STATISTICS IN CHEMISTRY

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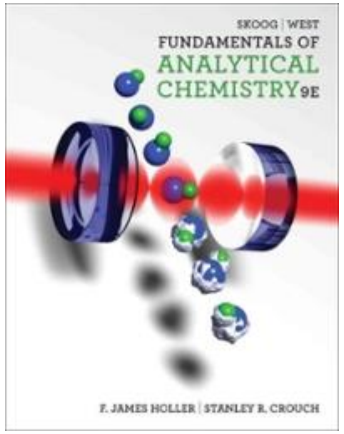
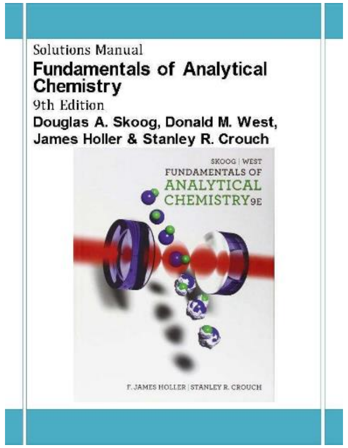


2.



1. Skoog DA, West DM, Holler FJ, Crouch SR. Fundamentals of Analytical Chemistry. Nelson Education; 2013.
2. Skoog DA, West DM, Holler FJ, Crouch SR. Solutions Manual of Fundamentals of Analytical Chemistry. Nelson Education; 2013.

Hypothesis testing, comparison of averages

Hypothesis testing

Hypothesis testing is often used in scientific studies to explain an observation. There are two different hypotheses. The first is the null hypothesis and the second is the alternative hypothesis. The null hypothesis is represented by H_0 and indicates that there is no significant difference between the magnitudes compared. It recognizes that numerical differences are the result of random errors. The alternative hypothesis is symbolized by H_a and assumes that there is a significant difference between the magnitudes compared and that the observed numerical difference is not solely caused by random errors, but that there are significant effects that lead to differentiation.

Hypotheses can be established in two different ways. In the unilateral hypothesis, whether one of the magnitudes compared is significantly larger than the other, the two- tailed hypothesis questions whether there is a significant difference between the magnitudes compared. In the bilateral hypothesis, the magnitudes compared can be larger or smaller than each other; in this test, it is not concerned with size or smallness, but only if there is a significant difference between them.

Generally, the following procedure is used in the hypothesis test:

* Null hypothesis (H_0) and alternative hypothesis (H_a) are stated.
* The relevant parameter is calculated (experimental parameter).
* The critical value of the relevant parameter is found in the table.
* If experimental parameter <critical parameter, Null hypothesis (H_0) is accepted, alternative hypothesis (H_a) is rejected.
* If the experimental parameter ≥ is the critical parameter, the Null hypothesis (H_0) is rejected and the alternative hypothesis (H_a) is accepted.

Comparison of the mean of the experiment with the known value

In the comparison of the mean of the experiment with the known value, it will be seen how to compare the value of μ_0 with the mean obtained from *N* experiments. The comparison can be made unilaterally or bilaterally.

The null hypothesis (H_0) and the alternative hypothesis (H_a) are established.

One-tailed hypothesis:

H_0: $\mu = \mu_0$

H_a: $\mu > \mu_0$ or H_a: $\mu < \mu_0$

Two- tailed hypothesis:

H_0: $\mu = \mu_0$

H_a: $\mu \neq \mu_0$

The relevant parameter is calculated (experimental parameter)

If σ is known;

$$z = \frac{\bar{x} - \mu_0}{\sigma/\sqrt{N}}$$

For small sample where σ value is unknown;

$$t = \frac{\bar{x} - \mu_0}{s/\sqrt{N}}$$

The critical value of the relevant parameter is found in the table.

The tables z and t are suitable for the two- tailed hypothesis test as in these notes.

To use these tables unilaterally, areas on both sides outside the forehead under the Gaussian curve are taken into account. At 95% confidence level, 2.5% area remains on both sides of the Gaussian curve. Accordingly, if a unilateral hypothesis test is to be performed at 95% confidence level, z or t values are found using a 90% confidence level with 5% area remaining on one side, ie 10% area on both sides.

If the experimental parameter < critical parameter;

$z < z_{crit}$ or $t < t_{crit}$

Null hypothesis (H_0) is accepted, alternative hypothesis (H_a) is rejected.

If the experimental parameter ≥ critical parameter;

$z \geq z_{crit}$ or $t \geq t_{crit}$

The null hypothesis (H_0) is rejected, the alternative hypothesis (H_a) is accepted.

Comparison of two experimental means

Since the analysis is generally performed with a small number of experiments, t statistic is used to compare the two test means. However, if a comparison is made with a large number of experiments, the z-statistic is used. Only the t statistic will be used here. If necessary, the z statistic can also be applied with appropriate modification.

The null hypothesis (H_0) and the alternative hypothesis (H_a) are established.

One-tailed hypothesis:
H_0: $\mu_1 = \mu_2$
H_a: $\mu_1 > \mu_2$ or H_a: $\mu_1 < \mu_2$

Two-tailed hypothesis:
H_0: $\mu_1 = \mu_2$
H_a: $\mu_1 \neq \mu_2$

The relevant parameter is calculated (experimental parameter).

$$t = \frac{|\bar{x}_1 - \bar{x}_2|}{s_b / \sqrt{\frac{N_1 + N_2}{N_1 \cdot N_2}}}$$

$$s_{pooled} = \sqrt{\frac{(N_1 - 1) \cdot s_1^2 + (N_2 - 1) \cdot s_2^2 + (N_3 - 1) \cdot s_3^2 + \cdots \ldots .}{N_1 + N_2 + N_3 + \cdots \ldots . - N_I}}$$

The critical value of the relevant parameter t is found in the table.

The t-table is suitable for the two-tailed hypothesis test as in these notes. To use this table unilaterally, areas on both sides outside the forehead under the Gaussian curve are taken into account. At 95% confidence level, 2.5% area remains on both sides of the Gaussian curve. Accordingly, if the unilateral hypothesis test is to be applied at 95% confidence level, t values are found using the 90% confidence level, where 5% area remains on one side, ie 10% area remains on both sides.

If experimental t parameter < critical t parameter that is; $t < t_{crit}$
Null hypothesis (H_0) is accepted, alternative hypothesis (H_a) is rejected.

If experimental t parameter is ≥ critical t parameter, ie; $t \geq t_{crit}$
The null hypothesis (H_0) is rejected, the alternative hypothesis (H_a) is accepted.