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# Appendix

## Reproducibility and Repeatibility

Reproducibility may be described as a comparison of the precision between two methods or two laboratories or two analysts (9). Repeatibility may be described as a comparison of the precision by same method or same laboratory or same analyst.

## Mean

$$\overline{X} = \frac{X_1 + X_2 + ... + X_n}{n}$$

n = numbers of measurements



## Standard Deviation

The standard deviation ($\sigma$) of an infinite set of experimental data is theoretically the square root of the mean of the squares of the difference between the individual measured values, $X_i$, and the mean of the infinite number of measurements, $\mu$ (which should represent the "true" value) (10).

$$s = \sqrt{\frac{\sum (x_i - \bar{x})^2}{(N-1)}}$$

This equation holds strictly only as $N \rightarrow \infty$. In practice, we must calculate the individual deviations from the mean of a limited number of measurements, Mean (X), in which it is anticipated that $X \rightarrow \mu$.

For a set of N measurements, it is possible to calculate N independently variable deviations from some reference number. But if reference number chosen is mean (X), the sum of individual deviations must necessarily add up to zero, and so values of N-1 deviations are adequate to define the N th.

Estimated standard deviation (S.D.) of a finite set of experimental data (generally $N < 30$) more nearly approximates $\sigma$ if the number of degrees of freedom is substituted for N (N-1 adjusts for the difference between X and $\mu$).

$$\text{S.D.} = \sqrt{\frac{(X_i - \overline{X})^2}{(N-1)}}$$

**<u>Relative Standard Deviation (RSD.)</u>**

$$\text{RSD.} = \frac{\text{S.D.}}{\overline{X}}$$

## Standard Error

Standard Error (S.E.) is referred to the standard deviation of the mean.

$$S.E. = \frac{S.D.}{\sqrt{N}}$$

## Correlation Coefficient

The correlation coefficient (r) is used as a measure of the correlation between two variables. When variables X and Y are correlated rather than being functionally related (i.e., are not directly dependent upon one another), we do not speak of the "best" Y value corresponding to a given X value, but only of the most "probable" value. The closer the observed values are to the most probable values, the more definite is the relationship between X and Y. This postulate is the basis for various numerical measures of the degree of correlation.

The **Pearson Correlation Coefficient** is one of the most convenient to calculate. This is given by

$$r = \sum \frac{(X_i - \overline{X})(Y_i - \overline{Y})}{nS_xS_y}$$

r = correlation coefficient

n = number of observations

$S_x$, $S_y$ = standard deviation of X and Y, respectively

$X_i$, $Y_i$ = individual values of the variables X and Y, respectively

X, Y = mean of the variables X and Y, respectively

The use of differences in the calculation is frequently cumbersome, and the equation can be transformed to a more convenient form:

$$r = \frac{n\sum X_iY_i - \sum X_i \sum Y_i}{\sqrt{[n\sum X_i^2 - (\sum X_i)^2][n\sum Y_i^2 - (\sum Y_i)^2]}}$$

The maximum value of r is 1. When this occurs, there is exact correlation between the two variables. When the value of r is zero (this occurs when XY is equal to zero), there is complete independence of the variables. The minimum value of r is -1. A negative correlation coefficient indicates that the assumed dependence is to opposite to what exists and is therefore a positive coefficient for the reversed relation.

# VITA

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