STATISTICS IN CHEMISTRY

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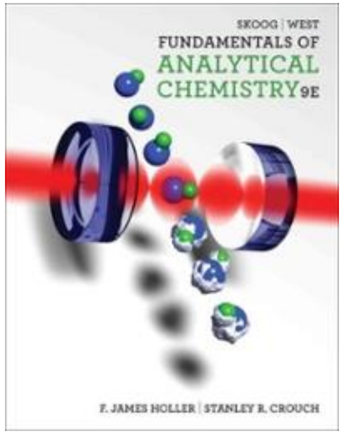
1.


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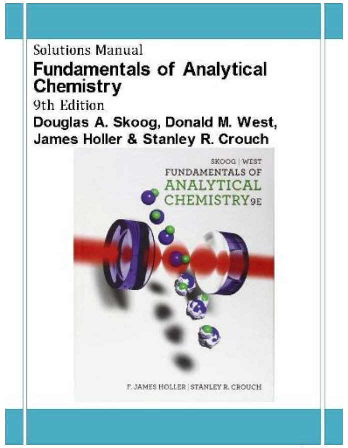

1. Skoog DA, West DM, Holler FJ, Crouch SR. Fundamentals of Analytical Chemistry. Nelson Education; 2013.
2. Skoog DA, West DM, Holler FJ, Crouch SR. Solutions Manual of Fundamentals of Analytical Chemistry. Nelson Education; 2013.

Processing and Evaluation of Statistical Data, Confidence Intervals

Confidence Levels, Confidence Intervals and Significance Tests

Confidence Intervals

In chemical analyzes, the actual average (σ) cannot be found with a small number of measurements. However, with the help of statistics, the range where the population mean (μ) can be determined at a certain probability level, with the sample mean obtained from a limited number of measurements ($\bar{x}$) at the center.

Confidence interval when σ is known or when s is near σ

The value σ can be known about a method based on past experience and experiments. In the previous section, it is stated that the areas under the Gaussian curve can be calculated by changing the z value at different intervals. Accordingly, the area under the Gaussian curve can be given as 68.3% when z is between (1 and +1). According to this; The confidence interval for 68 can be said to be in the range $\bar{x} \mp 1 \cdot \sigma$ with a probability of 68.3%. From here, the confidence interval for μ can be written as

Confidence Interval for $\mu = \bar{x} \mp z \cdot \sigma$

This equation gives the confidence interval obtained for a single measurement.

According to the sample mean obtained from N measurements, the confidence interval (CI) is calculated as follows:

CI for μ $= \bar{x} \mp \frac{z \cdot \sigma}{\sqrt{N}}$

The z value will be different according to the desired confidence level. This statistic is called z statistic.

Confidence level %	z
50	0,67
68	1,00
80	1,28
95	1,96
95,4	2,00
99,7	3,00
99,9	3,29

σ Confidence interval when unknown

If we do not have any information about σ based on previous experience, *t*-statistic is used to find the confidence interval somewhat similar to *z*-statistic. *t* value for a single measurement;

$$t = \frac{x - \mu}{s}$$

If t value for *N* measurements;

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

Equations are calculated. Accordingly, the confidence interval for the average of the *N* measurements ($\bar{x}$) can be calculated from the following equation.

Confidence Interval for μ :

$$\bar{x} \mp \frac{ts}{\sqrt{N}}$$

t values are given in the tables for different probability levels and different degrees of freedom

Degree of Freedom	80%	90%	95%	99%	99.9%
1	3.08	6.31	12.7	63.7	637
2	1.89	2.92	4.30	9.92	31.6
3	1.64	2.35	3.18	5.84	12.9
4	1.53	2.13	2.78	4.60	8.61
6	1.44	1.94	2.45	3.71	5.96
8	1.40	1.86	2.31	3.36	5.04
10	1.37	1.81	2.23	3.17	4.59
15	1.34	1.75	2.13	2.95	4.07
20	1.32	1.73	2.09	2.84	3.85
40	1.30	1.68	2.02	2.70	3.55
∞	1.28	1.64	1.96	2.58	3.29

If the line ∞ is taken into consideration in this table, it will be seen that t value becomes z values for the same probability levels.