Quantiles and Quantile Based Plots
Percentiles and Quantiles

The $k$-th percentile of a set of values divides them so that $k\%$ of the values lie below and $(100 - k)\%$ of the values lie above.

- The 25th percentile is known as the lower quartile.
- The 50th percentile is known as the median.
- The 75th percentile is known as the upper quartile.

It is more common in statistics to refer to quantiles. These are the same as percentiles, but are indexed by sample fractions rather than by sample percentages.
Some Difficulties

The previous definition of quantiles and percentiles is not completely satisfactory. For example, consider the six values:

\[ \begin{align*}
3.7 & \quad 2.7 & \quad 3.3 & \quad 1.3 & \quad 2.2 & \quad 3.1
\end{align*} \]

What is the lower quartile of these values?

There is no value which has 25% of these numbers below it and 75% above.

To overcome this difficulty we will use a definition of percentile which is in the spirit of the above statements, but which (necessarily) makes them hold only approximately.
Defining Quantiles

We define the quantiles for the set of values:

\[ 3.7 \quad 2.7 \quad 3.3 \quad 1.3 \quad 2.2 \quad 3.1 \]

as follows.

First sort the values into order:

\[ 1.3 \quad 2.2 \quad 2.7 \quad 3.1 \quad 3.3 \quad 3.7 \]

Associate the ordered values with sample fractions equally spaced from zero to one.

<table>
<thead>
<tr>
<th>Sample fraction</th>
<th>0</th>
<th>.2</th>
<th>.4</th>
<th>.6</th>
<th>.8</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantile</td>
<td>1.3</td>
<td>2.2</td>
<td>2.7</td>
<td>3.1</td>
<td>3.3</td>
<td>3.7</td>
</tr>
</tbody>
</table>
Defining Quantiles

The other quantiles of

```
1.3  2.2  2.7  3.1  3.3  3.7
```

can be obtained by linear interpolation between the values of the table.

The median corresponds to a sample fraction of .5. This lies half way between 0.4 and 0.6. The median must thus be
\[ .5 \times 2.7 + .5 \times 3.1 = 2.9 \]

The lower quartile corresponds to a sample fraction of .25. This lies one quarter of the way between .2 and .4. The lower quartile must then be
\[ .75 \times 2.2 + .25 \times 2.7 = 2.325. \]
The General Case

Given a set of values $x_1, x_2, \ldots, x_n$ we can define the quantiles for any fraction $p$ as follows.

Sort the values in order

$$x_{(1)} \leq x_{(2)} \leq \cdots \leq x_{(n)}.$$

The values $x_{(1)}, \ldots, x_{(n)}$ are called the order statistics of the original sample.

Take the order statistics to be the quantiles which correspond to the fractions:

$$p_i = \frac{i - 1}{n - 1}, \quad (i = 1, \ldots, n),$$
The Quantile Function

In general, to define the quantile which corresponds to the fraction $p$, use linear interpolation between the two nearest $p_i$.

If $p$ lies a fraction $f$ of the way from $p_i$ to $p_{i+1}$ define the $p$th quantile to be:

$$Q(p) = (1 - f)Q(p_i) + fQ(p_{i+1})$$

As special cases, define the median and quartiles by:

- Median: $Q(.5)$
- Lower Quartile: $Q(.25)$
- Upper Quartile: $Q(.75)$

The function $Q$ defined in this way is called the Quantile Function.
Computing Quantiles with R

The R function `quantile` can be used to compute the quantiles of a set of values.

```r
> x = c(1.3, 2.2, 2.7, 3.1, 3.3, 3.7)

> quantile(x)
   0% 25% 50% 75% 100%
 1.300 2.325 2.900 3.250 3.700

> quantile(x, seq(0, 1, by=.1))
   0% 10% 20% 30% 40% 50% 60% 70%
 1.30 1.75 2.20 2.45 2.70 2.90 3.10 3.20
   80% 90% 100%
 3.30 3.50 3.70
```
Plots Based on Quantiles

- Boxplots
- QQ plots
- Empirical shift function plots
- Symmetry plots
Boxplots and Variations

- Real name *box-and-whisker plots*.

- Draw a box from the lower quartile to the upper quartile.

- Extend a whisker from the ends of the box to the furthest observation which is no more than 1.5 times inter-quartile range from the box.

- Mark any observations beyond this as “outliers.”
Producing Boxplots With R

A single boxplot, vertically aligned.

```r
> boxplot(rain.nyc,
        main = "New York City Rainfall",
        ylab = "Inches")
```

The basic call can be heavily customized.

```r
> boxplot(rain.nyc,
         col = "lightgray",
         horizontal = TRUE,
         main = "New York City Rainfall",
         xlab = "Inches")
```
Comparing Samples with Boxplots

- It is possible to compare two or more samples with boxplots.

- By producing the plots on the same scale we are able to make direct comparisons of:
  - medians
  - quartiles
  - inter-quartile ranges

- The comparison of medians using boxplots can be regarded as the graphical equivalent of two-sample \( t \)-tests and one-way analysis of variance.
The New York Ozone Data

- The ozone levels in Yonkers and Stamford can be compared with boxplots.

- The two samples are passed to boxplot as separate arguments.

- Labels can be provided to label the two samples.

```r
> boxplot(yonkers, stamford,
    names = c("Yonkers", "Stamford"),
    main = "New York Ozone Levels",
    ylab = "Ozone Levels (ppb)")
```
Transformations

- The median ozone level in Stamford is higher than that in Yonkers.

- The spread of the values in Stamford is also larger than the spread in Yonkers.

- When there is a difference in data spreads it is common to transform the values so that the spreads are equal.

- This makes it possible to compare the medians in the absence of any other differences.

> `boxplot(log10(yonkers), log10(stamford),
      names = c("Yonkers", "Stamford"),
      main = "New York Ozone Levels",
      ylab = "Log10 Ozone Levels (ppb)")`
New York Ozone Levels

Log10 Ozone Levels (ppb)
Significance Testing

- The boxplot function can be used to carry out a formal significance test of whether there is difference between the median levels of the underlying populations.

- This is done by specifying `notch=TRUE` as an argument.

- If the resulting notches in the sides of the boxplots do not overlap then there is a significant difference between the medians of the underlying values.

```r
> boxplot(log10(yonkers), log10(stamford),
          names = c("Yonkers", "Stamford"),
          main = "New York Ozone Levels",
          ylab = "Log10 Ozone Levels (ppb)",
          notch = TRUE)
```
New York Ozone Levels

Log10 Ozone Levels (ppb)

Yonkers

Stamford
Quantile Plots

- Quantile plots directly display the quantiles of a set of values.
- The sample quantiles are plotted against the fraction of the sample they correspond to.
- There is no built-in quantile plot in R, but it is relatively simple to produce one.

```r
> x = rain.nyc
> n = length(x)
> plot((1:n - 1)/(n - 1), sort(x), type="l",
     main = "Quantiles for the NYC Rain Data",
     xlab = "Sample Fraction",
     ylab = "Sample Quantile")
```
Quantiles for the NYC Rain Data

Sample Fraction

Sample Quantile

Sample Fraction

Sample Quantile
Quantile-Quantile Plots

- Quantile-quantile plots allow us to compare the quantiles of two sets of numbers.

- This kind of comparison is much more detailed than a simple comparison of means or medians.

- There is a cost associated with this extra detail. We need more observations than for simple comparisons.
Drawing Quantile-Quantile Plots

- Obtain the sample fraction values for the larger batch of values.

- For each batch, compute the quantiles corresponding to the computed fractions.

- Plot the computed quantiles against each other.

```r
> n = max(length(x), length(y))
> p = (1:n - 1)/(n - 1)
> qx = quantile(x, p)
> qy = quantile(y, p)
> plot(qx, qy)
```

But there is an easier way …
The R Quantile-Quantile Plot Function

- Q-Q plots are an important tool in statistics and there is an R function which implements them.

- The function is called \texttt{qqplot}.

- The first two arguments to \texttt{qqplot} are the samples of values to be compared.
Modelling The Relationship

The points in the plot fall close to a straight line. This suggests that the quantiles of the two samples satisfy:

\[ \text{stamford} = a + b \times \text{yonkers} \]

or

\[ \text{stamford} = b \times \text{yonkers} \]

One way to check which of these situations applies is to add some straight lines to the plot.

We also need to expand the limits on the graph, because we want to check whether the points lie on a line through and origin.
An Improved Plot

First we get the ranges of the two samples.

```r
> xlim = range(0, yonkers)
> ylim = range(0, stamford)
```

Now we produce a Q-Q plot with the expanded limits and mark in the line $y = x$.

```r
> qqplot(yonkers, stamford,
        xlim = ylim, ylim = ylim,
        xlab = "Yonkers",
        ylab = "Stamford",
        main = "Ozone Levels (ppb)"
)

> abline(a=0, b=1, lty="dotted")
```
A Multiplicative Relationship

The model “stamford = \( b \times \text{yonkers} \)” seems to explain the relationship. What is the value of \( b \)?

We can find out by averaging the ratios of the quantiles.

```r
> y = yonkers
> s = stamford
> n = max(length(y), length(s))
> mean(quantile(s, seq(0, 1, length = n))/
    quantile(y, seq(0, 1, length = n)))
[1] 1.589835
```

The values in Stamford are about 1.6 times those in Yonkers.
An Alternative Procedure

A alternative way to proceed here is to work with the logs of the data values. This has the advantage of turning multiplication into addition.
Investigating Further . . .

The distance between the two lines is about .2. Since

$$10^{0.2} = 1.584893$$

we come to same conclusion this way.
Theoretical Quantile Quantile Plots

- Quantile-quantile plots can be used to compare the distributions of two sets of numbers.
- They can also be used to compare the distributions of one set of values with some theoretical distribution.
- Most commonly, the yardstick distribution is the standard normal distribution:
  \[ P[X \leq x] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-t^2/2} \, dt \]
- If the values being plotted resemble a sample from a normal distribution, they will lie on a straight line with intercept equal to the mean of the values and slope equal to the standard deviation.
1 R Functions

- The function `qqnorm` produces a basic Q-Q plot comparing a set of values with the normal distribution.

- The function `qqline` adds a straight line to the plot. The line passes through the point defined by the lower quartiles and the point defined by the upper quartiles.

```r
> qqnorm(rain.nyc, 
        main = "New York Precipitation")
> qqline(rain.nyc)
```
2 Deviations From Normality

- The NYC rainfall plot shows a systematic deviation from normality.

- Detecting such deviations is important because many statistical techniques depend on the data they are applied to having an approximately normal distribution.

- Note: The importance of normality is often overstated in elementary statistics courses. The NYC rainfall would be fine to use for most normally based statistical techniques.
Some Departures from Normality

(a) Normally Distributed  (b) Heavy Tails  (c) Light Tails
(d) Skewed to the Left  (e) Skewed to the Right  (f) Separate Clusters
Distribution Symmetry

- Suppose we have a collection of values $x_1, \ldots, x_n$. We will say that the values are symmetrically distributed if their quantile function satisfies:

  $Q(.5) - Q(p) = Q(1 - p) - Q(0.5), \quad \text{for } 0 < p < .5.$

- This says that the $p$th quantile is the same distance below the median as the $(1 - p)$th quantile is above it.

- When a set of values is “close” to normally distributed, a normal Q-Q plot can help to detect departures from symmetry,
A Symmetry Plot

- The obvious way to check the symmetry of a set of numbers is to plot the values $Q(1 - p_1), \ldots, Q(1 - p_{n/2})$ against the values of $Q(p_1), \ldots, Q(p_{n/2})$.

- If the plotted points fall on the line $y = x$, then $x_1, \ldots, x_n$ are symmetrically distributed.

- There is no built-in R function which produces symmetry plots, but it is very easy to create such a plot.
R Code

```r
symplot = function(x) {
  n = length(x)
  n2 = n %/% 2
  sx = sort(x)
  mx = median(x)
  plot(mx - sx[1:n2], rev(sx)[1:n2] - mx,
       xlab = "Distance Below Median",
       ylab = "Distance Above Median")
  abline(a = 0, b = 1, lty = "dotted")
}

symplot(rain.nyc)
```
Transforming to Symmetry

- There appears to be evidence of lack of symmetry in the symmetry plot.

- The upper quantiles of the distribution are further from the median than the corresponding lower quartiles.

- This indicates that the distribution of values is skewed to the right.

- It can sometimes be useful to transform skewed distributions to more symmetric ones. Transformations which can be used to do this are: square roots, cube and other roots, logarithms and reciprocals.
Transforming to Symmetry

- In the case of the rainfall data, it is hard to find a transformation which makes the distribution more symmetric.

- This is because of the internal clustering present in the values.

- Negative reciprocals do a fairly good job.

```r
> symplot(-1/rain.nyc)
```
Sample Size Considerations

- Both normal Q-Q plots and symmetry plots require large sample sizes to reliably represent the population being sampled.

- This is especially true for symmetry plots.

- Sample sizes of at least 1000 are desirable, although the plots do tend to get used on much smaller sample sizes.

- Running the command below repeatedly can show just how unstable the plots are with smaller sample sizes.

  ```r
  > symplot(rnorm(100))
  ```
Stability of QQ Plots

- Elementary statistics courses often recommend using normal qq plots to assess normality.

- They don’t tend to explain that qq plots are very variable, especially in the tails.

- Unless the sample size is larger than 1000, the plots cannot really be trusted when judging normality.
Code: Confidence Bounds by Simulation

```r
nrep = 1000
n = 100
x = qnorm(1:n/(n+1))
y = matrix(rnorm(nrep * n), nc = n)
for(i in 1:nrep)
    y[i,] = sort(y[i,])
y95 = apply(y, 2, quantile, c(.025, .975))
plot(x, x, ylim = range(y95), type = "n",
    xlab = "Theoretical Quantiles",
    ylab = "95% Bounds on Observed Quantiles",
    main = paste("Sample Size =", p))
polygon(c(x, rev(x)), c(y95[1,], rev(y95[2,])),
    col = "grey")
```