Evaluation of analytical data

In the analytical Chemistry there is different methods used in the analysis, so one have to choos the method which it used for definit analysis.

For example, the methods for determining the concentration of lead (Pb) in drinking water, insoluble lead salts such as $PbSO_4$ and $PbCrO_4$ can form the basis for (gravimetric method).

In the other hand Lead forms several soluble complexes that can be used it a (complexation titrimetric method) or, if the complexes are highly absorbing in a (spectrophotometric method). The availability of multiple oxidation state (Pb, Pb^{+2}, Pb^{+4}) makes

coulometric, potentiometric and voltammetric methods feasible.

However in choosing a method consideration is given to some or all the following design criteria:

1- accuracy, 2- precision,
3- sensitivity, 4- selectivity, 5- robustness
6- scale of operation, 7- analysis time
8- availability of equipment, 9- cost (lower cost is better).

It is important to notice that the measurements in the Laboratory for the analysis might be exposed to (uncertainity). To avoid this uncertainty it must be make repitition to the measurements. Therefor it is usfull to discriminate between the accuracy and precision.

Accuracy: indicate the closeness of the measurements to the true or accepted value and is expressed by the error.

For the relative errors:

$$Er = \frac{\text{obtained result} - \text{expected result}}{\text{expected result}} \times 100$$

For absolute errors:

$$E = X_i - X_t$$

X_i is the value obtained

X_t is the true or accepted value.

Precision: describe the agreement among several results obtained in the same way.

Note: The true value is difficult to determind so that, use the (most probable value) as a true value and always using the (average value) of the measurements as a true value.

Sources of errors

Determinat errors (systematic errors)

1- Instrumental errors
2- Methodic errors
3- operative errors
4- Personal errors

Indeterminant errors (Random errors)

- depend on the probability Laws
- (unknown the sources)

The determinant errors classified by the two groups of errors

Constant errors

independant on the volume or quantity of the sample

proportional errors

depend on the volume and quantity of the sample

Sensitivity : A measure of a method's ability to distinguish between two samples reported as the change in signal per unit change in the amount of analyte.

Selectivity: A measure of a method's freedom from interferences as defined by the method's selectivity coefficient.

Therefore using one of the statistical methods is necessary to make accuracy of the results. One of these methods is the determination of standard deviation.

① Mean: $(\bar{X})$ is the average of a set of data (X).

$$\bar{X} = \frac{\sum X_1 + X_2 + \cdots X_n}{n}$$

n: is the number of values, $X_1, X_2, X_3 \cdots X_n$

② Range: is the numerical difference between the Largest and smallest values in a data set.

③ Median: is the value for aset of ordered data for which half of the data is larger in value and

half is smaller in value (X_{n+1}) When the number of value ($2n+1$) or is $\frac{1}{2}(X_n + X_{n+1})$ When the number of values is ($2n$).

④ variance : is the squar of the standard deviation (s^2).

⑤ standard deviation : A statistical measure of the «average» deviation «spread» of data from the data's mean value (s).

⑥ Deviation : (d) the difference between value of a set data X_n and the mean ($\bar{X}$).

$$d = X_n - \bar{X}$$

⑦ Average deviation : $\bar{d}$. is the sum of the deviation's value devided by the number of values (n)

⑧ standard deviation = $S = \sqrt{\frac{\sum(X_i - \bar{X})^2}{n-1}}$

$$= \sqrt{\frac{\sum d^2}{n-1}}$$

X_i is a value measured

$\bar{X}$ is a mean

$$\text{Variance} \Rightarrow S^2 = \frac{\sum (X_i - \bar{X})^2}{n-1}$$

$$\text{Average deviation} \Rightarrow \bar{d} = \frac{\sum d}{n} = \frac{\sum X_i - \bar{X}}{n}$$

$$\text{Variance Coefficient} = \frac{S}{\bar{X}} \times 100$$

Example: in an experiment of liquid volume measurements of 6 students as follow.

24.32, 24.38, 24.45, 24.29, 24.3, 24.31 Cm^3

Calculate the mean, Range, median, standard deviation, and variance for the measurements.

$X_i (cm^3)$	Deviation $d (cm^3)$	squard $d^2 (cm^3)^2$
24.32	− 0.022	
24.38	+ 0.038	
24.45	+ 0.108	
24.29	− 0.052	
24.30	− 0.042	
24.31	− 0.032	

1) $\text{Mean} = \bar{X} = \frac{\sum X_i}{n} = \frac{24.32 + 24.38 + 24.45 + 24.29 + 24.30 + 24.31}{6}$

$$\therefore \quad \bar{X} = \frac{145.05}{6} = 24.34 \text{ cm}^3$$

② Range $= 24.45 - 24.29 = 0.16 \text{ cm}^3$

③ Median $= 24.29, 24.30, 24.31, 24.32, 24.38, 24.45$

$$= \frac{1}{2}(X_n + X_{n+1})$$

$$= \frac{1}{2}(24.31 + 24.32) = 24.315$$

④ standard deviation:

$$S = \sqrt{\frac{\sum(X_i - \bar{X})^2}{n-1}} = \sqrt{\frac{\sum d^2}{n-1}} \quad \text{(find it)}$$

⑤ Variance: $S^2 = \frac{\sum(X_i - \bar{X})^2}{n-1} = \frac{\sum d^2}{n-1}$ (find it)

Problems . Determine the Sd, median, Rang, Deviation, averag deviation and variance for the following numbers.

1- 7, 13, 16, 20, 23, 27, 29.

2- 25, 28, 7, 13, 16, 20, 18, 12