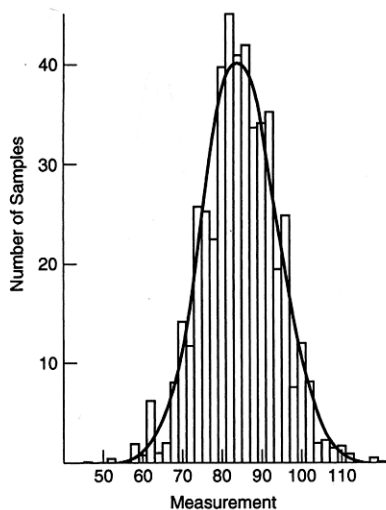


Appendix B

Treatment of Data



Bar graph and standard error curve for the multiple analysis of a sample.

Confidence in a scientific theory depends on the reliability of the experimental data on which the theory is based. For this reason, a scientist must be concerned about the quality of the data he or she collects. Of prime importance is the **accuracy** of the data—how closely the measured values lie to the true values.

To obtain accurate data we must use instruments that are carefully calibrated with known standards of measurement. A balance, for example, is periodically calibrated using very accurately known masses to ensure proper adjustment. But even with accurate measuring devices we find that repeated measurements of the same quantity produce slightly different numerical values. These errors are called **systematic errors**. One reason for these errors is that we are often forced to estimate the last digit in the measurement, the last significant figure of the measurement (see Laboratory Data on page 5). Measuring the volume of a liquid in a graduated cylinder to the nearest tenth of a milliliter, for example, requires an estimate of the tenths place. If you measure a series of samples of, say, 10.2 mL, the actual volumes would fluctuate somewhat around 10.2 mL; some would be slightly larger and some slightly smaller. The measurement has three significant figures. These systematic errors are unavoidable and result from natural difficulties in judging volumes with this measuring device.

All experimental measurements are subject to these systematic errors. Because of this, scientists are very concerned about the **precision** of their data—that is, how closely the measured values lie to one another. These errors are called **random errors**. When the random errors are small, all measurements are close to one another and we say the data are of high precision. When the random errors are large, the values cover a much broader range and the data are of low precision. *Generally*, data of high precision are also of high accuracy, especially if the measuring device is properly calibrated. Remember that all measurements are to be expressed with the correct number of significant figures, the number being reflective of the measuring instrument.

Methods of analyzing experimental data, based on statistics, provide information on the degree of precision of the measured values. Applying the methods is simple, as you will see, but to understand their significance, examine briefly the **standard error curve** (Figure B.1a).

If we make a large number of measurements of a quantity, the values would fluctuate about the average value (also called the mean value). The **average, or mean, value** is obtained by dividing the sum of all the measured values by the total number

Average (or Mean) Value, \bar{x}

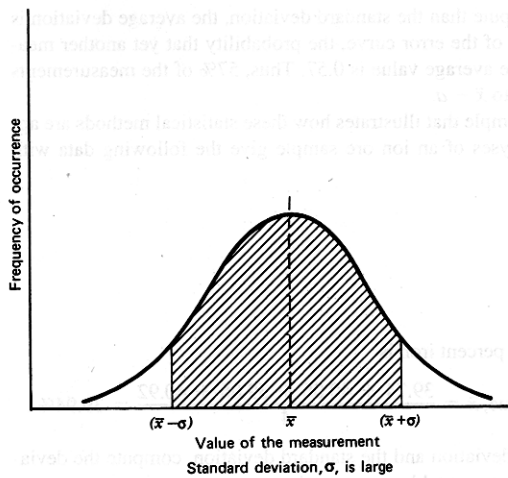


Figure B.2b Data set with a large standard deviation.

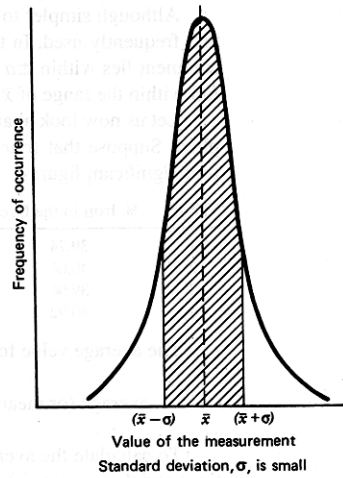


Figure B.2c Data set with a small standard deviation.

Statistics gives us methods for computing quantities that tell us about the width of the error curve for our data and, therefore, about the precision of the data, even when the amount of data is relatively small. One of the most important statistical measures of precision is the **standard deviation**, σ (Greek letter sigma). To calculate the standard deviation, we first compute the average value, \bar{x} . The next step is to compute the *deviation*, d , from the average value for *each* measurement—the difference between the average and each measured value:

$$\text{deviation, } d_i = \bar{x} - x_i \quad (\text{B.2})$$

d_i is the deviation for the measured value, x_i . The standard deviation σ is obtained by squaring these deviations, adding the squared values together, dividing this sum by $n - 1$ (where n is the number of measurements), and then taking the square root.

$$\text{standard deviation } \sigma = \sqrt{\frac{d_1^2 + d_2^2 + \dots + d_n^2}{(n - 1)}} \quad (\text{B.3})$$

The standard deviation means that if we make yet another measurement, the probability that its value will lie within $\pm\sigma$ of the average value is 0.68. In other words, 68% of the measurements lie within $\pm\sigma$ of the average value (i.e., within the range $\bar{x} - \sigma$ to $\bar{x} + \sigma$). On the error curve in Figure B.2a, this represents the measurements falling within the shaded area. If we obtain a large calculated σ from a set of measured values, it means that the error curve for our data is broad and the precision of the data is low (Figure B.2b); a small value of σ for a set of data means that the error curve is narrow and the precision of the data is high (see Figure B.2c). Thus, σ is a statistical measure of the precision of the data.

Standard Deviation, σ

Another quantity that serves as a statistical measure of precision is the **average deviation**, a . To compute it we simply add all the deviations (Equation B.2) together, take their absolute values, and then divide this sum by the number of measurements.

$$\text{average deviation, } a = \frac{|d_1| + |d_2| + |d_3| + \dots + |d_n|}{n} \quad (\text{B.4})$$

Average Deviation, a

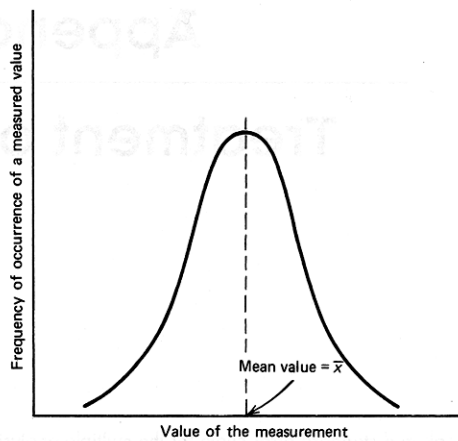


Figure B.1a The standard error curve.

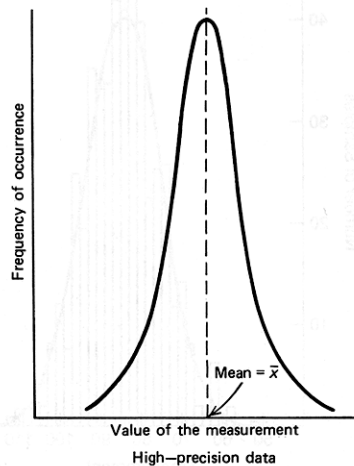


Figure B.1b Error curve for high-precision data.

of values. If x_1, x_2, x_3 , etc., are measured values, and there are n of them, then the average value, \bar{x} , is computed as

$$\text{average (or mean) value, } \bar{x} = \frac{x_1 + x_2 + x_3 + \cdots + x_n}{n} \quad (\text{B.1})$$

Most values lie close to the average, but some lie further away. If we plot the frequency with which a measured value occurs versus the value of the measurement, we obtain the curve in Figure B.1a. When the random errors are small (high-precision data, Figure B.1b), the curve is very narrow and the peak is sharp. When the random errors are large (low-precision data, Figure B.1c), the data are more “spread out,” and the error curve is broader and less sharp.

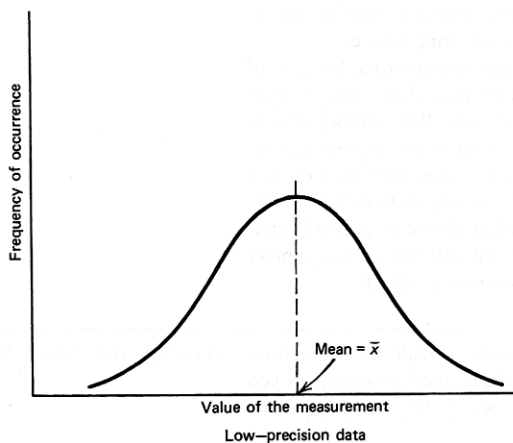


Figure B.1c Error curve for low-precision data.

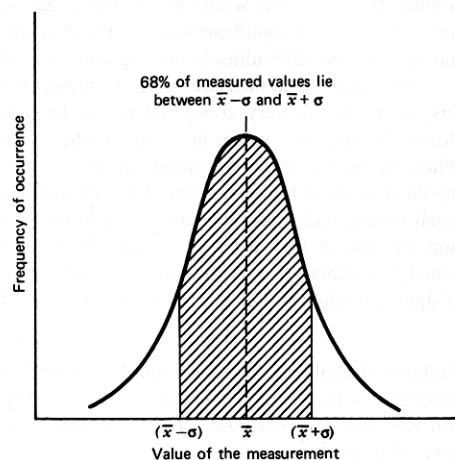


Figure B.2a Relationship of the standard deviation to the error curve.

Although simpler to compute than the standard deviation, the average deviation is less frequently used. In terms of the error curve, the probability that yet another measurement lies within $\pm a$ of the average value is 0.57. Thus, 57% of the measurements fall within the range of $\bar{x} + a$ to $\bar{x} - a$.

Let us now look at an example that illustrates how these statistical methods are applied. Suppose that four analyses of an iron ore sample give the following data with four significant figures:

Trial	% Iron in the Ore
1	39.74
2	40.06
3	39.06
4	40.92

The average value for the percent iron is

$$\text{average (or mean) value, } \bar{x} = \frac{39.74 + 40.06 + 39.06 + 40.92}{4} = 39.94\%$$

To calculate the average deviation and the standard deviation, compute the deviations and their squares. Let's set up a table.

Trial	Measured Values	$d_i = \bar{x} - x_i$	$ d_i $	d_i^2
1	39.74	0.20	0.20	0.040
2	40.06	-0.12	0.12	0.014
3	39.06	0.88	0.88	0.77
4	40.92	-0.98	0.98	0.96
	$\bar{x} = 39.94$		Sum = 2.18	Sum = 1.78

$$\text{average deviation, } a = \frac{2.18}{4} = 0.54$$

$$\text{standard deviation, } \sigma = \sqrt{\frac{1.78}{4 - 1}} = 0.77$$

If we wish to express the precision of our analysis in terms of an average deviation, the percent iron is reported as $39.94 \pm 0.54\%$; this means that 57% of all subsequent analyses of the iron ore sample should be in the range of $39.94 \pm 0.54\%$ iron. If we choose to express our precision in terms of a standard deviation, the percent iron is reported as $39.94 \pm 0.77\%$, meaning that 68% of all subsequent analyses should be in the range of $39.94 \pm 0.77\%$ iron.

Percent Error

Scientists check the *accuracy* of their measurements by comparing their results with values that are well established and are considered "accepted values." Many reference books, such as the Chemical Rubber Company's (CRC) *Handbook of Chemistry and Physics*, are used to check a result against an accepted value. To report the percent error in *your* result, take the absolute value of the difference between your value and the accepted value, divide this difference by the accepted value, and then multiply by 100. Taking x to be your measured value and y to be the accepted value,

$$\text{percent error} = \frac{|x - y|}{y} \times 100$$