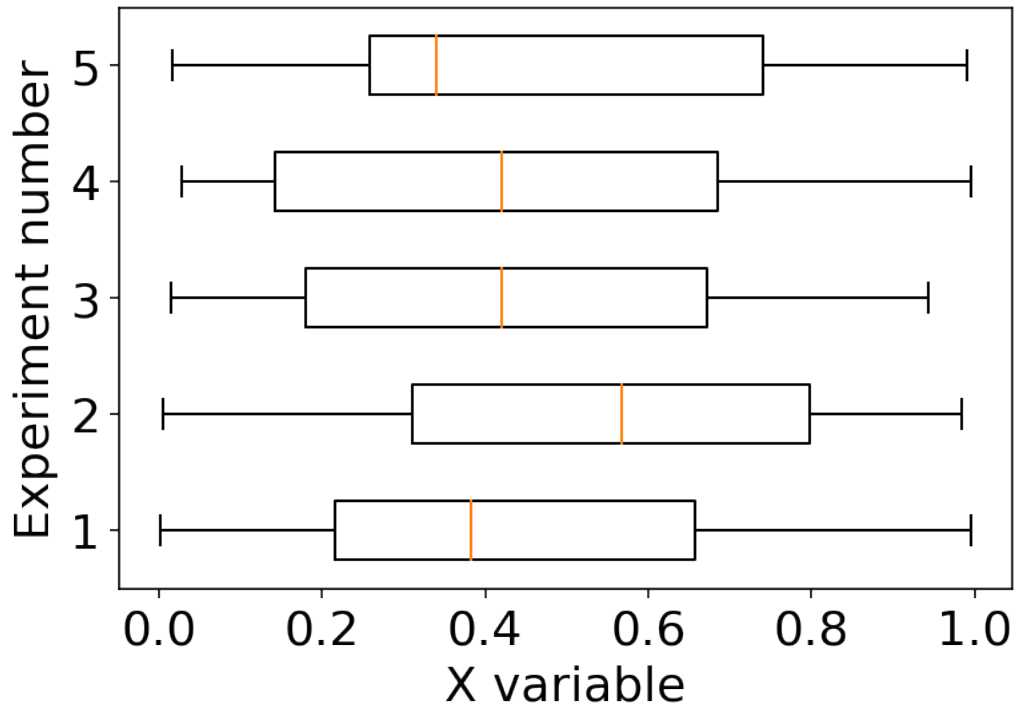




Compactly summarizing many distributions

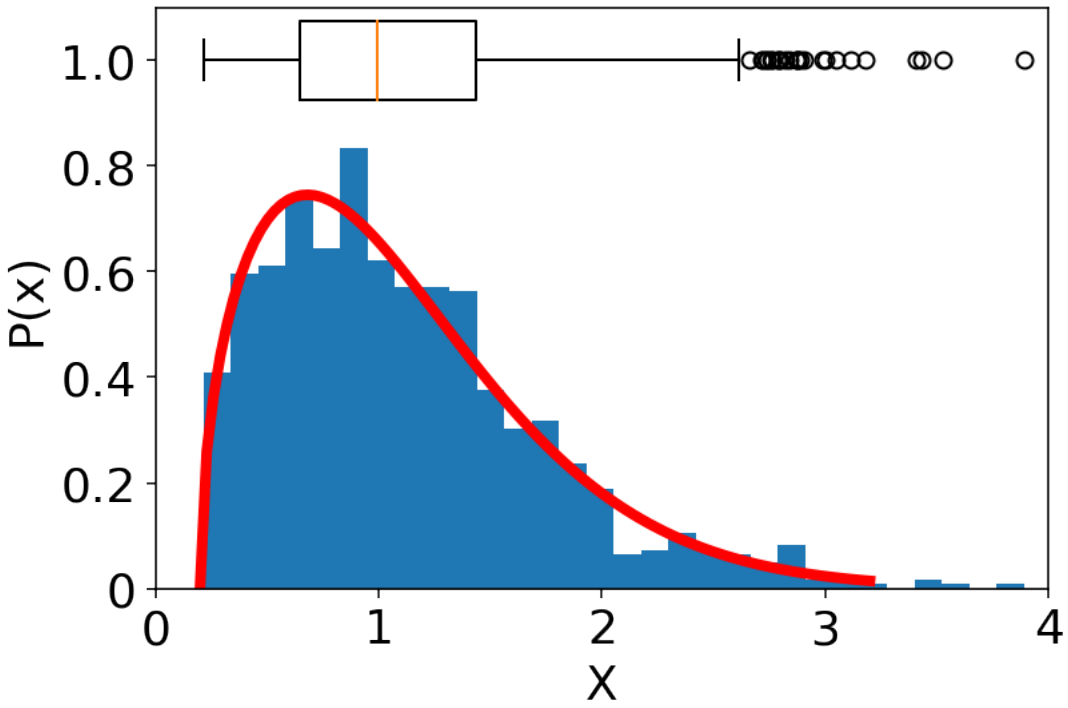
- Trade off quality (details within a single distribution) for quantity

[10]:
```
datasets=[]
for i in np.arange(5):
    data = np.random.random(50)
    datasets.append(data)

plt.boxplot(datasets,vert=False);
plt.xlabel("X variable"); plt.ylabel("Experiment number")
plt.show()
```



Of course, the underlying distribution need not be **Gaussian** (normal):

[11]:
```
def weibull(x, n,a):
    """PDF of weibull distribution"""
    return (a/n)*(x/n)**(a-1) * np.exp(-(x/n)**a)

data = np.random.weibull(1.5,1000)+0.2

plt.hist(data, 30, density=True)
x = np.linspace(0,3,100)

plt.boxplot(data,vert=False, )#positions=[0.95]);
plt.plot(x+0.2, weibull(x, 1., 1.5), 'r-', lw=4)


plt.xlim(0,4)
plt.ylim(0,1.1)
yts = [0,0.2,0.4,0.6,0.8,1.0]
plt.yticks(yts,yts)
plt.xlabel("X")
plt.ylabel("P(x)")
plt.show()
```

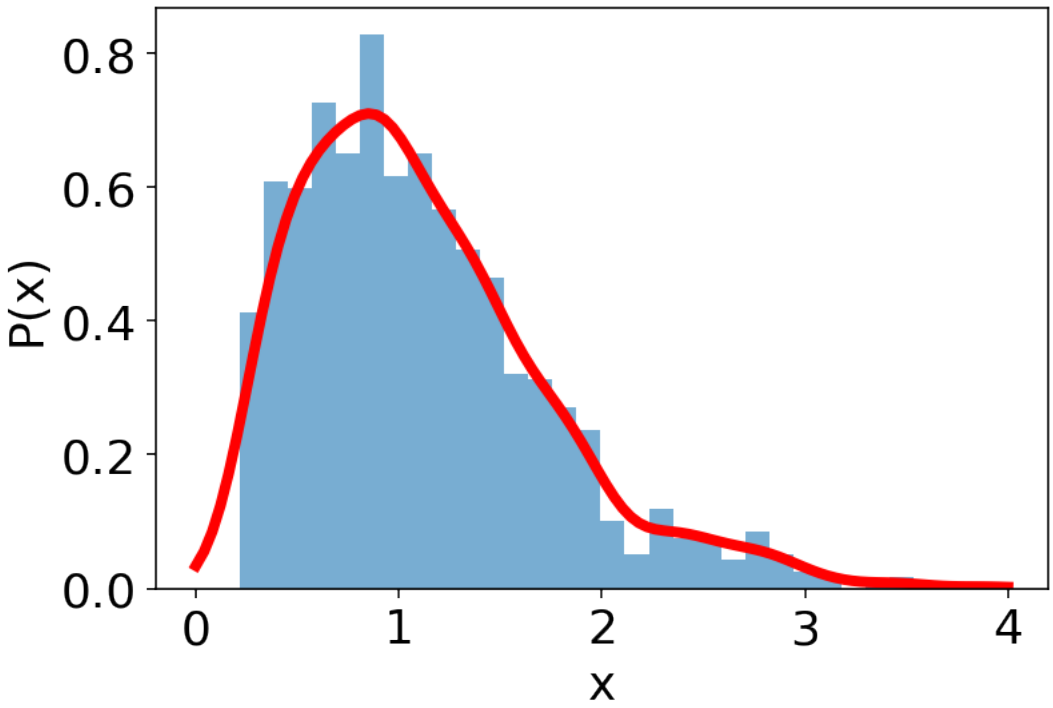


Kernel density estimation (KDE)

Recall that KDE is a technique for "smoothing" out a histogram.

- Sometimes you want to make things **pretty**, and these pictures are a little old-fashion.
- Plus if the data are noisy, the histograms look **jagged**.

[12]:
```
# scipy!!!
from scipy.stats.kde import gaussian_kde


# obtaining the KD-estimate of the Probability distribution function
# or PDF (kde_pdf is a function!)
kde_pdf = gaussian_kde( data ) # weibull data, from above...

# plotting the result
x = np.linspace(0,4,100)
plt.plot(x,kde_pdf(x),'r', linewidth=4) # distribution function
plt.hist(data,numbins,density=True,alpha=.6) # histogram
plt.xlabel("x"); plt.ylabel("P(x)")
plt.show()
```

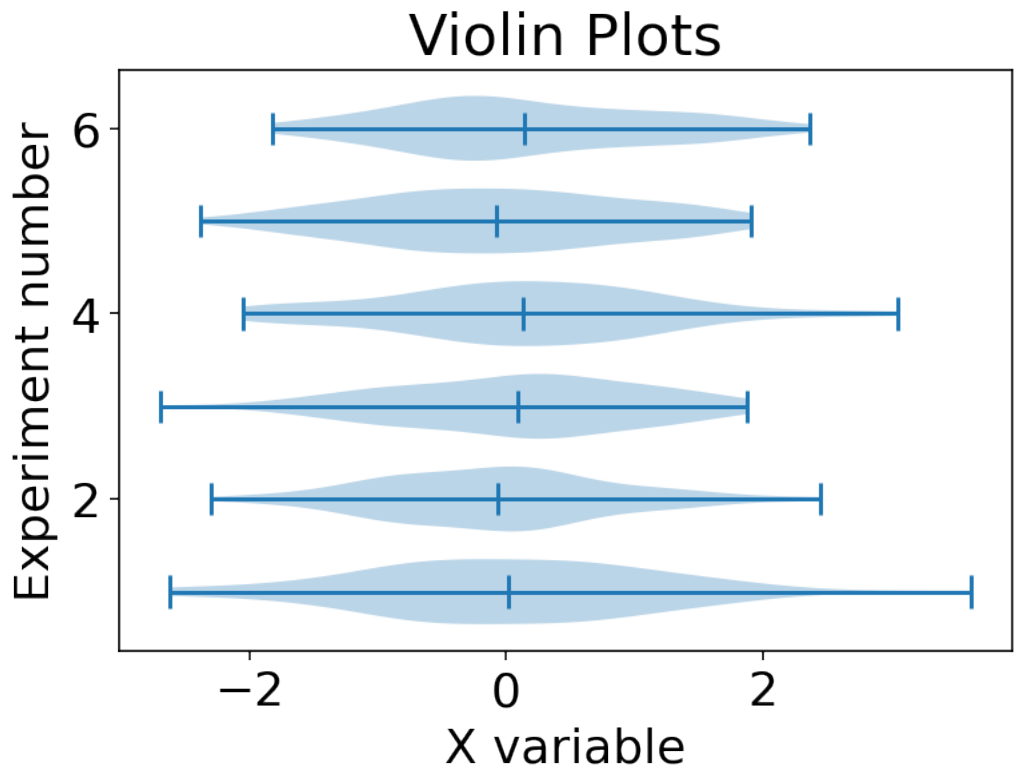


You can also **combine** boxplots and KDE in a nice way:

Violin plots

Slightly fancier box plots. Crossing box plots with KDEs.

[13]:
```
# fake data
fs = 10 # fontsize
pos = [1,2,3,4,5,6] # y-variable...?
data = [np.random.normal(size=100) for i in pos]

plt.violinplot(data, pos,
               points=80, vert=False, widths=0.7,
               showmeans=True, showextrema=True)

plt.title('Violin Plots')
plt.xlabel("X variable")
plt.ylabel("Experiment number")
plt.show()
```



Here's an example in action, from a paper of mine (and with an alumnus of this very course!):

[14]:
```
Image("figures/violin_plots_in_action.png", width=700)
```

[14]:

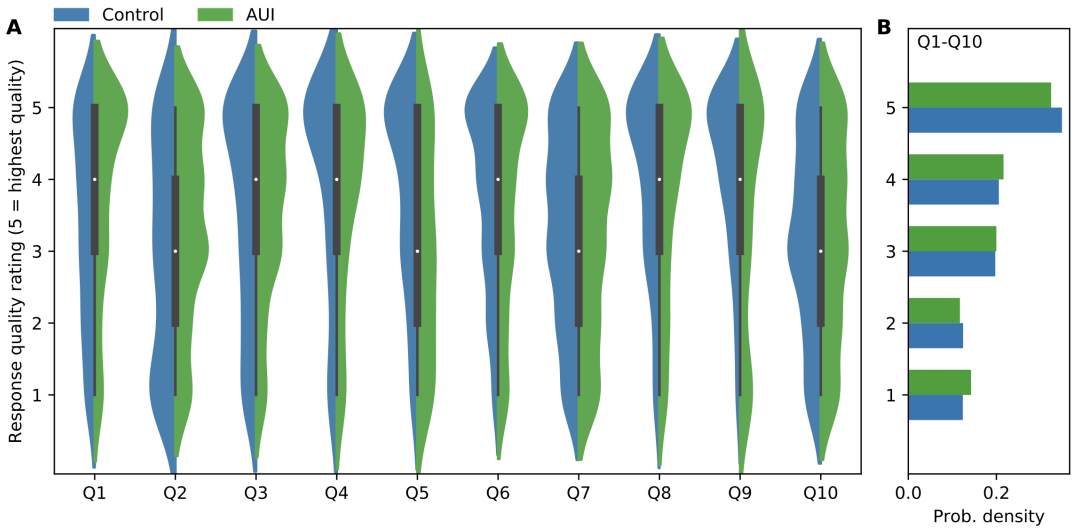


Figure 5: Quality of responses. All question-response pairs were rated independently by workers on a 1-5 scale of perceived quality (1–lowest quality, 5–highest quality).

Here's an incredibly useful and powerful idea (slides).

Cumulative probability distribution

Read the notation as "The probability that a randomly chosen piece of data is less than a particular value x". (More precisely, "the probability that a *random variable* X takes on a value less than x".)

- Also known as the "Cumulative Distribution Function" (CDF) or even "Distribution Function".
- I sometimes like to denote this as $P_<(x)$, dispensing with the X.
- For a continuous distribution:
$$P(X < x) = \int_{-\infty}^{x} P(x)dx$$
- For a discrete random variable:
$$P(X \leq x) = \sum_{x_i \leq x} P(X = x_i) = \sum_{x_i \leq x} P(x_i)$$
- Complementary cumulative distribution $P(X \geq x) = 1 - P(X < x)$
- Standard practice to use uppercase variable for CDF to correspond to the lowercase variable for the PDF, $F(x)$ (cdf) vs. $f(x)$ (pdf).

So by sorting the data we have computed an ***empirical estimate*** of the CDF!

$$P(X \leq x) = \frac{\text{number of datapoints} \leq x}{\text{number of datapoints}} = \frac{1}{N}\sum_{i=1}^{N} \mathbf{1}_{x_i \leq x},$$

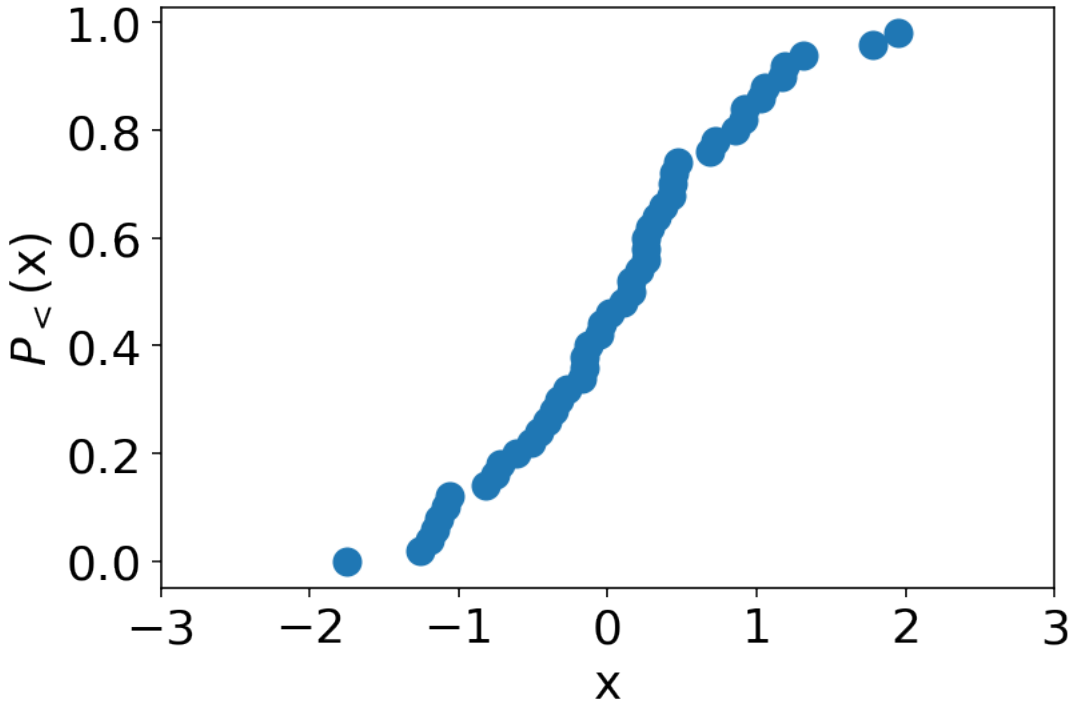
- Sorting generated all these counts at once!
- Sometimes called the **ECDF** for "Empirical CDF"
  - a subscript N is used to distinguish the ECDF for a sample of N datapoints from the "real" or "true" or "underlying" CDF.
  - For example, $F_N(x)$ vs. $F(x)$.
- For $P(X \leq x)$ just use $i\,/N$ instead of $(i-1)/N$
- (Common to write {number of datapoints} as #{datapoints}. Other variants also used.)

Let's see it in action:

How to compute the table from the slides?

[15]:
```
N = 50
data = np.random.normal(size=N)

X = sorted(data)
Y = np.arange(N)/N # that's the whole calculation
                   # that's it!!!
# np.arange(N) gives [0,1,...,N-1]

plt.plot(X, Y, '.', markersize=20)
plt.xlabel("x"); plt.ylabel("$P_<$(x)");
```

```
plt.xlim(-3,3)
plt.show()
```



(Technically, we should plot this using `plt.step` because the ECDF is defined for all values of x.)

Let's compare to the **true CDF**:

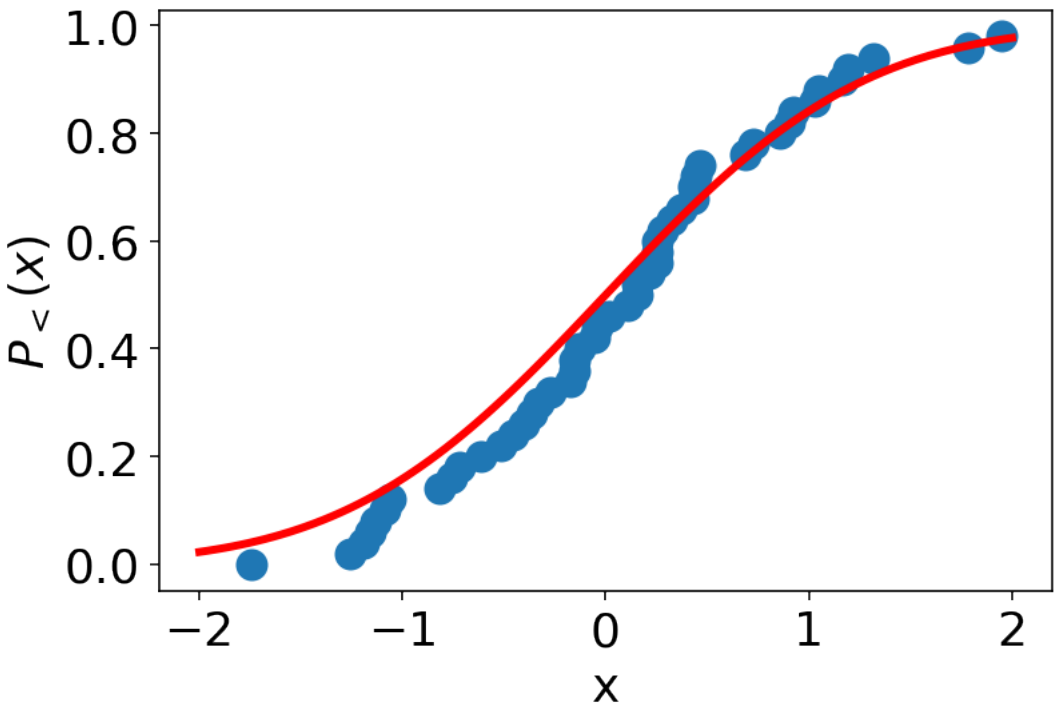
Remember that the PDF for a **normal distribution** with mean μ and variance σ^2 is

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

By integrating, the CDF is

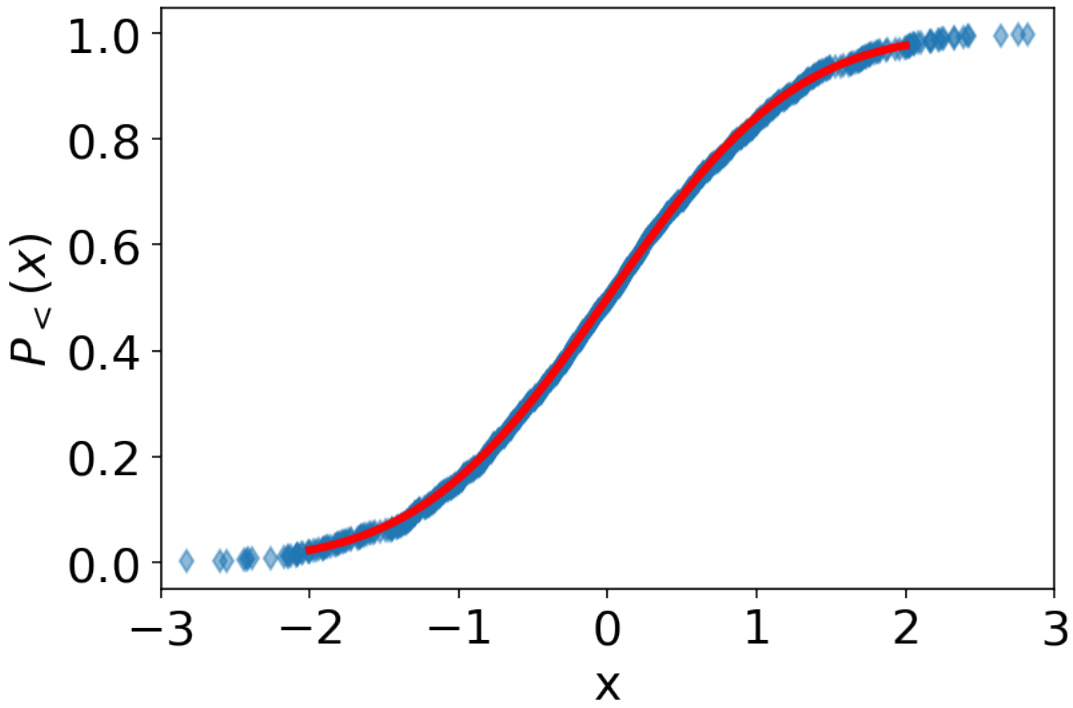
$$P(X < x) = \int_{-\infty}^{x} P(x)dx = \frac{1}{2}\left[1 + \text{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right]$$

[16]:
```
x_true = np.linspace(-2,2,100)
y_true = [0.5*(1+math.erf(x/math.sqrt(2))) for x in x_true] # integral of gaussian

#plt.plot(X,Y, 'bx', x_true,y_true, 'r-');
plt.plot(X,Y, '.', markersize=22)
plt.plot(x_true,y_true, 'r-', lw=3);

plt.xlabel("x")
plt.ylabel("$P_<(x)$")
plt.show()
```



Pretty good agreement with $N = 50$ points. What if we have more?

[17]:
```
N = 1000
data = np.random.normal(size=N)

X = sorted(data)
Y = 1.0*np.arange(N)/N

plt.plot(X,     Y,      'd', alpha=0.5)
plt.plot(x_true,y_true, 'r-', lw=3);
plt.xlabel("x"); plt.ylabel("$P_<(x)$");
plt.xlim(-3,3)
plt.show()
```



Pros CDF vs. PDF

- CDF uses ***all*** the data, nothing is lost.
- CDF has no choices for binning or kernel bandwidth — method is automatic!
- Works equally well for continuous and discrete data

Cons

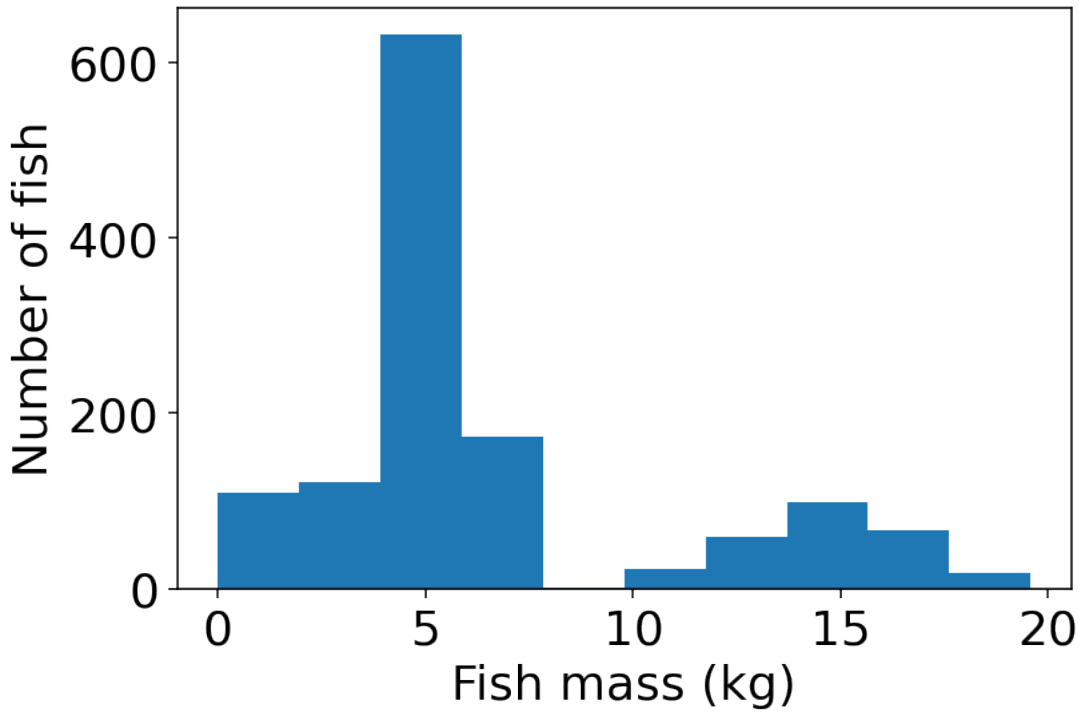
- It is harder to think about for people, especially those who have weak calculus backgrounds
- Because it's cumulative, a bias at one region will affect all regions to the right (we will address this shortly)

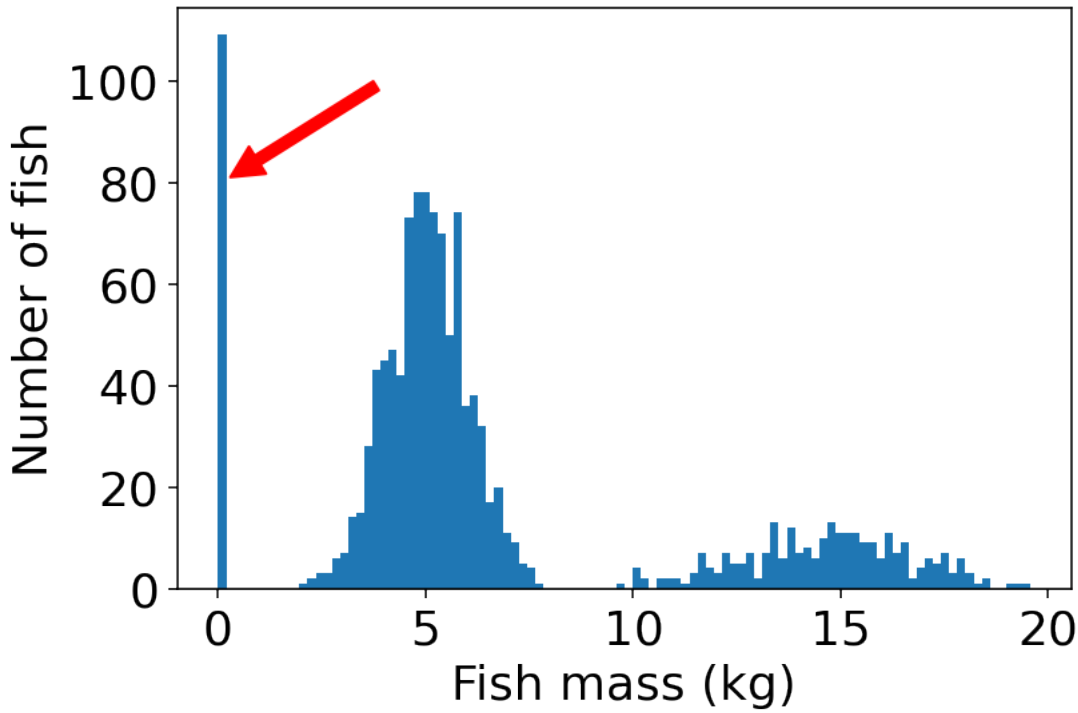
Recall our **fish mass** data?

A bad binning hides a third mode of data:

[18]:
```
data = []
for line in open("fishMass_kilograms.txt"):
    data.append( float(line.strip()) )


plt.hist(data)

# pretty up the figure a little
plt.xlabel("Fish mass (kg)");
plt.ylabel("Number of fish");

# more bins with an arrow annotation:
plt.figure()
plt.hist(data, bins=100);
```

```
plt.gca().annotate('', xy=(0.1, 80), xytext=(4, 100),
  arrowprops=dict(facecolor='red', edgecolor='red',shrink=0.05),
)

plt.xlabel("Fish mass (kg)");
plt.ylabel("Number of fish");
plt.show()
```

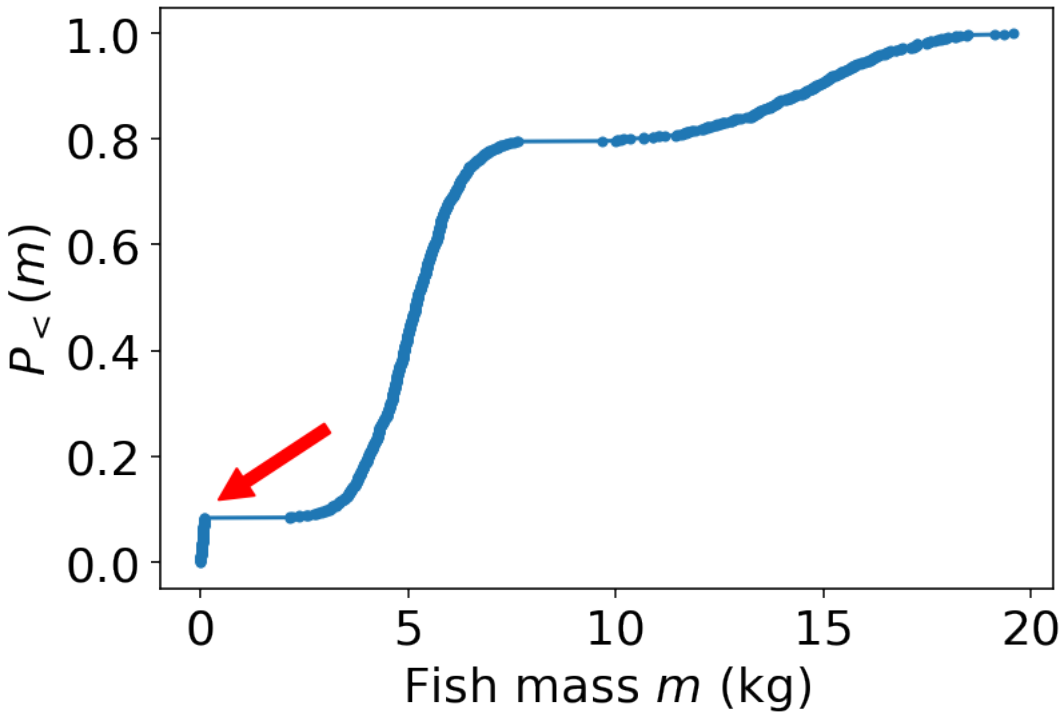




Question
How many fish are very small? It looks like a lot, but it's hard to read out the **proportion of data** in that position from just the histogram.

Now let's try the CDF:

[19]:
```
X = sorted(data)
N = len(data)
Y = 1.0*np.arange(N)/N

plt.plot(X,Y,'.-')
#plt.step(X,Y, where='pre', lw=4)

plt.gca().annotate('', xy=(0.3, 0.11), xytext=(3.2, 0.26),
  arrowprops=dict(facecolor='red', edgecolor='red',shrink=0.05),
)

plt.xlabel("Fish mass $m$ (kg)")
plt.ylabel("$P_<(m)$") # shorthand for P(M < m)
plt.show()
```



Ahh, we see immediately that it's around 10% of the data!

CDFs are **easier** to read than PDFs in one sense: * To find the proportion of data between two values, just look at how much the CDF travels vertically. For example, in the plot above the CDF is at about 10% for 2.5kg and about 80% for 7.5 kg. Therefore, we can immediately tell that about 70% of the data lie in the second mode.

- To find this value for a histogram requires estimating the *area* of the second mode relative to the total area. This is a *much harder visual task*.

Using CDFs to examine broadly distributed data

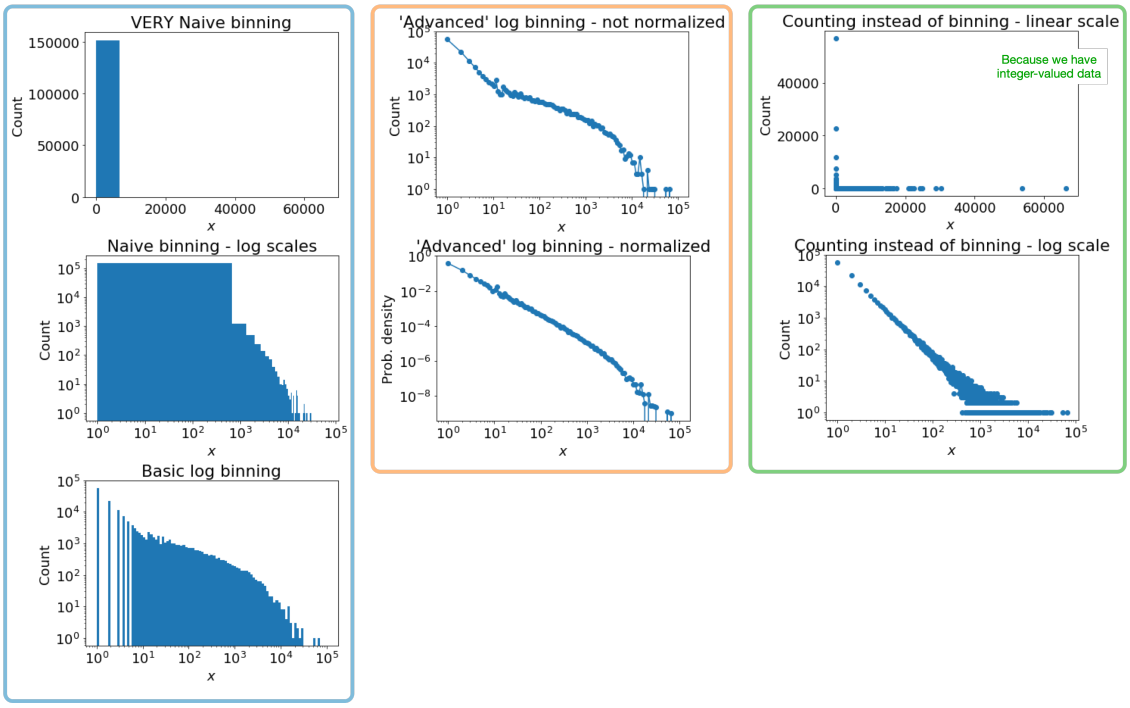
Recall our **skewed/broad** data?

Summarizing from the previous lecture:

1. Simple binning
2. "Advanced" binning
3. Counting

[20]:
```
print()
Image("figures/broad-data-binning-summary.png", width=800)
```

[20]:



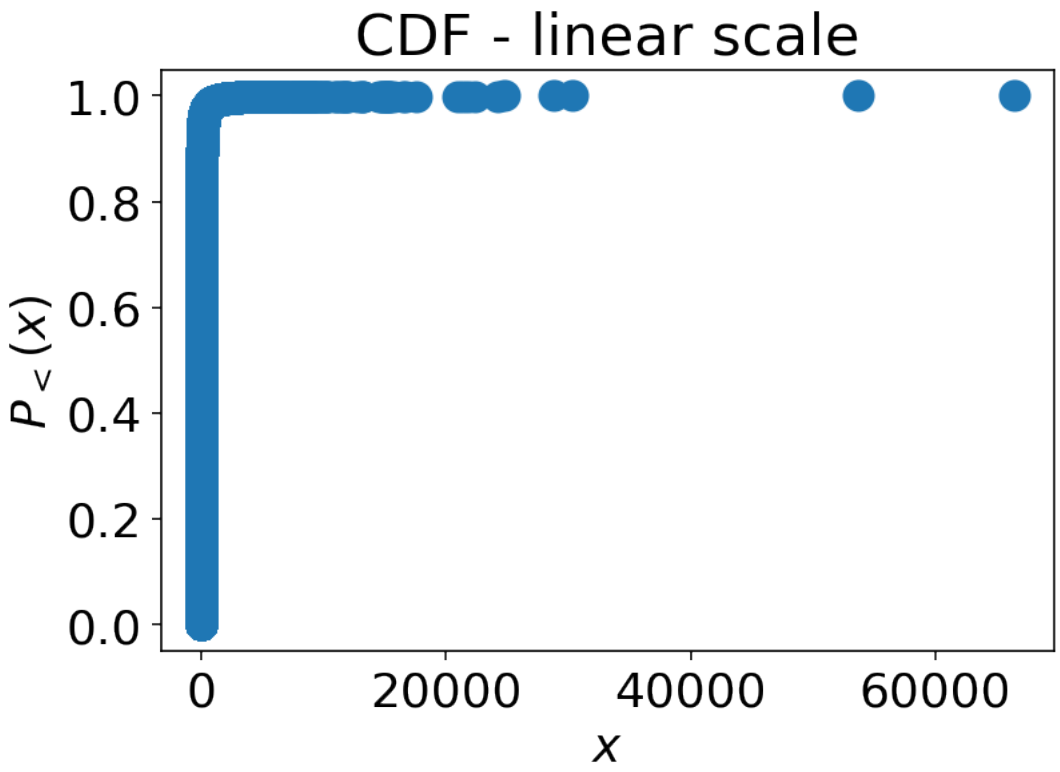
Takeaway?

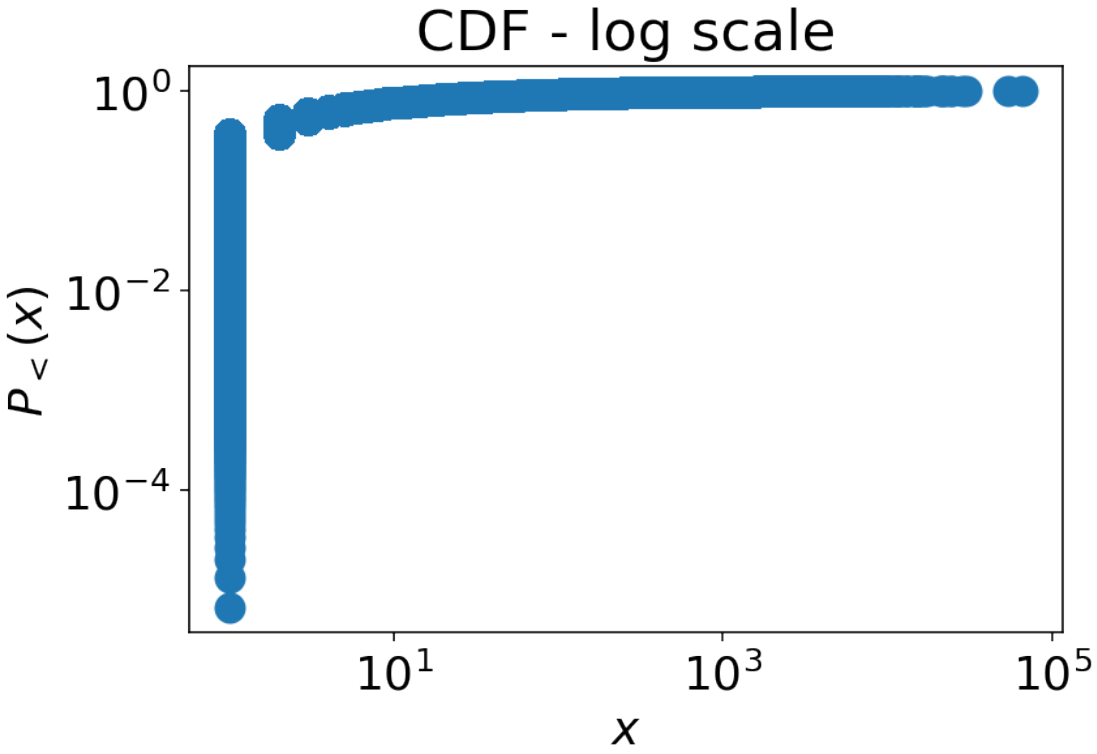
So many different option, between the linear/log scales and the (vast) set of binning options.

What can we do?

Use the Cumulative distribution!

[21]:
```
data = [float(line) for line in open("7impact_counts.txt")]

X = sorted(data)
N = len(data)
Y = 1.0*np.arange(N)/N

plt.plot(X,Y, '.', markersize=22)
plt.xlabel("$x$");plt.ylabel("$P_<(x)$")
plt.title("CDF - linear scale")
plt.show()

plt.loglog(X,Y, '.', markersize=22)
plt.xlabel("$x$");plt.ylabel("$P_<(x)$")
plt.title("CDF - log scale")
plt.show()
```

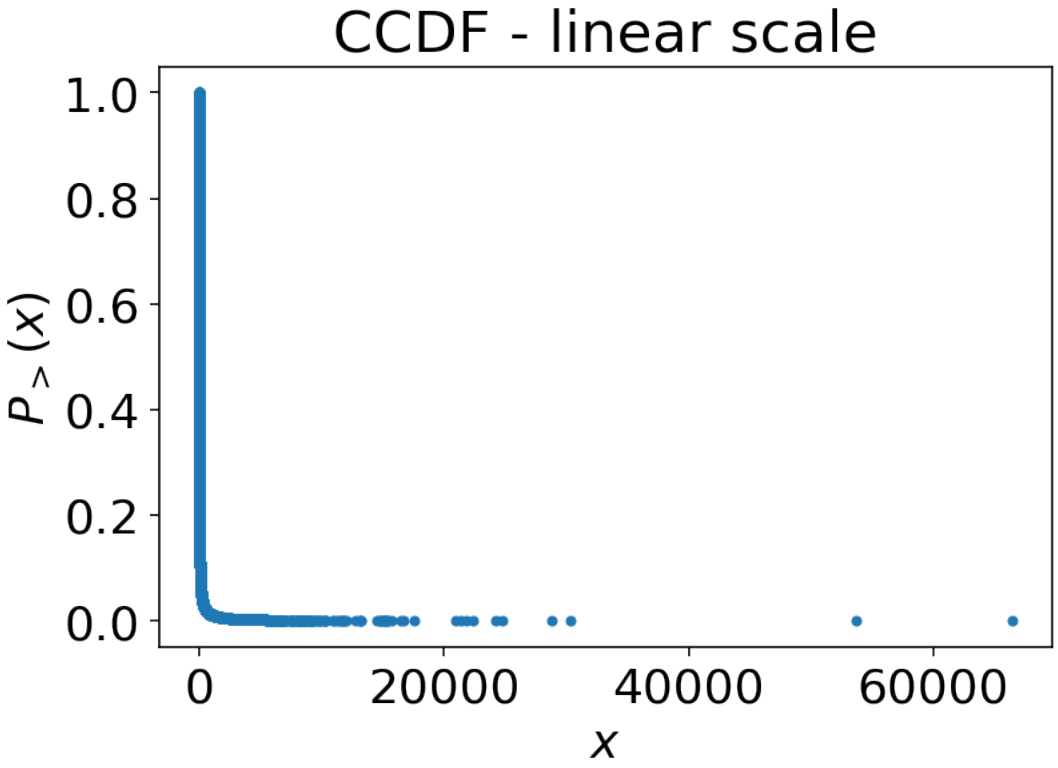

CDF - linear scale
1.0
0.8
0.6
0.4
0.2
0.0
$P_<(x)$
0
20000
40000
60000
x

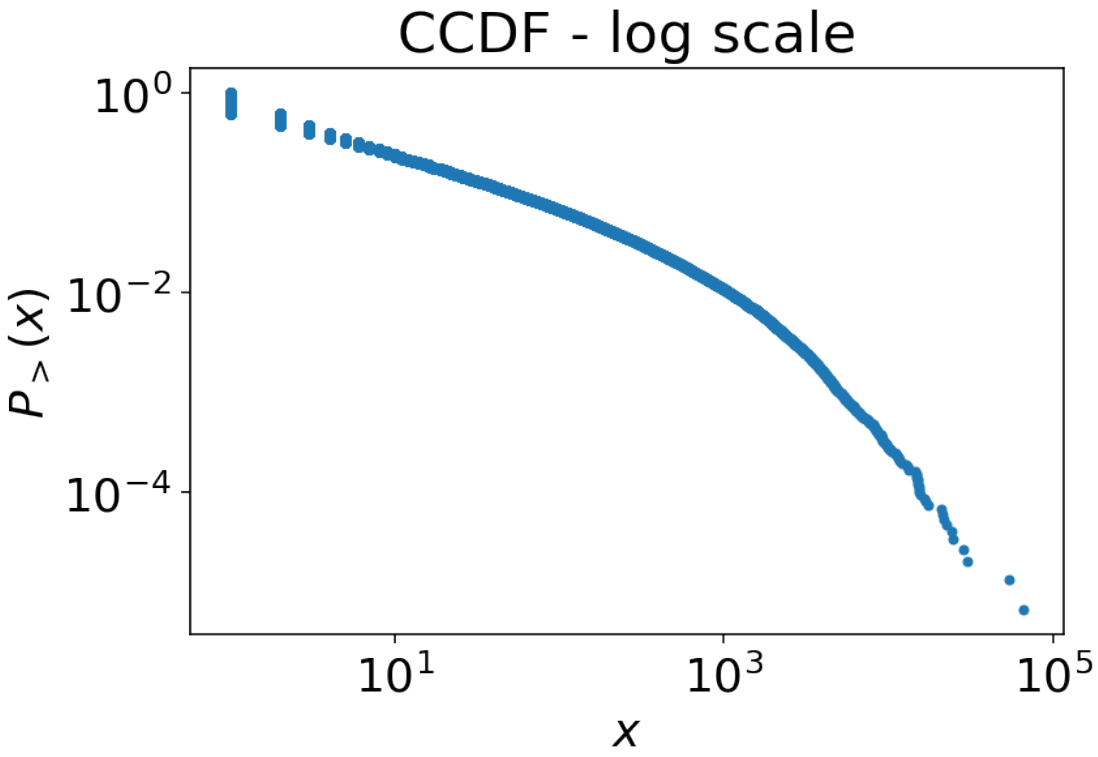

CDF - log scale
10^0
10^{-2}
10^{-4}
$P_<(x)$
10^1
10^3
10^5
x

Turns out to not be so helpful. Why? Because we are looking at $P(X < x)$. Let's look at $P(X > x)$:

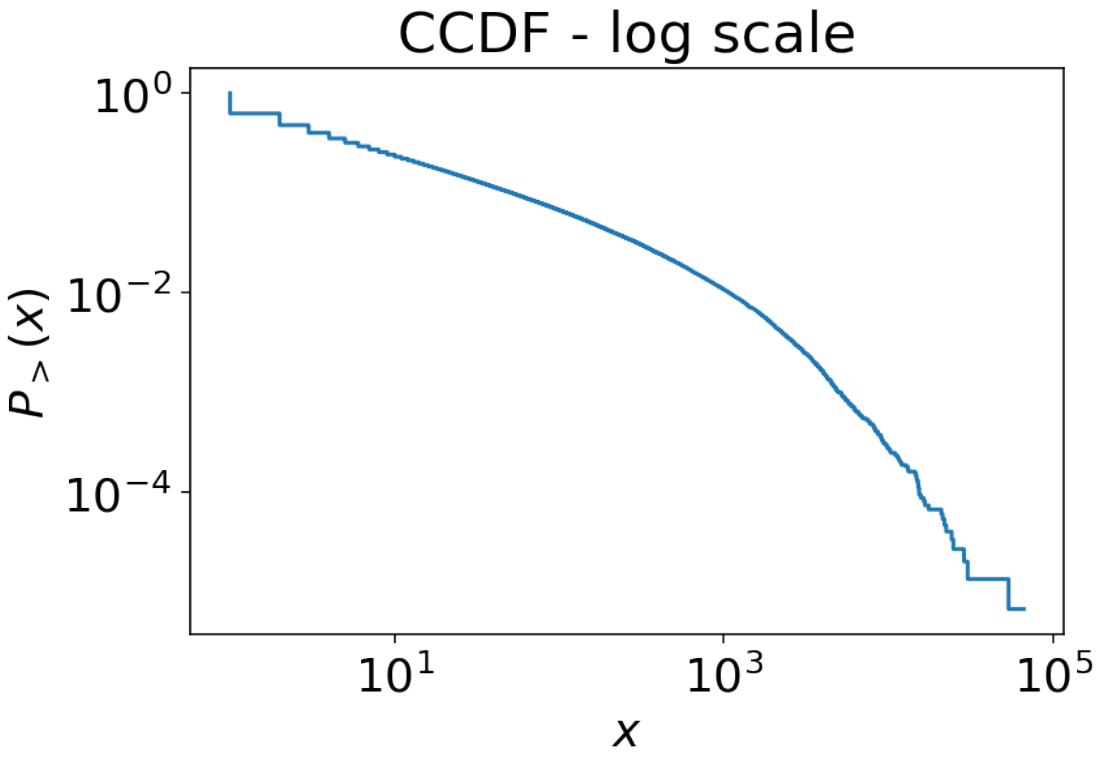
- This is sometimes called the CCDF (complementary CDF), but some fields define CDF and CCDF in reverse compared with other fields

[22]:
```
Y = 1 - 1.0*np.arange(N)/N # CCDF

plt.plot(X,Y, '.')
plt.xlabel("$x$");plt.ylabel("$P_>(x)$")
plt.title("CCDF - linear scale")
plt.show()

plt.loglog(X,Y, '.')
plt.xlabel("$x$");plt.ylabel("$P_>(x)$")
plt.title("CCDF - log scale")
plt.show()
```





[23]:
```
plt.step(X,Y)
plt.xscale('log')
plt.yscale('log')
plt.xlabel("$x$");plt.ylabel("$P_>(x)$")
plt.title("CCDF - log scale")
plt.show()
```



I cannot impress upon you more strongly just how *useful* and *powerful* the CDF is, even for just basic data exploration. I use it all the time. Even when I go back and report a histogram because it's simpler for presenting (interdisciplinary) research, I still **start** with the CDF.

- Python has a `cumulative=True` option for histograms, but it's still binning! ***They got it wrong!!!*** Easier to just sort!
- I've been a little lax in some details. For example, the limits $x \to -\infty$ and $x \to \infty$. At the largest datapoint, the ECDF curve jumps vertically from a y = (N-1)/N to y = 1. Likewise, the distinction between $P(X < x)$ and $P(X \leq x)$; this can be easily worked out by comparing i/N instead of $(i-1)/N$.

Errors and sampling in CDFs

(This addresses the cumulative bias that a sampling effect or error in one region of the ECDF will affect all regions to the right.)

We just saw how much better the data represents the distribution when $N = 1000$ than when $N = 50$.

- How many data points do we need?

There are some beautiful results relating the **empirical** distribution function $F_n(x)$ to the true **distribution** $F(x)$.

1. **Glivenko–Cantelli** (1933):

$$\sup_{x \in \mathbb{R}} \left| F_N(x) - F(x) \right| \to 0 \text{ as } N \to \infty$$

assuming the data $x_1, \ldots, x_N$ are iid real numbers.

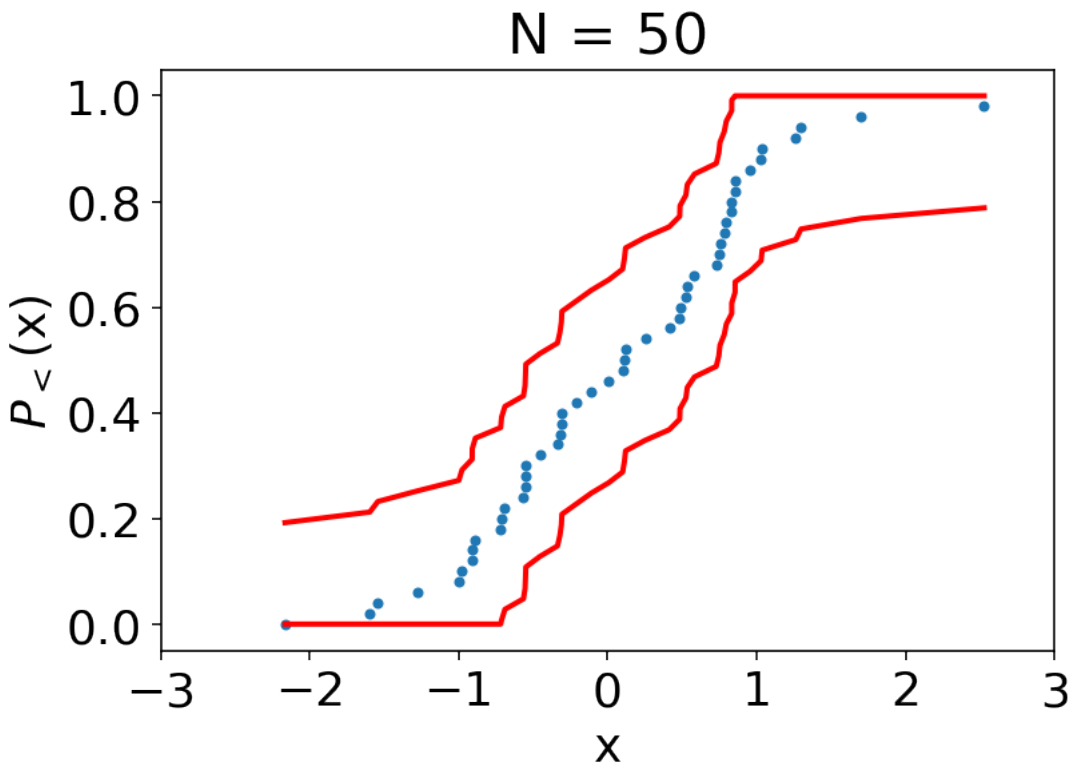
2. This result was strengthened, **Dvoretzky–Kiefer–Wolfowitz** inequality (1956) and Massart (1990).

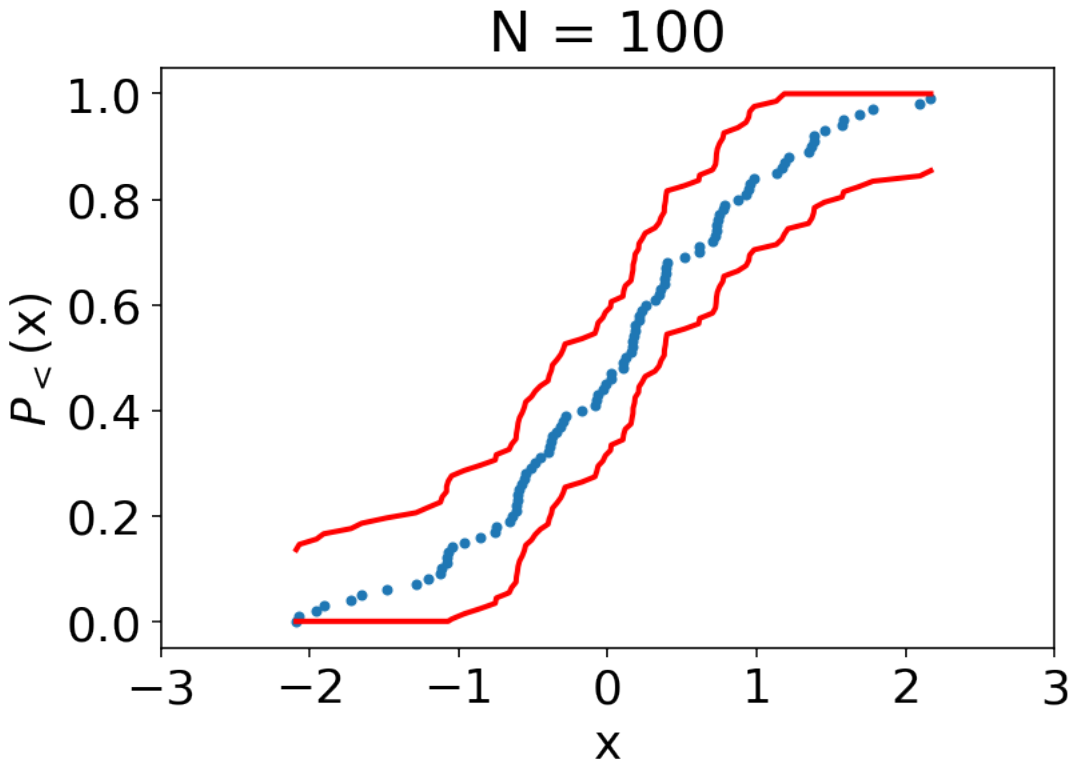
$$\Pr\left(\sup_{x\in\mathbb{R}} |F_n(x) - F(x)| > \varepsilon\right) \leq 2e^{-2n\varepsilon^2} \qquad \text{for every } \varepsilon > 0.$$

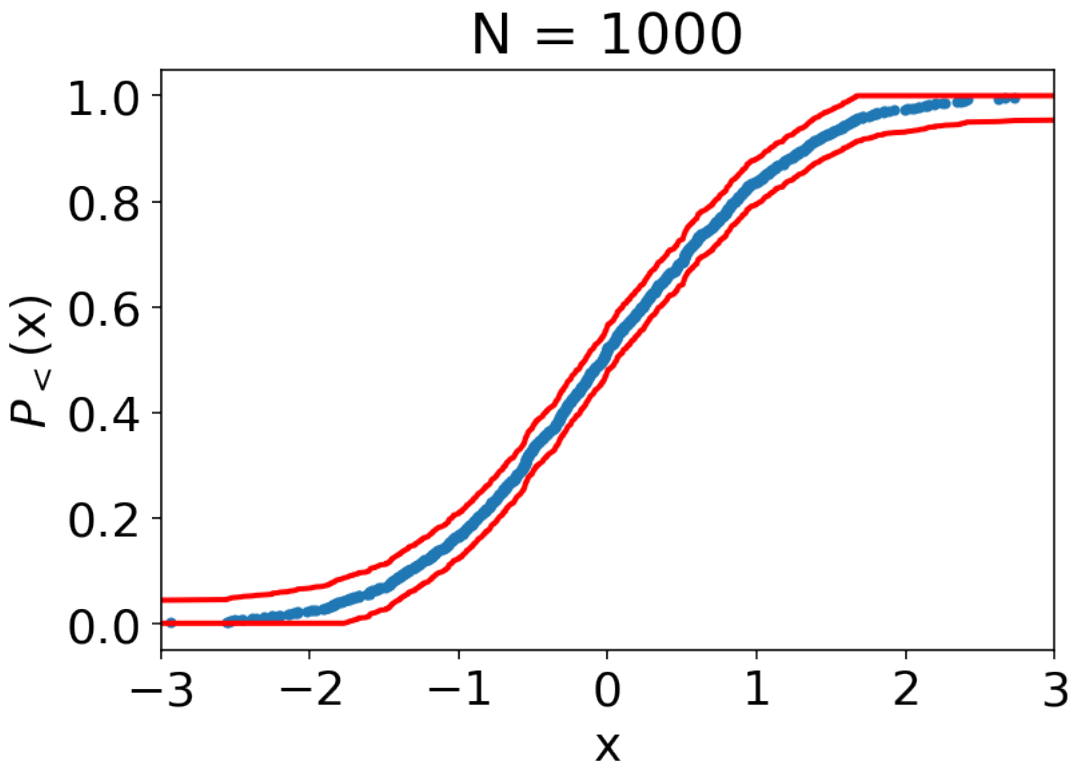
This shows that not only does F_N converge to F but how quickly!

Let's implement it by reversing DKW to find the largest value of ϵ that gives $\Pr\left(\sup_{x\in\mathbb{R}} |F_n(x) - F(x)| > \varepsilon\right) = \alpha$, for a given α:

[24]:
```
def DKW_CI(ecdf, alpha=0.05):
    """Dvoretzky-Kiefer-Wolfowitz confidence intervals at significance level alpha"""
    N = len(ecdf)
    eps = np.sqrt(np.log(2./alpha) / (2 * N))
    lower = np.clip(ecdf - eps, 0, 1)
    upper = np.clip(ecdf + eps, 0, 1)
    return lower, upper

for N in [50,100,1000]:
    plt.figure()
    data = np.random.normal(size=N)

    # get the ecdf:
    X = sorted(data)
    Y = 1.0*np.arange(N)/N

    plt.plot(X, Y, '.')

    lower,upper = DKW_CI(Y)

    plt.plot(X, lower, 'r-', X, upper, 'r-', lw=2)

    plt.xlabel("x"); plt.ylabel("$P_<$(x)");
    plt.xlim(-3,3);
    plt.title("N = %i" % N)
    plt.show()
```


N = 50
1.0
0.8
0.6
0.4
0.2
0.0
$P_<(x)$
−3
−2
−1
0
1
2
3
x


N = 100
1.0
0.8
0.6
0.4
0.2
0.0
$P_<(x)$
−3
−2
−1
0
1
2
3
x



Pros and cons of CDF vs. histogram

Pros

- No need to bin
- All data is used, nothing is lost
- Very easy to code up!
- Easy to tell how much of the data falls between two values x_L and x_R: just subtract: $P(X < x_R) - P(X < x_L)$. For the PDF you need to find the total *area* between x_L and x_R.

Cons

- **None!**

OK, OK!

Cons people mention that are not big deals:

- Every data point is plotted, which can lead to large figure files
  - This can be avoided by removing ties, but you need to be a little bit careful
- Errors compound as the data are "accumulated" left-to-right — An unusual value at the start of the function will change all subsequent values
  - This is addressed by the DKW confidence intervals derived above.

The one true con of CDFs over PDFs/histograms:

- Harder to communicate to some audiences; less intuitive

  - Need calculus skills. The CDF is the integral of the PDF, so you need to be comfortable with looking at a curve and seeing its derivative—the **steepness** of the curve tells you how much data is there.

Advice

I **always** go to the CDF to start, but I will also check the histogram: If the PDF via the histogram works well, I will tend to use that.

- Don't overcomplicate things

Takeaways

- **Boxplots** - May be a leftover artifact of limited computing resources but still useful for comparing many distributions
- **CDF** - Cumulative Distribution Function - sorting is integrating (!) - MANY advantages(!)
  - I never explore data with histograms. I only use (E)CDFs!

X-data
If you have X-data you want to understand, think about summarizing it using it's statistics (mean, median, IQR, etc.) and drawing the underlying distribution (histogram, KDE, etc.)