In the other category, model-dependent statistics, we lump the whole subject of fitting data to a theory, parameter estimation, least-squares fits, and so on. Those subjects are introduced in Chapter 15.

Section 14.1 deals with so-called *measures of central tendency*, the moments of a distribution, the median and mode. In §14.2 we learn to test whether different data sets are drawn from distributions with different values of these measures of central tendency. This leads naturally, in §14.3, to the more general question of whether two distributions can be shown to be (significantly) different.

In §14.4–§14.7, we deal with *measures of association* for two distributions. We want to determine whether two variables are "correlated" or "dependent" on one another. If they are, we want to characterize the degree of correlation in some simple ways. The distinction between parametric and nonparametric (rank) methods is emphasized.

Section 14.8 introduces the concept of data smoothing, and discusses the particular case of Savitzky-Golay smoothing filters.

This chapter draws mathematically on the material on special functions that was presented in Chapter 6, especially §6.1–§6.4. You may wish, at this point, to review those sections.

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14.1 Moments of a Distribution: Mean, Variance, Skewness, and So Forth

When a set of values has a sufficiently strong central tendency, that is, a tendency to cluster around some particular value, then it may be useful to characterize the set by a few numbers that are related to its *moments*, the sums of integer powers of the values.

Best known is the *mean* of the values $x_1, \ldots, x_N$,

$$\overline{x} = \frac{1}{N} \sum_{j=1}^{N} x_j \tag{14.1.1}$$

which estimates the value around which central clustering occurs. Note the use of an overbar to denote the mean; angle brackets are an equally common notation, e.g., $\langle x \rangle$. You should be aware that the mean is not the only available estimator of this quantity, nor is it necessarily the best one. For values drawn from a probability distribution with very broad "tails," the mean may converge poorly, or not at all, as the number of sampled points is increased. Alternative estimators, the *median* and the *mode*, are mentioned at the end of this section.

Having characterized a distribution's central value, one conventionally next characterizes its "width" or "variability" around that value. Here again, more than one measure is available. Most common is the *variance*,

$$\mathrm{Var}(x_1 \dots x_N) = \frac{1}{N-1} \sum_{j=1}^{N} (x_j - \overline{x})^2 \tag{14.1.2}$$

or its square root, the *standard deviation*,

$$\sigma(x_1 \dots x_N) = \sqrt{\mathrm{Var}(x_1 \dots x_N)} \tag{14.1.3}$$

Equation (14.1.2) estimates the mean squared deviation of x from its mean value. There is a long story about why the denominator of (14.1.2) is $N-1$ instead of N. If you have never heard that story, you may consult any good statistics text. Here we will be content to note that the $N-1$ *should* be changed to N if you are ever in the situation of measuring the variance of a distribution whose mean $\overline{x}$ is known *a priori* rather than being estimated from the data. (We might also comment that if the difference between N and $N-1$ ever matters to you, then you are probably up to no good anyway — e.g., trying to substantiate a questionable hypothesis with marginal data.)

As the mean depends on the first moment of the data, so do the variance and standard deviation depend on the second moment. It is not uncommon, in real life, to be dealing with a distribution whose second moment does not exist (i.e., is infinite). In this case, the variance or standard deviation is useless as a measure of the data's width around its central value: The values obtained from equations (14.1.2) or (14.1.3) will not converge with increased numbers of points, nor show any consistency from data set to data set drawn from the same distribution. This can occur even when the width of the peak looks, by eye, perfectly finite. A more robust estimator of the width is the *average deviation* or *mean absolute deviation*, defined by

$$\mathrm{ADev}(x_1 \dots x_N) = \frac{1}{N} \sum_{j=1}^{N} |x_j - \overline{x}| \tag{14.1.4}$$

One often substitutes the sample median x_{med} for $\overline{x}$ in equation (14.1.4). For any fixed sample, the median in fact minimizes the mean absolute deviation.

Statisticians have historically sniffed at the use of (14.1.4) instead of (14.1.2), since the absolute value brackets in (14.1.4) are "nonanalytic" and make theorem-proving difficult. In recent years, however, the fashion has changed, and the subject of *robust estimation* (meaning, estimation for broad distributions with significant numbers of "outlier" points) has become a popular and important one. Higher moments, or statistics involving higher powers of the input data, are almost always less robust than lower moments or statistics that involve only linear sums or (the lowest moment of all) counting.

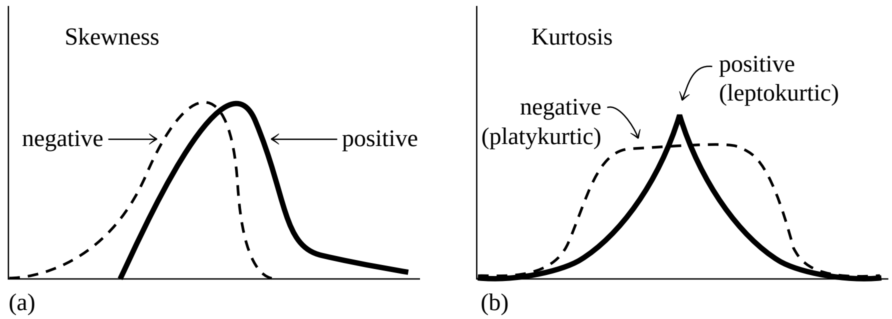

Figure 14.1.1. Distributions whose third and fourth moments are significantly different from a normal (Gaussian) distribution. (a) Skewness or third moment. (b) Kurtosis or fourth moment.

That being the case, the *skewness* or *third moment*, and the *kurtosis* or *fourth moment* should be used with caution or, better yet, not at all.

The skewness characterizes the degree of asymmetry of a distribution around its mean. While the mean, standard deviation, and average deviation are *dimensional* quantities, that is, have the same units as the measured quantities x_j, the skewness is conventionally defined in such a way as to make it *nondimensional*. It is a pure number that characterizes only the shape of the distribution. The usual definition is

$$\text{Skew}(x_1 \dots x_N) = \frac{1}{N}\sum_{j=1}^{N}\left[\frac{x_j - \overline{x}}{\sigma}\right]^3 \tag{14.1.5}$$

where $\sigma = \sigma(x_1 \dots x_N)$ is the distribution's standard deviation (14.1.3). A positive value of skewness signifies a distribution with an asymmetric tail extending out towards more positive x; a negative value signifies a distribution whose tail extends out towards more negative x (see Figure 14.1.1).

Of course, any set of N measured values is likely to give a nonzero value for (14.1.5), even if the underlying distribution is in fact symmetrical (has zero skewness). For (14.1.5) to be meaningful, we need to have some idea of *its* standard deviation as an estimator of the skewness of the underlying distribution. Unfortunately, that depends on the shape of the underlying distribution, and rather critically on its tails! For the idealized case of a normal (Gaussian) distribution, the standard deviation of (14.1.5) is approximately $\sqrt{15/N}$. In real life it is good practice to believe in skewnesses only when they are several or many times as large as this.

The kurtosis is also a nondimensional quantity. It measures the relative peakedness or flatness of a distribution. Relative to what? A normal distribution, what else! A distribution with positive kurtosis is termed *leptokurtic*; the outline of the Matterhorn is an example. A distribution with negative kurtosis is termed *platykurtic*; the outline of a loaf of bread is an example. (See Figure 14.1.1.) And, as you no doubt expect, an in-between distribution is termed *mesokurtic*.

The conventional definition of the kurtosis is

$$\text{Kurt}(x_1 \dots x_N) = \left\{\frac{1}{N}\sum_{j=1}^{N}\left[\frac{x_j - \overline{x}}{\sigma}\right]^4\right\} - 3 \tag{14.1.6}$$

where the -3 term makes the value zero for a normal distribution.

The standard deviation of (14.1.6) as an estimator of the kurtosis of an underlying normal distribution is $\sqrt{96/N}$. However, the kurtosis depends on such a high moment that there are many real-life distributions for which the standard deviation of (14.1.6) as an estimator is effectively infinite.

Calculation of the quantities defined in this section is perfectly straightforward. Many textbooks use the binomial theorem to expand out the definitions into sums of various powers of the data, e.g., the familiar

$$\text{Var}(x_1 \dots x_N) = \frac{1}{N-1}\left[\left(\sum_{j=1}^{N} x_j^2\right) - N\overline{x}^2\right] \approx \overline{x^2} - \overline{x}^2 \tag{14.1.7}$$

but this can magnify the roundoff error by a large factor and is generally unjustifiable in terms of computing speed. A clever way to minimize roundoff error, especially for large samples, is to use the *corrected two-pass algorithm* [1]: First calculate $\overline{x}$, then calculate $\text{Var}(x_1 \dots x_N)$ by

$$\text{Var}(x_1 \dots x_N) = \frac{1}{N-1}\left\{\sum_{j=1}^{N}(x_j - \overline{x})^2 - \frac{1}{N}\left[\sum_{j=1}^{N}(x_j - \overline{x})\right]^2\right\} \tag{14.1.8}$$

The second sum would be zero if $\overline{x}$ were exact, but otherwise it does a good job of correcting the roundoff error in the first term.

```
SUBROUTINE moment(data,n,ave,adev,sdev,var,skew,curt)
INTEGER n
REAL adev,ave,curt,sdev,skew,var,data(n)
    Given an array of data(1:n), this routine returns its mean ave, average deviation adev,
    standard deviation sdev, variance var, skewness skew, and kurtosis curt.
INTEGER j
REAL p,s,ep
if(n.le.1)pause 'n must be at least 2 in moment'
s=0.                          First pass to get the mean.
do 11 j=1,n
    s=s+data(j)
enddo 11
ave=s/n
adev=0.                       Second pass to get the first (absolute), second, third, and fourth
var=0.                            moments of the deviation from the mean.
skew=0.
curt=0.
ep=0.
do 12 j=1,n
    s=data(j)-ave
    ep=ep+s
    adev=adev+abs(s)
    p=s*s
    var=var+p
    p=p*s
    skew=skew+p
    p=p*s
    curt=curt+p
enddo 12
adev=adev/n                   Put the pieces together according to the conventional definitions.
var=(var-ep**2/n)/(n-1)           Corrected two-pass formula.
sdev=sqrt(var)
```

```
if(var.ne.0.)then
    skew=skew/(n*sdev**3)
    curt=curt/(n*var**2)-3.
else
    pause 'no skew or kurtosis when zero variance in moment'
endif
return
END
```

Semi-Invariants

The mean and variance of independent random variables are additive: If x and y are drawn independently from two, possibly different, probability distributions, then

$$\overline{(x+y)} = \overline{x} + \overline{y} \qquad \text{Var}(x+y) = \text{Var}(x) + \text{Var}(x) \tag{14.1.9}$$

Higher moments are not, in general, additive. However, certain combinations of them, called *semi-invariants*, are in fact additive. If the centered moments of a distribution are denoted M_k,

$$M_k \equiv \left\langle (x_i - \overline{x})^k \right\rangle \tag{14.1.10}$$

so that, e.g., $M_2 = \text{Var}(x)$, then the first few semi-invariants, denoted I_k are given by

$$\begin{aligned} &I_2 = M_2 \qquad I_3 = M_3 \qquad I_4 = M_4 - 3M_2^2 \\ &I_5 = M_5 - 10M_2M_3 \qquad I_6 = M_6 - 15M_2M_4 - 10M_3^2 + 30M_2^3 \end{aligned} \tag{14.1.11}$$

Notice that the skewness and kurtosis, equations (14.1.5) and (14.1.6) are simple powers of the semi-invariants,

$$\text{Skew}(x) = I_3/I_2^{3/2} \qquad \text{Kurt}(x) = I_4/I_2^2 \tag{14.1.12}$$

A Gaussian distribution has all its semi-invariants higher than I_2 equal to zero. A Poisson distribution has all of its semi-invariants equal to its mean. For more details, see [2].

Median and Mode

The median of a probability distribution function $p(x)$ is the value x_{med} for which larger and smaller values of x are equally probable:

$$\int_{-\infty}^{x_{\text{med}}} p(x)\,dx = \frac{1}{2} = \int_{x_{\text{med}}}^{\infty} p(x)\,dx \tag{14.1.13}$$

The median of a distribution is estimated from a sample of values $x_1, \ldots, x_N$ by finding that value x_i which has equal numbers of values above it and below it. Of course, this is not possible when N is even. In that case it is conventional to estimate the median as the mean of the unique *two* central values. If the values x_j $j = 1, \ldots, N$ are sorted into ascending (or, for that matter, descending) order, then the formula for the median is

$$x_{\text{med}} = \begin{cases} x_{(N+1)/2}, & N \text{ odd} \\ \frac{1}{2}(x_{N/2} + x_{(N/2)+1}), & N \text{ even} \end{cases} \tag{14.1.14}$$

If a distribution has a strong central tendency, so that most of its area is under a single peak, then the median is an estimator of the central value. It is a more robust estimator than the mean is: The median fails as an estimator only if the area in the tails is large, while the mean fails if the first moment of the tails is large; it is easy to construct examples where the first moment of the tails is large even though their area is negligible.

To find the median of a set of values, one can proceed by sorting the set and then applying (14.1.14). This is a process of order $N \log N$. You might rightly think that this is wasteful, since it yields much more information than just the median (e.g., the upper and lower quartile points, the deciles, etc.). In fact, we saw in §8.5 that the element $x_{(N+1)/2}$ can be located in of order N operations. Consult that section for routines.

The *mode* of a probability distribution function $p(x)$ is the value of x where it takes on a maximum value. The mode is useful primarily when there is a single, sharp maximum, in which case it estimates the central value. Occasionally, a distribution will be *bimodal*, with two relative maxima; then one may wish to know the two modes individually. Note that, in such cases, the mean and median are not very useful, since they will give only a "compromise" value between the two peaks.

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Chan, T.F., Golub, G.H., and LeVeque, R.J. 1983, *American Statistician*, vol. 37, pp. 242–247. [1]

Cramér, H. 1946, *Mathematical Methods of Statistics* (Princeton: Princeton University Press), §15.10. [2]

14.2 Do Two Distributions Have the Same Means or Variances?

Not uncommonly we want to know whether two distributions have the same mean. For example, a first set of measured values may have been gathered before some event, a second set after it. We want to know whether the event, a "treatment" or a "change in a control parameter," made a difference.

Our first thought is to ask "how many standard deviations" one sample mean is from the other. That number may in fact be a useful thing to know. It does relate to the strength or "importance" of a difference of means *if that difference is genuine*. However, by itself, it says nothing about whether the difference *is* genuine, that is, statistically significant. A difference of means can be very small compared to the standard deviation, and yet very significant, if the number of data points is large. Conversely, a difference may be moderately large but not significant, if the data