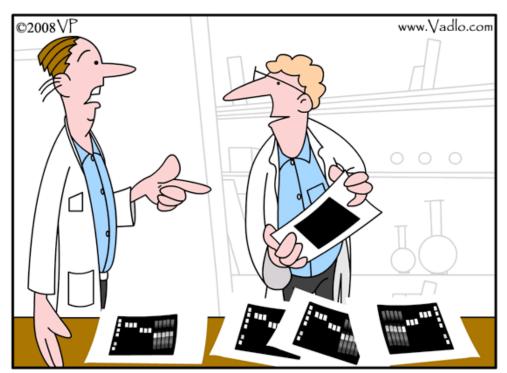
Other Statistical Calculations

- Comparison of Two Experimental Means
- Q-Test for the Rejection of Data Points
- Propagation of Errors



Robert Corn - Chem M3LC UC Irvine

Data don't make any sense, we will have to resort to statistics.

Comparison of Two Experimental Means

Used to determine whether two experimentally measured values are statistically different.

Experiment A: Experiment B:

Number of data points: N_A Number of data points: N_B

Mean: x_A Mean: x_B

Std. Dev: s_A Std. Dev: s_B

Are x_A and x_B statistically different?

i) Calculate the pooled standard deviation (s_P):

$$s_P = \sqrt{\frac{\sum_{i=1}^{N_A} (x_i - x_A)^2 + \sum_{j=1}^{N_B} (x_j - x_B)^2}{N_A + N_B - 2}}$$

Note that the total DOF is $N_A + N_B - 2$

Comparison of Two Experimental Means

Used to determine whether two experimentally measured values are statistically different.

ii) Calculate a t-value (t_{calc}) using the equation:

$$t_{calc} = \frac{|x_A - x_B|}{s_P} \sqrt{\frac{N_A N_B}{N_A + N_B}}$$

iii) Compare t_{calc} with the t-value in the 95% table for the total DOF (t_{table}):

If $t_{calc} > t_{table}$, then the two numbers are statistically different.

(95% Confidence Level)

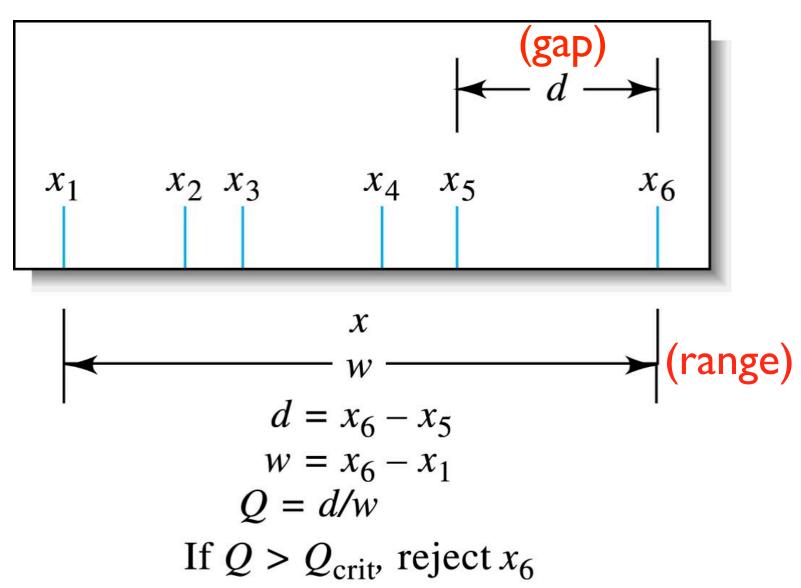
Q-Test for the Rejection of Data Points

Used to determine whether a data point can be rejected on the basis of determinate error.

$$Q = \frac{gap}{range}$$

Compare to the tabulated value of Q_{crit} reject if $Q > Q_{crit}$

Example of a Q-test:



© 2004 Thomson - Brooks/Cole

TABLE 7-5

Critical Values for the Rejection Quotient, Q*

 Q_{crit} (Reject if $Q > Q_{\text{crit}}$)

Number of Observations	90% Confidence	95% Confidence	99% Confidence
3	0.941	0.970	0.994
4	0.765	0.829	0.926
5	0.642	0.710	0.821
6	0.560	0.625	0.740
7	0.507	0.568	0.680
8	0.468	0.526	0.634
9	0.437	0.493	0.598
10	0.412	0.466	0.568

^{*}Reprinted with permission from D. B. Rorabacher, *Anal. Chem.*, **1991**, *63*, 139. Copyright 1991 American Chemical Society.

© 2004 Thomson - Brooks/Cole

At a 95% Confidence Level, Q must be greater than 0.625 to reject the data point.

Propagation of Errors

If you have multiple sources of error, you calculate the Standard Deviation using the method of "Propagation of Errors."

Propagation of Errors.

R. Corn - Chem M3LC.

Addition and Subtraction: sum of the squares of the absolute standard deviations:

$$y = a + b - c$$

$$s_y^2 = s_a^2 + s_b^2 + s_c^2$$

Multiplication and Division: sum of the squares of the relative standard deviations:

$$y = a b/c$$

$$\left(\frac{S_y}{y}\right)^2 = \left(\frac{S_a}{a}\right)^2 + \left(\frac{S_b}{b}\right)^2 + \left(\frac{S_c}{c}\right)^2$$

Please see my handout on "Propagation of Errors for more information.