

# **Review of Fundamentals**

CHEM-5181

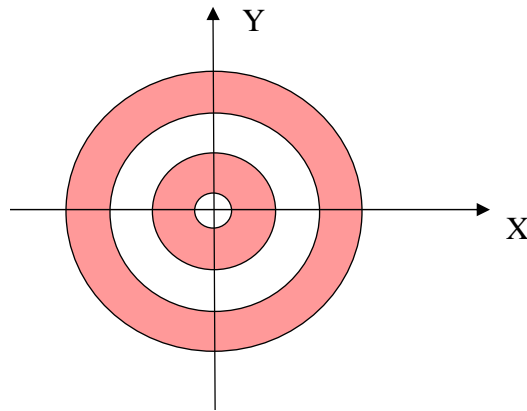
Fall 2007

*Prof. Jose L. Jimenez*

## **Business Items**

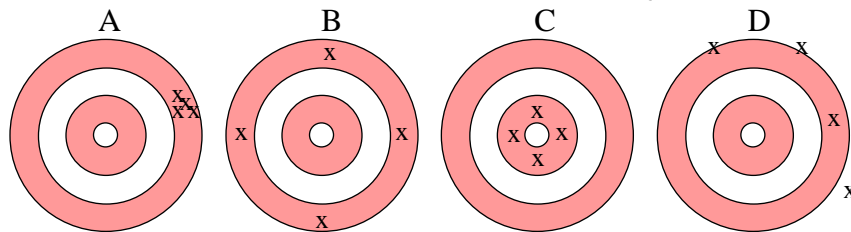
- Fundamentals review used to be a homework, trying clickers this year
- Homework assigned later today
  - Fundamentals
    - Partially based on clicker responses
  - TOFMS

## Precision vs. Accuracy I



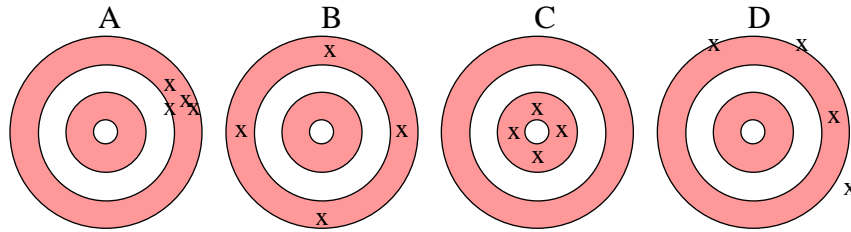
- Measure two variables
  - E.g. concentration of  $\text{Na}^+$  and  $\text{Cl}^-$  in seawater
- Accepted value at origin

## Precision vs. Accuracy II



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

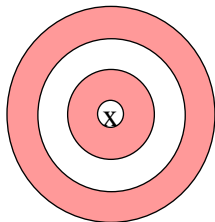
## Precision vs. Accuracy III



- 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

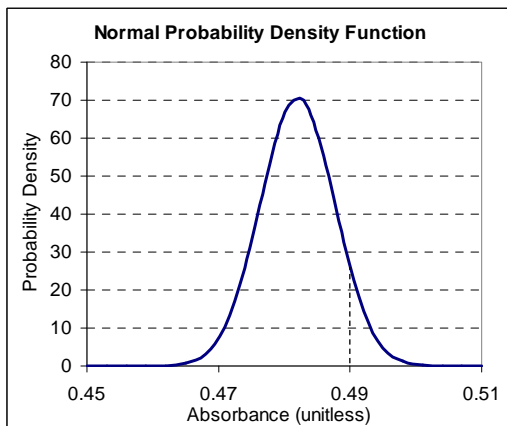
- Precision
  - Agreement between two or more measurements made in an identical fashion
- Accuracy
  - Accuracy is the nearness of a measurement to the accepted value



- 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



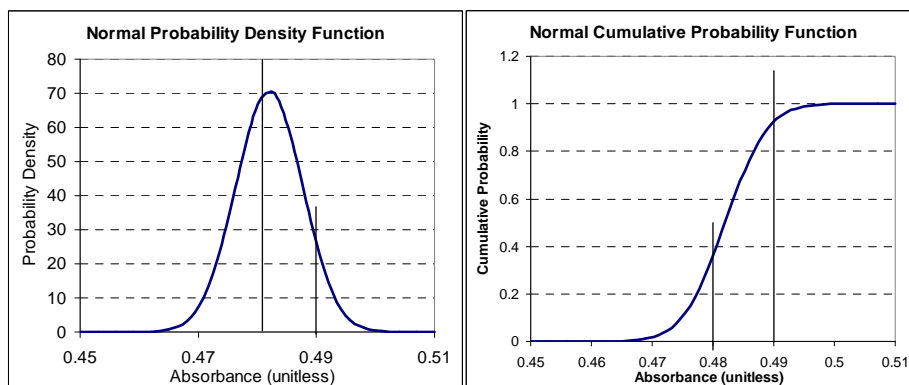
CQ: the probability that the absorbance is exactly 0.49 is:

- 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](http://www.chem.uoa.gr/Applets/AppletCentralLimit/Appl_CentralLimit2.html)

## PDF vs CDF

- Probability Density vs. Cumulative Probability

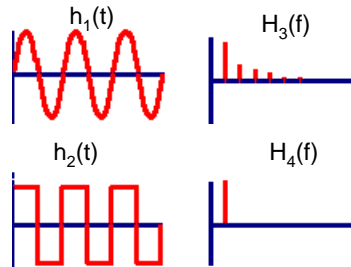


CQ: the probability that the absorbance is between 0.48 and 0.49 is:

- 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](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.  $1.6 \times 10^{-13}$  Newtons
  - C.  $1.6 \times 10^{-13}$  Newtons / meter
  - D.  $10^6$  Newtons
  - E. Zero

### Clicker Q

- What the force acting on a singly charged (+) potassium ion with zero velocity in a 1 Tesla magnetic field
  - A. 1 Newton
  - B.  $1.6 \times 10^{-19}$  Newtons
  - C. Zero
  - D. It depends on the relative alignment
  - E. 1 Tesla

### Clicker Q

- What is true for the distribution of molecular speeds of  $N_2$  at ambient T & P
  - A. The average speed is  $\sim 472$  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  $\text{SF}_6$  at ambient T & P is
  - A. Smaller than that of  $\text{N}_2$
  - B. Larger than that of  $\text{N}_2$
  - C. Same as that of  $\text{N}_2$
  - 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  $\mu$ s
  - C. 100  $\mu$ s
  - D. 10 ms
  - E. 3 s

### Clicker Q

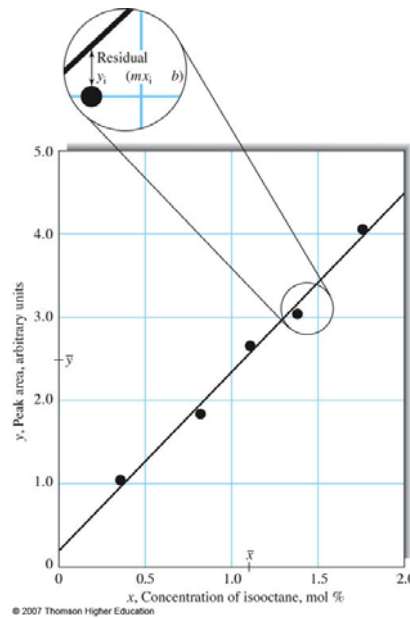
- What is the condition for laminar flow in a tube?
  - A. Pressure  $\leq$  1 atmosphere
  - B. Reynolds number  $< 1$
  - C. Reynolds number  $< 2000$
  - D.  $T < T_{\text{critical}}$  and  $P < P_{\text{critical}}$
  - E. What is laminar flow?

## 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

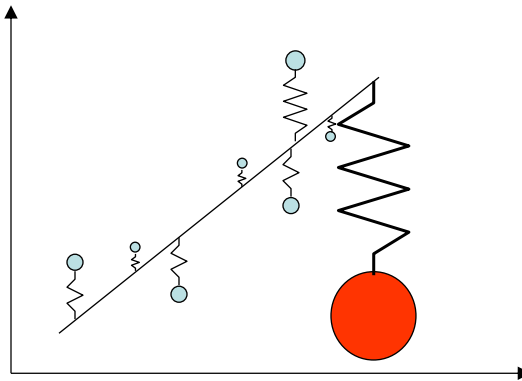
## Linear Regression

- 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



## 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

