

Review of Fundamentals

CHEM-5181

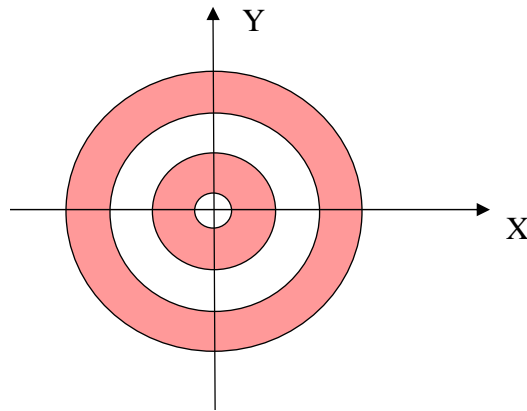
Fall 2009

*Prof. Jose L. Jimenez
Tue 1-Sep-2009*

Business Items

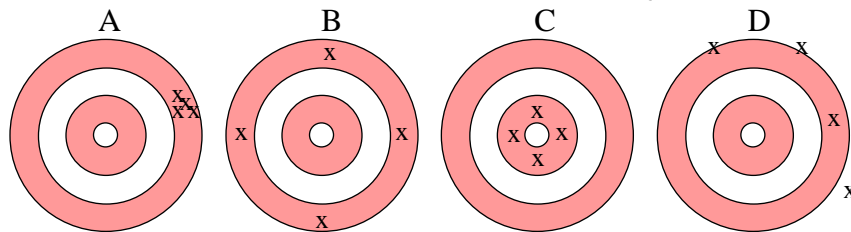
- Discuss syllabus
 - Time for class on Thu
- Sign up for Labs
- Fundamentals review used to be a homework, trying clickers this year
- Homework assigned later today
 - Fundamentals
 - Partially based on clicker responses
 - TOFMS

Precision vs. Accuracy I



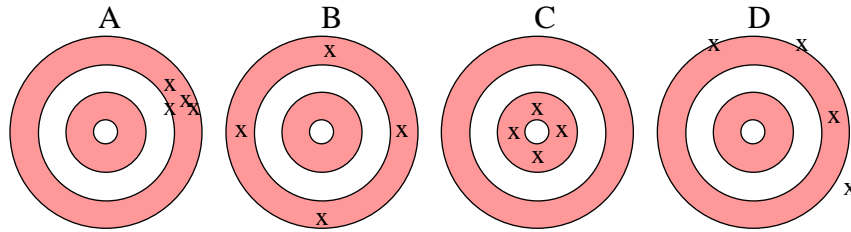
- Measure two variables
 - E.g. concentration of Na^+ and Cl^- in seawater
- Accepted value at origin

Precision vs. Accuracy II



- CQ: Which is the most precise?
 - A
 - B
 - C
 - D
 - I don't know

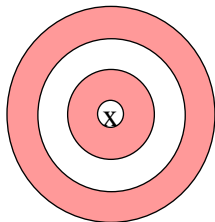
Precision vs. Accuracy III



- CQ: Which is the most accurate?
 - A
 - B
 - C
 - D
 - I don't know
- Follow up: Which is better, A or B?

Precision vs. Accuracy IV

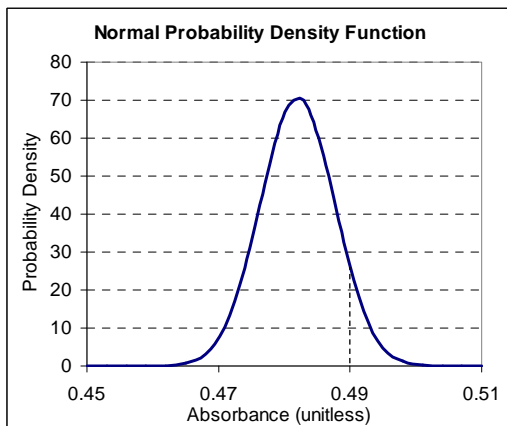
- Precision
 - Agreement between two or more measurements made in an identical fashion
- Accuracy
 - Accuracy is the nearness of a measurement to the accepted value



- CQ: This measurement is
- A. Accurate
 - B. Precise
 - C. Precise and Accurate
 - D. Neither
 - E. I don't know

Clicker Q

- Random errors are often distributed according to the normal error law



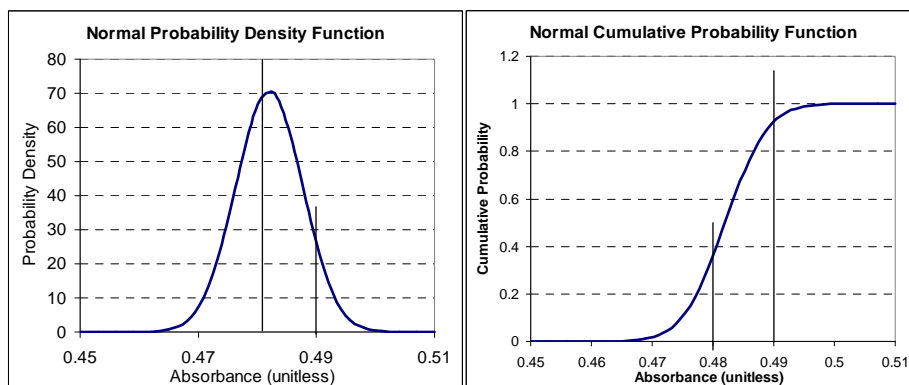
CQ: the probability that the absorbance is exactly 0.49 is:

- A. 0.49
- B. 25
- C. infinity
- D. zero
- E. I don't know

CLT: http://www.chem.uoa.gr/Applets/AppletCentralLimit/Appl_CentralLimit2.html

PDF vs CDF

- Probability Density vs. Cumulative Probability

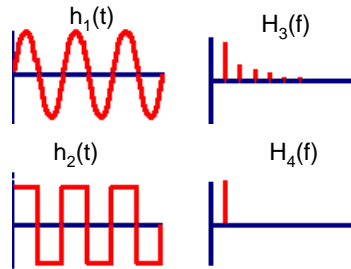


CQ: the probability that the absorbance is between 0.48 and 0.49 is:

- A. zero
- B. It is not defined
- C. 0.37
- D. 0.56
- E. I don't know

Fourier Analysis

- A. H_3 is the Fourier transform of h_1
- B. H_3 is the FT of h_2
- C. H_4 is the FT of h_1
- D. B and C are true
- E. All are false



http://www.chem.uoa.gr/Applets/AppletFourAnal/App1_FourAnal2.html

Clicker Q

- What is the strength of the electric field between two parallel plates at -1000 and 1000 V with respect to ground, if they are separated by 5 mm?
 - A. 2000 Tesla
 - B. 400,000 Volts/meter
 - C. Zero
 - D. 400,000 Newtons/Coulomb
 - E. 2000 Coulombs

Clicker Q

- What is the strength of the electric field between two parallel plates at +2000 and +4000 V with respect to ground, if they are separated by 5 mm?
 - A. 2000 Tesla
 - B. 400,000 Volts/meter
 - C. Zero
 - D. 400,000 Newtons/Coulomb
 - E. 2000 Coulombs

Clicker Q

- What is the net electric force on a neutral mercury atom in an electric field of 10^6 V/m?
 - A. It depends on the polarizability of Hg
 - B. 1.6×10^{-13} Newtons
 - C. 1.6×10^{-13} Newtons / meter
 - D. Zero
 - E. I don't know

Clicker Q

- What is the force acting on a singly charged (+) potassium ion with zero velocity in a 1 Tesla magnetic field
 - A. 1 Newton
 - B. 1.6×10^{-19} Newtons
 - C. Zero
 - D. It depends on the relative alignment
 - E. I don't know

Clicker Q

- What is true for the distribution of molecular speeds of N_2 at ambient T & P
 - A. The average speed is ~ 472 m/s
 - B. The minimum speed is 0 m/s
 - C. The maximum speed is not bound
 - D. None of the above
 - E. A, B, and C

Clicker Q

- The average thermal speed of SF_6 at ambient T & P is
 - A. Smaller than that of N_2
 - B. Larger than that of N_2
 - C. Same as that of N_2
 - D. None of the above
 - E. A, B, and C

Clicker Q

- Air molecules in this classroom are colliding with each other approximately:
 - A. Once a second
 - B. 100 times per second
 - C. 10,000 times per second
 - D. 10^6 times per second
 - E. 10^{10} times per second

Clicker Q

- The time between collisions for air molecules in an ionizer at a pressure of 10^{-4} Torr is approximately:
 - A. 0.1 ns
 - B. 1 μ s
 - C. 100 μ s
 - D. 10 ms
 - E. 3 s

Clicker Q

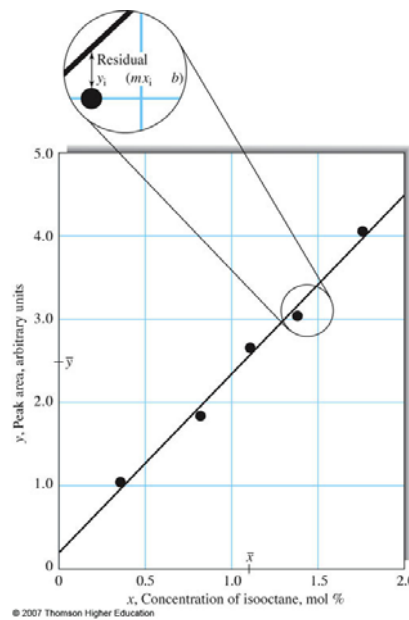
- What is the condition for laminar flow in a tube?
 - A. Pressure \leq 1 atmosphere
 - B. Reynolds number < 1
 - C. Reynolds number < 2000
 - D. $T < T_{\text{critical}}$ and $P < P_{\text{critical}}$
 - E. What is laminar flow?

Clicker Q

- What is the vapor pressure of water at 100 degrees C?
 - A. 1012 Torr
 - B. 760 mbar
 - C. 1 bar
 - D. 1 atmosphere
 - E. 15 Torr

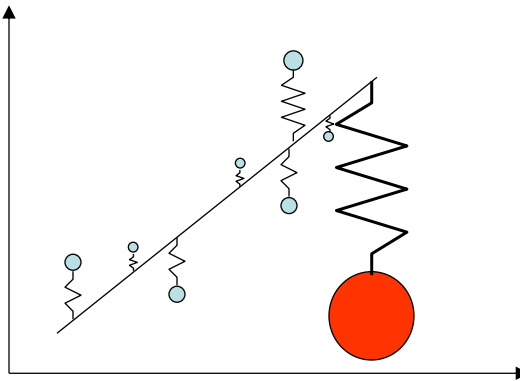
Linear Regression

- Standard regression minimizes sum of squared residuals
 - Residual = vertical distance between datapoint and line
- Depending how much scatter there is in the data, the slope and intercept will have more or less error
 - $y = (m \pm s_m) * x + (b \pm s_b)$
 - Not displayed in simple regression in Excel
 - Only gives $y = m * x + b$
 - Need to use advanced reg.

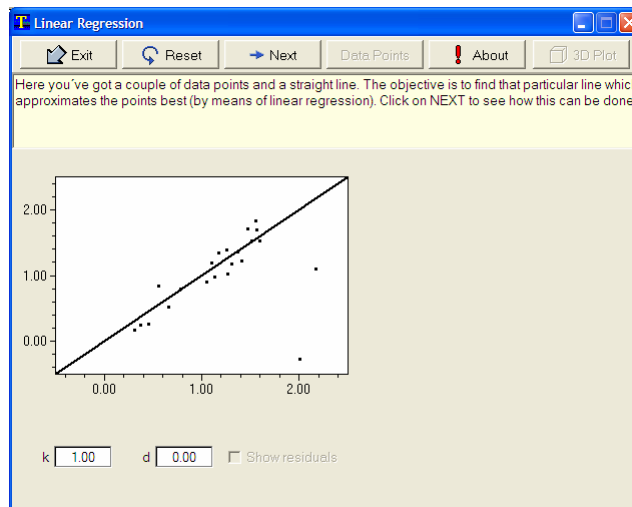


The Trouble w/ Standard Regression

- Every point pulls the line towards itself
 - With a weight equal to the squared residual
 - Noisy points, outliers, can seriously distort fit



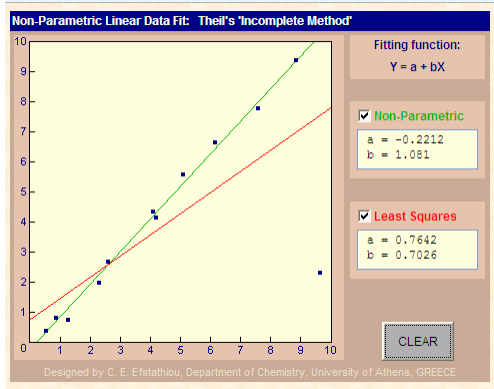
Regression Demo Program



–http://www.vias.org/simulations/simusoft_linregr.html

Example of Non-Parametric Regression

- Goal: reduce the pull of outliers



- A. Green line is a better fit
- B. Red line is a better fit
- C. Neither line is a good fit
- D. The difference in the lines is the uncertainty of the regression
- E. I don't know

<http://www.chem.uoa.gr/applets/AppletTheil/AppletTheil2.html>

More Complete Regression

- Nonparametric regression
 - Does not assume a distribution
 - Typical linear regression assumes no errors on X, Gaussian errors on Y
 - More robust in the presence of outliers
 - <http://www.chem.uoa.gr/Applets/AppletTheil/AppletTheil2.html>
- Regression with errors in X and Y
- Weighted linear regression
 - Different points have more or less error
- Numerical recipes for explanations
 - Chapters 14 & 15
 - <http://www.nr.com/>
- Different regressions in many programs

